Theoretical Physics Prof. Ruiz, UNC Asheville, doctorphys on YouTube Chapter K Notes. Spinors Part II: The Pauli Equation

K1. Measurement. Our eigenvector analysis in the previous chapter is the key to understanding measurement in quantum mechanics. An operator stands for some measurement you make and if the state is an eigenstate of that operator, you get the eigenvalue. Below we measure a state in the third energy level.

$$H\psi_3 = E_3\psi_3$$

The H is none other than the left side of the Schrödinger equation, called the Hamiltonian. Sometimes we prefer to work with the abstract operator symbols, a hallmark of Heisenberg's approach to quantum mechanics.

PK1 (Practice Problem). Show $H\psi_3 = E_3\psi_3$ for a particle in a one-dimensional box. Most of the solution is given below.



When you calculate $H\psi_3 = E_3\psi_3$ you will get the energy eigenvalue. Compare your answer to the third energy level found from the formula we found earlier.

Since we know
$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$
, you must find $E_3 = \frac{3^2 \pi^2 \hbar^2}{2mL^2} = \frac{9\pi^2 \hbar^2}{2mL^2}$

Below we make a measurement and find the electron in a spin-up state.

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

But since the actual measured value will be h-bar over two from experiment, we write

$$S_z = \frac{\hbar}{2}\sigma_z$$

as the measurement operator for the electron spin-1/2 particles. If you make two measurements A and B where the state is an eigenstate of each operator, then

$$A\psi = a\psi$$
 and $B\psi = b\psi$, with
 $AB\psi = A(b\psi) = bA\psi = ba\psi$
 $BA\psi = B(a\psi) = aB\psi = ab\psi$

and all is well. The measurements can be accomplished in either order. Note that when this happens, the measurement operators commute, which you can see by subtracting the above pair of equations.

$$(AB-BA)\psi = (ba-ab)\psi = 0$$
 and $[A,B] = 0$

But remember the operator action of the Pauli matrix σ_x on our spin-up state?

σ_x	1	=	0	1	$\begin{bmatrix} 1 \end{bmatrix}$	1]_		
	0		1	0	0	_	1	

We do not get the same state back. In fact we kicked the state into something else. The electron now has spin down. So you can disturb the states. When this happens, the measurement operators do not commute. Before hitting the state with σ_x the electron was spin up.

	[1]		1	0]	[1]		1	
σ_z	0	=	0	-1	0	=	0	,

But afterwards, we get

$$\sigma_{z}\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = -\begin{bmatrix}0\\1\end{bmatrix}.$$

Checking the commutator, you find something you already have calculated in the previous chapter.

$$[\sigma_{x},\sigma_{z}] = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$
$$[\sigma_{x},\sigma_{z}] = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} = 2 \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} = -2i \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = -2i\sigma_{y}$$

Here is your general result from the last chapter.

$$\left[\sigma_{j},\sigma_{k}\right]=2i\varepsilon_{jkl}\sigma_{l}$$

When operators do not commute, the measurements disturb the states.

There is an Uncertainty Relation!

K2. Heisenberg Uncertainty Relation.



Werner Heisenberg (1901-1976)

Courtesy School of Mathematics and Statistics University of St. Andrews, Scotland

Now we consider position and momentum. Recall from our chapter introducing quantum mechanics that

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

Therefore, we have the momentum operator in one dimension as

$$p = -i\hbar \frac{d}{dx}$$

Does the position operator x commute with the momentum operator p? Let's check.

$$x(p\psi) = x \left[-i\hbar \frac{d}{dx} \right] \psi = -i\hbar x \frac{d\psi}{dx}$$
$$p(x\psi) = \left[-i\hbar \frac{d}{dx} \right] (x\psi) = -i\hbar \psi - i\hbar x \frac{d\psi}{dx}$$

Subtracting these,

$$(xp)\psi - (px)\psi = i\hbar\psi$$

and we obtain for the commutator

$$[x, p] = i\hbar$$

So if you make a position measurement first, then measure the momentum, you kick the state and no longer have the position you just measured. There is an uncertainty in the combined position and momentum measurements. The above commutator is an elegant form for Heisenberg's Uncertainty relation.

