2 Foundations of Quantum mechanics

2.1 The Stern-Gerlach experiments

Two ways of learning Quantum Mechanics:

- historical perspective: experimental findings between 1905 to 1922
- concentrate on one of these experiments: the need for a "new physics"

We will do the latter. We choose the Stern-Gerlach experiments to demonstrate to us the need for a "new" physical theory to explain important concepts.

1. Silver atoms are heated in an oven that has a small hole through which some atoms escape.

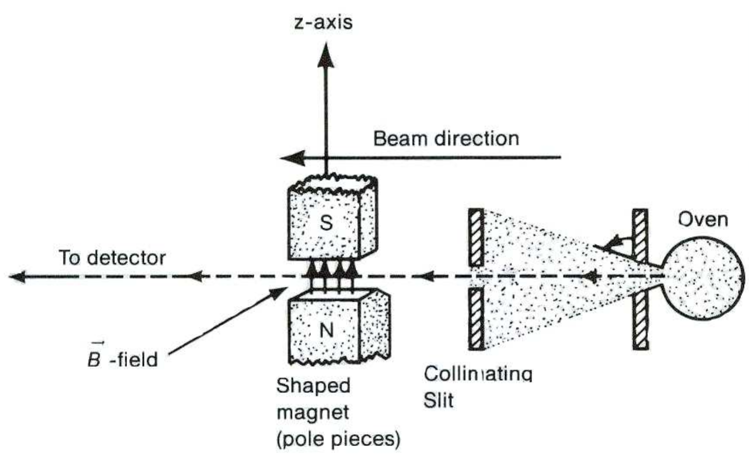


Figure 5: The Stern-Gerlach experimental setup.

2. The atoms go through a region that contains a magnetic field as seen in the figure. What happens?
3. To understand what happens let us analyze the silver atoms.
   - The atomic number for silver is 47.
   - So it has 46 electrons that are paired (*i.e.* upspin-downspin partners) and there is one electron that is unpaired.
   - Classical theory of magnetism : a "spinning electron" behaves as a magnet and the heavy silver atom has a magnetic moment due to the one extra (unpaired) 47th electron. *So each silver atom is like a tiny magnet due to that extra, unpaired electron.*
   - *This is also consistent with our description of magnetization in the previous section.*

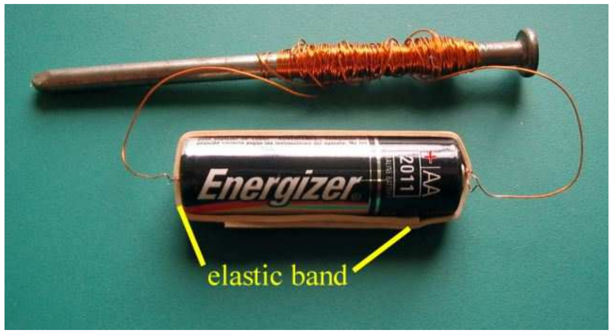


Figure 6: The current carrying copper wire in the above figure creates a magnetic field in the metallic nail.

- Any magnet that is placed in a magnetic field, experiences a force due to the magnetic field which bends its path.
- Hence each silver atom that escapes from the oven into the region of the magnetic field experiences a force that bends its path.
- But we can do better and quantify this.
- To explain this, a little understanding of magnetism helps:
- Force on the silver atom that drags it along the direction of the magnetic field is proportional to the magnetic moment of the silver atom.

$$F_z = \frac{\partial}{\partial z}(\mu \cdot B) = \mu_z \frac{\partial B_z}{\partial z} \tag{2.1.1}$$

- **Vector algebra? $\rightarrow$ review handout in Section II . Note: Section II will not be discussed in class. You are responsible for the material, but please see us if you have trouble.**
- The equation above implies there is a force on the silver atom due to its magnetic moment. This force is along z (the direction of the magnetic field).
- And proportional to the component of the magnetic moment along the direction of the magnetic field (μ_z).
- The magnetic moment of the silver atom is proportional to the spin of the extra electron

$$\mu \propto \mathbf{S} \tag{2.1.2}$$

- Hence the force on each silver atom (which drags the silver atom and bends its path) is proportional to the spin component of the extra electron along the z-axis direction.

$$F_z \propto \mathbf{S_z}, \tag{2.1.3}$$

$$F_z = C\mathbf{S_z} \tag{2.1.4}$$

where C is some constant.