Think of the Schrödinger picture of quantum mechanics as the way with differential equations. The Heisenberg picture involves operators. Both ways are equivalent formulations. Thus we credit two physicists as architects of quantum mechanics.



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

Werner Heisenberg (1901-1976)



 $H\psi = E\psi$ $[x, p] = i\hbar$



Max Born (1882-1970)

Courtesy School of Mathematics and Statistics University of St. Andrews, Scotland

But we should include Max Born among the architects of quantum mechanics since he gave us the interpretation of the wave function in terms of probability.

$$P(x)dx = \psi^*(x)\psi(x)dx$$

Nobel Prizes for Quantum Mechanics Heisenberg (1932) Schrödinger (1933) Born (1954)

Also Grand pop to Olivia Newton-John

Schrödinger shared his prize with Dirac and Born shared the prize with another scientist honored for another achievement in physics.

K3. Angular Momentum. We continue with the powerful language of operators.

The angular momentum operator is found from the definition in classical physics,

 $\vec{L} = \vec{r} \times \vec{p}$, but now we treat these as operators.

$$\vec{r} \times \vec{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = \hat{i}(yp_z - zp_y) - \hat{j}(xp_z - zp_x) + \hat{k}(xp_y - yp_x)$$

Note that the order of position and momenta do not matter in the above equation since the pairs have different spatial dimensions. We could not be cavalier if we had xp_x . We could not switch to p_xx . We find

$$L_{x} = yp_{z} - zp_{y},$$
$$L_{y} = zp_{x} - xp_{z},$$
$$L_{z} = xp_{y} - yp_{x}.$$

Let's find a commutator.

$$[L_{x}, L_{y}] = [yp_{z} - zp_{y}, zp_{x} - xp_{z}]$$

$$[L_{x}, L_{y}] = [yp_{z}, zp_{x}] - [yp_{z}, xp_{z}] - [zp_{y}, zp_{x}] + [zp_{y}, xp_{z}]$$

$$[L_{x}, L_{y}] = yp_{x}[p_{z}, z] - yx[p_{z}, p_{z}] - p_{y}p_{x}[z, z] + xp_{y}[z, p_{z}]$$

$$[L_{x}, L_{y}] = yp_{x}(-i\hbar) - yx \cdot 0 - p_{y}p_{x} \cdot 0 + xp_{y}(i\hbar)$$

$$[L_{x}, L_{y}] = yp_{x}(-i\hbar) + xp_{y}(i\hbar) = i\hbar(xp_{y} - yp_{x}) = i\hbar L_{z}$$

PK2 (Practice Problem). Show that along with

$$[L_x, L_y] = i\hbar L_z, \text{ we have } [L_y, L_z] = i\hbar L_x \text{ and } [L_z, L_x] = i\hbar L_y.$$

Since each angular momentum component commutes with itself, we can write

$$\begin{bmatrix} L_j, L_k \end{bmatrix} = i\hbar \varepsilon_{jkl} L_l$$

But wait, this looks very similar to

$$\left[\sigma_{j},\sigma_{k}
ight]=2iarepsilon_{jkl}\,\sigma_{l}$$

This suggests that the Pauli spin matrices are proportional to a type of angular momentum that has only two values from working with these operators on spinors! But angular momentum has units of h-bar. So we do two things.

1. Insert the h-bar to get angular momentum units.

2. Get rid of that 2 so the commutation relation looks like the L relations.

Then,

$$S_{x} = \frac{\hbar}{2}\sigma_{x} \qquad S_{y} = \frac{\hbar}{2}\sigma_{y} \qquad S_{z} = \frac{\hbar}{2}\sigma_{z}$$
$$\left[S_{j}, S_{k}\right] = i\hbar\varepsilon_{jkl}S_{l}$$

Summary:

Orbital Angular Momentum:
$$\vec{L} = \vec{r} \times \vec{p}_{with} [L_j, L_k] = i\hbar \varepsilon_{jkl} L_l$$

Intrinsic Angular Momentum for the Electron: $\vec{S} = \frac{\hbar}{2} \vec{\sigma}_{\text{with}} [S_j, S_k] = i\hbar \varepsilon_{jkl} S_l$

Total Angular Momentum: $ec{J} = ec{L} + ec{S}$



K4. General Spin Eigenstates.

We choose our coordinate system as shown in the figure, following the convention used in physics. Note that in math classes, the angle definitions are often interchanged.

Let the unit vector n point along the r direction, i.e., n = r. We want to find the eigenvectors for a spinor along such an arbitrary direction.

We start with our spin-up and spin-down cases along the z-direction to be



which are eigenvectors for σ_z . We

work with Pauli matrices because the math is faster. you can always put the h-bar in and 1/2 later to get the actual spin.

$$\hat{n} = \hat{r} = \sin \theta \cos \phi \hat{i} + \sin \theta \sin \phi \hat{j} + \cos \theta \hat{k}$$

$$\hat{n} = \hat{\sigma} = \sin \theta \cos \phi \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \sin \theta \sin \phi \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} + \cos \theta \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\hat{n} \cdot \vec{\sigma} = \begin{bmatrix} \cos \theta & \sin \theta (\cos \phi - i \sin \phi) \\ \sin \theta (\cos \phi + i \sin \phi) & -\cos \theta \end{bmatrix}$$

$$\hat{n} \cdot \vec{\sigma} = \begin{bmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{bmatrix}$$

Eigenvalues. We now set up the eigenvalue problem.

$$\stackrel{\wedge}{n} \stackrel{\rightarrow}{\sigma} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \lambda \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

For the solution of the eigenvalues, the following determinant must vanish.

$$\begin{vmatrix} \cos \theta - \lambda & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta - \lambda \end{vmatrix} = 0$$

The result for the vanishing determinants

$$-(\cos^{2} \theta - \lambda^{2}) - \sin^{2} \theta = 0$$
$$-\cos^{2} \theta + \lambda^{2} - \sin^{2} \theta = 0$$
$$\lambda^{2} = \cos^{2} \theta + \sin^{2} \theta = 1$$
$$\lambda = \pm 1$$

Eigenvectors. We proceed to find the eigenvectors. We will give the eigenvector that goes with $\lambda = +1$ the name \mathcal{X}_{\uparrow} and for $\lambda = -1$ we will use \mathcal{X}_{\downarrow} . We use a and b as temporary parameters for the components we use. For the first case we find

$$\begin{bmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix}$$
$$\begin{bmatrix} a\cos\theta + b\sin\theta e^{-i\phi} \\ a\sin\theta e^{i\phi} - b\cos\theta \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix}$$

For the upper component

$$a\cos\theta + b\sin\theta e^{-i\phi} = a$$
$$b\sin\theta e^{-i\phi} = a(1 - \cos\theta)$$
$$\frac{b}{a} = \frac{(1 - \cos\theta)}{\sin\theta} e^{i\phi}$$

Do you remember an elegant identity involving a half angle and/or double angle from trig you studied some time ago? It will unlock the secret to spinor rotations? Recall that we derived these two identities earlier in our course.

$$\cos(\alpha + \beta) = \cos\alpha\cos\beta - \sin\alpha\sin\beta$$
$$\sin(\alpha + \beta) = \cos\alpha\sin\beta + \sin\alpha\cos\beta$$

From the above, we obtain.

$$\sin 2\theta = 2\sin \theta \cos \theta$$
 and $\cos 2\theta = \cos^2 \theta - \sin^2 \theta$
 $\sin \theta = 2\sin \frac{\theta}{2} \cos \frac{\theta}{2}$ and $\cos \theta = \cos^2 \frac{\theta}{2} - \sin^2 \frac{\theta}{2}$

Summary:

$$\frac{b}{a} = \frac{(1 - \cos \theta)}{\sin \theta} e^{i\phi}$$
$$\sin \theta = 2\sin \frac{\theta}{2} \cos \frac{\theta}{2}$$
$$\cos \theta = \cos^2 \frac{\theta}{2} - \sin^2 \frac{\theta}{2}$$