2.1.1 Detour: the Zeeman effect: Splitting the m, magnetic quantum numbers

The p orbitals are triply degenerate, each degenerate state characterized by m values in the range +1 to -1 (since for p orbital, $l = 1$). The 3d orbital has a degeneracy of 5, each degenerate state characterized by m values in the range +2 to -2 (for the d orbital $l = 2$). We may recall that the solution to the hydrogen that wave functions with magnetic quantum numbers +m and -m only differ due to $\exp[\imath m\phi]$ factor. Furthermore, the energy for the $\pm m$ levels are the same (which is why all the 2p orbitals for example have the same energy).

Is there a way to split this degeneracy? The z-component of the spin angular momentum interacts with an external magnetic field to give rise to a force on the silver atoms. (As seen above.) The angular momentum of a charged particle creates an internal magnetic field which interacts with the external magnetic field. There are two kinds of angular momenta in quantum mechanics, spin angular momentum and orbital angular momentum. As an illustration here we shown how the orbital angular momentum interacts with an external magnetic field but the same can be said about the spin angular momentum.

Using Eqs. (2.1.1) and (2.1.2) and realizing that force is the Negative of the derivative of the potential energy with respect to distance, We see that

$$E_B = CBS_z \tag{2.1.5}$$

A similar energy exists due to the orbital angular momentum and in that case the Constant is just the definition of the Bohr-magneton:

$$E_B = \frac{\beta_e}{\hbar} BL_z \tag{2.1.6}$$

where β_e is the Bohr magneton of an electron and $\beta_e = \frac{e\hbar}{2m_e}$.

And so now we are in a position to write the new Hamiltonian of the Hydrogen Atom in the presence of the magnetic field as

$$H_B = H + \frac{\beta_e}{\hbar} BL_z \tag{2.1.7}$$

where H is the Hydrogen atom Hamiltonian of Eq. (1.6.1). Since L_z commutes with H, the eigenstates of the Hamiltonian in Eq. (2.1.7) will be the same as the Hydrogen atom eigenstates. But now the eigenvalues get an additional m dependent term due the $\frac{\beta_e}{\hbar} BL_z$ factor since

$$H_B\Psi = \left[H + \frac{\beta_e}{\hbar} BL_z\right]\Psi = \left[E_{R_{CM}} + E_\mu + \beta_e Bm\right]\Psi \tag{2.1.8}$$

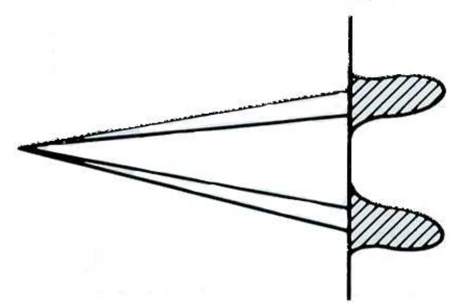
where $E_{R_{CM}}$ and E_μ are given by Eqs. (1.6.19) and (1.6.47), Ψ is the full hydrogen atom wavefunction discussed earlier. (**How do we know that the wavefunction in Eq. (2.1.8) is the H-atom wavefunction?**)

So the m quantum number states can be split in this fashion. This effect is called the Zeeman effect.

2.2 Spin quantization

4. Based on Eq. (2.1.8) we note that the beam of silver atoms must split into two depending on the m_z values of the 47th electron.