But wait!

$$1 - \cos\theta = \left[1 - \cos^2\frac{\theta}{2}\right] + \sin^2\frac{\theta}{2}$$

$$1 - \cos\theta = \left[\sin^2\frac{\theta}{2}\right] + \sin^2\frac{\theta}{2} = 2\sin^2\frac{\theta}{2}$$

Now we are ready. The result is

$$\frac{b}{a} = \frac{(1 - \cos\theta)}{\sin\theta} e^{i\phi} = \frac{2\sin^2\frac{\theta}{2}}{2\sin\frac{\theta}{2}\cos\frac{\theta}{2}} e^{i\phi}$$
$$\frac{b}{a} = \frac{\sin\frac{\theta}{2}}{\cos\frac{\theta}{2}} e^{i\phi}$$

We can pick

$$a = \cos \frac{\theta}{2}$$
 and $b = \sin \frac{\theta}{2} e^{i\phi}$ since $a * a + b * b = 1$

We are normalized.

The eigenvector is

$$\chi_{\uparrow} = \begin{bmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{bmatrix}$$

PK3 (Practice Problem). Use the lower component equation in

$$\begin{bmatrix} a\cos\theta + b\sin\theta e^{-i\phi} \\ a\sin\theta e^{i\phi} - b\cos\theta \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix}$$

and normalization to obtain the same result.

PK4 (Practice Problem). Show that the eigenvector for $\lambda = -1$ is

$$\chi_{\downarrow} = \begin{bmatrix} -e^{-i\phi} \sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{bmatrix}.$$

Summary:

$$\chi_{\uparrow} = \begin{bmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{bmatrix} \qquad \chi_{\downarrow} = \begin{bmatrix} -e^{-i\phi}\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{bmatrix}$$

The dual of
$$\chi_{\downarrow}$$
 is defined as $\left[\chi_{\downarrow}\right]^{\dagger} = \left[-e^{+i\phi}\sin\frac{\theta}{2} \quad \cos\frac{\theta}{2}\right]$

Then
$$\begin{bmatrix} \chi_{\downarrow} \end{bmatrix}^{\dagger} \chi_{\uparrow} = \begin{bmatrix} -e^{+i\phi} \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{bmatrix} \begin{bmatrix} \cos \frac{\theta}{2} \\ e^{i\phi} \sin \frac{\theta}{2} \end{bmatrix} = 0$$

The eigenstates are orthogonal.

K5. What Does It All Mean?



$$\chi_{\uparrow} = \begin{bmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{bmatrix} \quad \chi_{\downarrow} = \begin{bmatrix} -e^{-i\phi}\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{bmatrix}$$

Whenever you feel this question coming on, just look at friendly cases. Set $\theta = 0^{\circ}$. Then,

$$\chi_{\uparrow_{z-axis}} = \begin{bmatrix} 1\\ 0 \end{bmatrix} \qquad \chi_{\downarrow_{z-axis}} = \begin{bmatrix} 0\\ 1 \end{bmatrix}$$

We know what this means. The left spinor is an electron with spin aligned up. The right spinor is a spin state where the spin is aligned down. Now check out $\theta = 90^{\circ}$ with $\phi = 0^{\circ}$, which is along our x-axis.

$$\chi_{\uparrow_{x-axis}} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\1 \end{bmatrix}$$

This is an eigenstate of a spin measurement along the x-axis where the spin is up relative to the x-axis. But it is expressed in terms of a mixture or superposition of states relative to the z-axis.

$$\chi_{\uparrow x-axis} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\0 \end{bmatrix} + \frac{1}{\sqrt{2}} \begin{bmatrix} 0\\1 \end{bmatrix}$$

$$\chi_{\uparrow_{x-axis}} = \frac{1}{\sqrt{2}} \chi_{\uparrow_{z-axis}} + \frac{1}{\sqrt{2}} \chi_{\downarrow_{z-axis}}$$

So for the spin up along the x-axis, when measured with respect to the z-axis you can get either up or down. In fact the probability for each is 1/2.

What about when $\theta = 180^{\circ}$?

$$\chi_{\uparrow} = \begin{bmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{bmatrix}$$

becomes

$$\chi_{\uparrow}(\theta = 180^{\circ}) = \begin{bmatrix} 0\\ e^{i\phi} \end{bmatrix} = 0 \begin{bmatrix} 1\\ 0 \end{bmatrix} + e^{i\phi} \begin{bmatrix} 0\\ 1 \end{bmatrix}$$

$$\chi_{\uparrow_{-z-axis}} = c_1 \chi_{\uparrow_{z-axis}} + c_2 \chi_{\downarrow_{z-axis}}$$

The state for you, standing on your head, is up since it is your eigenstate. But for the person oriented along the positive z-axis, the spin is flipped. We get this result from the probabilities. The probability for regular z-axis spin up is $c_1^*c_1 = 0$. For spin down we find

$$c_2 * c_2 = e^{-i\phi} e^{i\phi} = 1$$
.

What about $\theta = 360^\circ$?

$$\chi_{\uparrow}(\theta = 360^{\circ}) = \begin{bmatrix} -1\\ 0 \end{bmatrix}$$

Well, we get 100% probability that we are spin up again since

$$c_1 * c_1 = (-1)(-1) = 1$$

But we DO NOT get the exact same thing back due to a phase factor. You have to go two complete 360° rotations for that due to the half angles.



Courtesy Council on Science and Technology, Princeton University

K6. The Pauli Equation

We will assume time-independent potentials in this section and thus work with the timeindependent form of the Schrödinger equation. We also consider spin-1/2 particles such as electrons.

To include spin we promote our wave function $\, arphi \,$ to

$$\boldsymbol{\psi} = \begin{bmatrix} \boldsymbol{\psi}_1 \\ \boldsymbol{\psi}_2 \end{bmatrix}$$

Replace the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

with

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

where the potential is a matrix potential

$$V = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix}$$

The H operator

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{becomes}}$$
$$H = -\frac{\hbar^2}{2m} \begin{bmatrix} 1 & 0\\ 0 & 1 \end{bmatrix} \nabla^2 + \begin{bmatrix} V_{11} & V_{12}\\ V_{21} & V_{22} \end{bmatrix}$$



Wolfgang Pauli (1900-1958) Courtesy School of Mathematics and Statistics University of St. Andrews, Scotland

The Pauli Effect. A joke, but taken seriously by Pauli and some others. Background: Physicists are either theorists or experimentalists for many years now. You either work with the math and calculations to explain observed phenomena or spend your career making the measurements and gathering the data. However, there are rare exceptions like the great Enrico Fermi.

Theorists have an image of being inept in lab. Instead, they feel at home with mathematical physics. So they might break things in lab, ruin experiments, or do something not too intelligent, even putting themselves and others in danger.

So the Pauli effect is this - if a theorist walks into a lab where an experimentalist is working, the experimental equipment will break or malfunction by just the mere presence of the theorist. It is said the greater the theorist, the greater the destruction.

A famous story is the mysterious failure of an experiment in a lab in Germany. But Pauli was not even present. However, later they discovered Pauli was at the train station in that town at the time of the malfunction.

Pauli and the famous psychiatrist Carl Jung, a student who broke away from Freud, analyzed this in terms of Jung's concept of synchronicity, where coincidences are believed to happen for a reason with some underlying connection.

A Famous Pauli Put Down. "Not only is it not right, it's not even wrong!"

Pauli Tough on a Student in Class. One day in lecture Pauli said something was trivial. The student did not see it, so the student asked Pauli for an explanation. Pauli left the room and came back a few minutes later. On his return, Pauli said "It is trivial!" Apparently Pauli left the lecture hall to check his comment out in his office and satisfied himself that it was indeed an easy calculation. This was not quite the answer the student was hoping for.

Max Born Comments on His Assistant Pauli. "Since the time when he was assistant in Göttingen, I knew he was a genius, comparable only to Einstein himself." (from *Quips, Quotes and Quanta: An Anecdotal History of Physics* by Anton Z. Capri).