5. Hence Stern and Gerlach saw two spots like what we have in the figure below.



6. This result at that point in time was quite earth shattering. To us it is not, because in some sense we have cheated and learned the theory first. Hence no surprise.

7. m_z has to be quantized and not continuous and can have only two values:

$$m_z = \pm\hbar/2 \tag{2.2.9}$$

   where h is a constant number derived by Planck and known as the Planck's constant. $\hbar$ is a simplified notation of $h/2\pi$.

   This was quite a surprising result at the time when classical mechanics and classical theory of electro-magnetics were considered complete. However, this was not the only experiment that exposed the limitation of the classical style of thinking. There were others: Planck's black body radiation and the Einstein-debye theory of specific heats to name a couple. We have chosen to concentrate here only on the Stern-Gerlach so as to quickly expose the short-comings. What we have arrived at above is known as **spin quantization**, a very important concept in quantum mechanics. *Spin is quantized not continuous.*

8. A little later we will understand this from a different perspective when we construct an analogy between the Stern-Gerlach experiments and polarized light. But, for now, lets proceed further to other even more surprising facts.

2.3 Sequential Stern-Gerlach experiments

The sequence of experiments that I consider here can be performed computationally using the java applet at:
http://www.indiana.edu/%7Essiweb/SG/spins.jar (you will need Java). You should try this yourself and if you have trouble using the applet you could see me during office hrs.

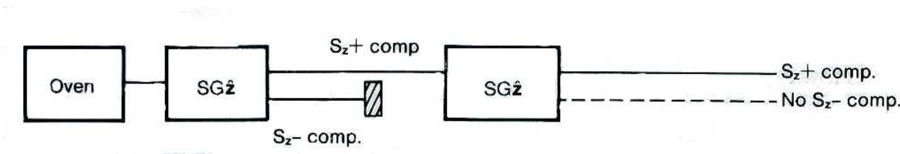


Figure 7:

1. What happens if we choose to pass $\mathbf{S_z^+}$ through a magnetic field oriented along the x-direction?

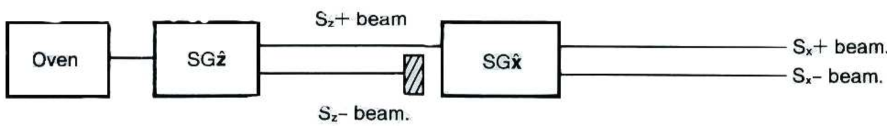


Figure 8:

2. We get the states $\mathbf{S_x^+}$ and $\mathbf{S_x^-}$.
3. This makes sense. Although $\mathbf{S_z^+}$ has a non-zero spin component along the positive z-axis, there is no definite information here regarding what the component along x-axis might be.
4. What happens when we block $\mathbf{S_x^-}$ and let $\mathbf{S_x^+}$ go through another magnetic field oriented along the z-direction

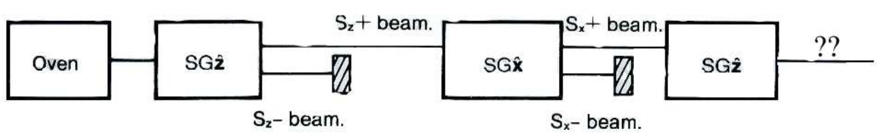


Figure 9:

5. A completely different story. *We are in for a shock.*
6. We find that both $\mathbf{S_z^+}$ and $\mathbf{S_z^-}$ are present in the result.
7. **How can this make any sense? We blocked off $\mathbf{S_z^-}$ before it entered into the x-directed magnetic field. Yet it makes its appearance after passing through the z-directed magnetic field. Whats going on?**

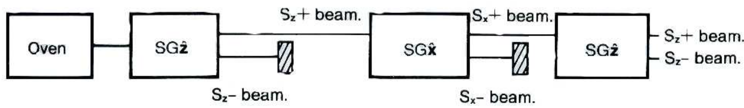


Figure 10:

8. This last part *most drastically* illustrates the peculiarities of quantum mechanics. And it is an observed fact and a complete surprise !!

9. How is it possible that $\mathbf{S_z^-}$ which we completely eliminated initially has resurfaced? It almost seems as if when we passed the $\mathbf{S_z^+}$ state through the x-magnetic field, it forgot that it was passed through the z-magnetic field before that. Weird!

10. Is there an explanation? Yes. And we will get into that in a little bit. But it is to be clearly understood that this problem encountered between $\mathbf{S_z}$ and $\mathbf{S_x}$ is not due to incompetence in the experiment and cannot be done away with by improving the quality of the experiment or such. There is a very fundamental concept here that we will get into next.

2.4 The spin states in the Stern-Gerlach experiment are analogous to the behavior of plane and circularly polarized light

1. We will show here that when we consider the behavior of plane and circularly polarized light (which are considered in wave-forms), then we get behavior identical to what was seen from the spin states in the Stern-Gerlach experiments.

2. With this we hope to convince ourselves that the spin states in the Stern-Gerlach experiment are *really acting like waves* thus making all our previous observations meaningful, and hence leading to the basis for the **wave particle duality** arguments later (in c.a. 1927) proposed by de Broglie.

3. **What is plane polarized light?**

   - Light is made of electric and magnetic fields.
   - These are vectors. See the link: http://www.indiana.edu/%7Essiweb/C561/movies/EandManim.gif for an animated rendering of the electric and magnetic fields in light.
   - And light is generally represented by a right handed (three-dimensional) set of vectors.
   - The electric and magnetic fields themselves are waves of the kind:

   $$E = E_0 \hat{x} \cos(kz - \omega t) \tag{2.4.10}$$

   where z is the direction in which the light waves are moving in time, and k and ω are the wave-vector and the frequency of light.

- The magnetic field vector of light is along the $\hat{y}$ direction.
- Note that in the equation above the electric field remains forever on the x-z plane. Such a wave is said to be plane-polarized with the direction of polarization along x-axis.

4. Now consider the following experiment with plane-polarized light.
   - Consider a filter that creates a plane-polarized light in the x-direction.
   - This is the same filter that you guys might have encountered in a general chemistry or P. Chem experiment.
   - The way this filter works is, it allows only plane-polarized light in the x-direction to come out of it. But you may remember that by rotating the knob you could get plane-polarization at different angles.
   - So lets remember that experiment before we move further:
     - There was a polarizer that light was fed into.
     - By rotating the knob you could see the intensity reduce or increase.
     - The following figure depicts this experiment completely.

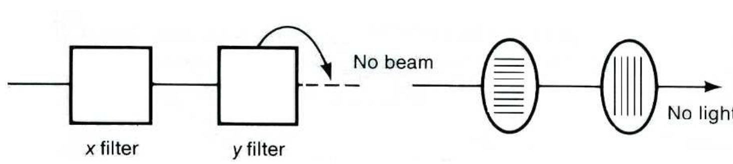


Figure 11: The plane-polarized light experiment

5. Now consider the following analogy between the Stern-Gerlach SG_z^+ filter and the x-filter. (We have chosen to use the term filter for the SG experiment, because thats what it does, it filters out everything but the state that has a +ve z-axis contribution of S_z.)

Figure 12:

6. Does this analogy make sense? The x-filter allows only plane polarized light in the x-direction. Similarly the SG_z^+ filter on the right side of the above figure only allows states with +ve z-axis contribution of S_z. Perhaps the following picture makes it clearer:

7. Now consider the following analogy between the Stern-Gerlach SG_z^- filter and the y-filter.

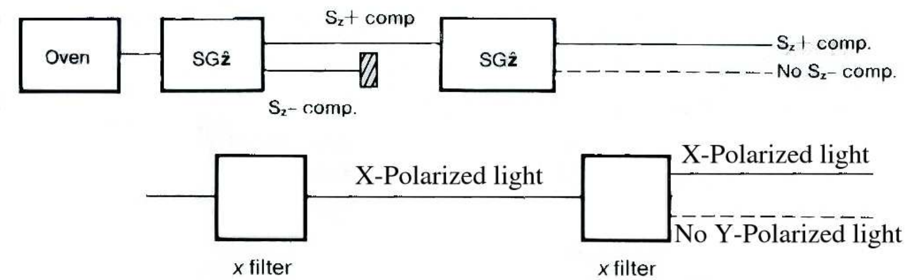
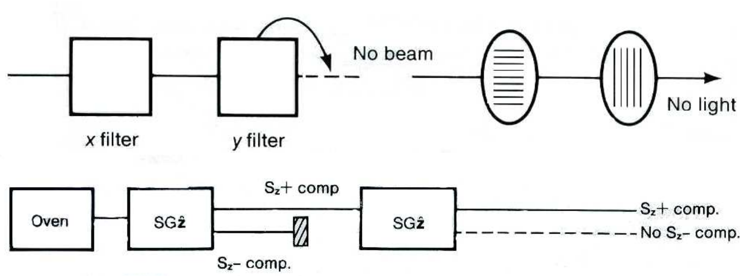


Figure 13:

Figure 14:

8. And a similar diagram like Fig. (6) can be drawn for the y-filter.

9. Note further that x-polarized light fed into a y-filter does not yield any light in a fashion similar to the fact that an SG_z^+ filter does not yield any states that have negative z-axis contribution of S_z. (Compare Fig. (11) and Fig. (7) which are both reproduced below for your convenience.)



10. Thus the analogy between the x- and y-filters with the SG_z^+ and SG_z^- filters in now complete.

11. *The Stern Gerlach experimental observations are hence very similar to observations conducted on plane-polarized light.*

12. Now lets consider an analogy for the SG_x^+ and SG_x^- filters.

13. Consider a polarization direction x′ that is 45 degrees rotated from the x-direction. (y-polarization direction is 90 degrees rotated from x-direction.)

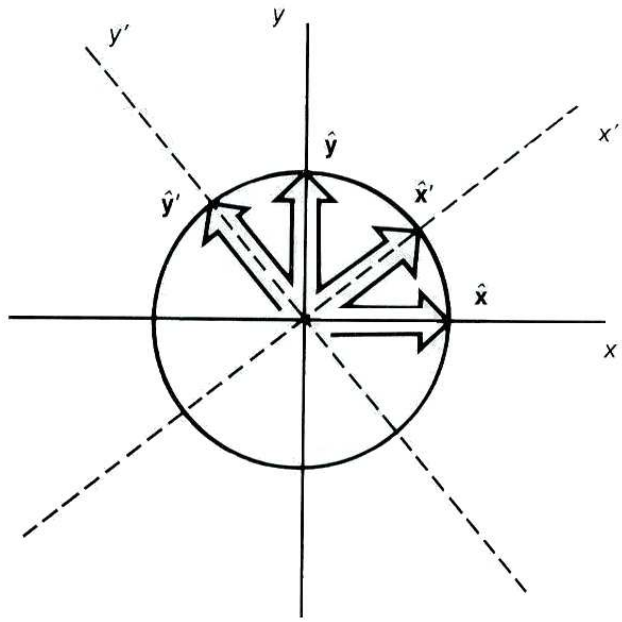


Figure 15: Direction of the x′ is 45 degrees rotated from the x-direction

14. Consider the following polarization sequence.

15. Compare Fig. (16) above with the Fig. (10) which are reproduced below for your convenience. It does seem like the x′ filter acts in a fashion similar to the SG_x^+ filter does.

16. Similarly the SG_x^- filter acts like the y′ filter.

17. If $SG_x^+ \leftrightarrow$ x′, can we say that $SG_x^- \leftrightarrow$ y′

18. But:
$$\hat{x'} = \frac{1}{\sqrt{2}}\left[\hat{x} + \hat{y}\right] \tag{2.4.11}$$
and
$$\hat{y'} = \frac{1}{\sqrt{2}}\left[\hat{x} - \hat{y}\right] \tag{2.4.12}$$
Due to analogy constructed we must be able to same the same for the Stern-Gerlach states:
$$SG_x^+ = \frac{1}{\sqrt{2}}\left[SG_z^+ + SG_z^-\right] \tag{2.4.13}$$

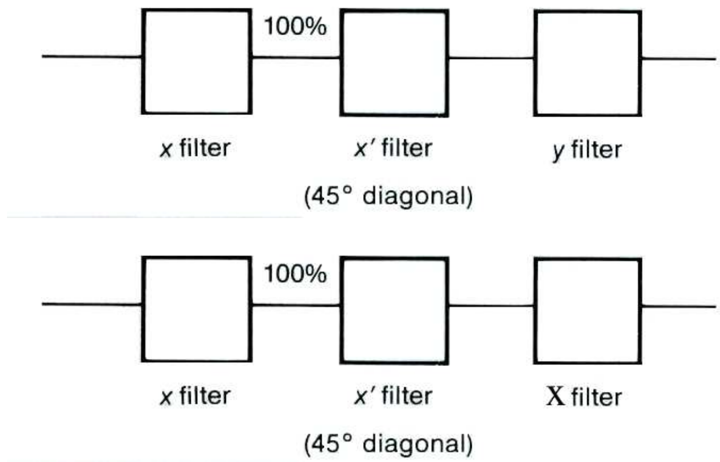
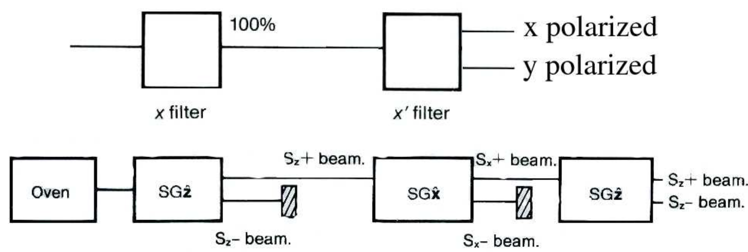


Figure 16: You get light from both. Compare this figure with Fig. (10).



and

$$SG_x^- = \frac{1}{\sqrt{2}} \left[SG_z^+ - SG_z^- \right] \tag{2.4.14}$$

19. Hence we may construct this analogy between polarized light and the states for the Stern-Gerlach experiment.

20. **But wait, we have now resolved the confusion we had in Figure (10). Now it all makes sense when we look at Figure (10) in the same manner as Figure (16).** (Or does it? Your homework will tell. :-))

21. So it must be that the spin states act in a fashion similar to plane polarized light (which are waves as we saw in Eq. (2.4.10)).

22. This is precisely what de Broglie was to realize (*the wave particle-duality*) a few years after Stern and Gerlach did this experiment. But now we can see how it all comes together.

23. But we now see that our earlier nonsensical remark in point (9) (page 15) after Fig. (10) does make sense after all !!! It must be true that when we made the X-direction measurement in Fig (10), we forgot that the z-direction had been measured before that.

24. In fact, it is true that the x′ polarizer changes an input x-polarized beam to an x′ polarized beam. So, something similar is going on here with respect to the SG$_x$ operation on an S$_z^+$ input.

25. *This is actually a very subtle concept in quantum mechanics that is completely non-existent in classical theories.* We will see later on that all makes perfect sense when the correct mathematical framework is utilized.

26. To understand these peculiarities it is required that we embark into some abstract mathematical theories (linear vector spaces). We have already seen that this nonsensical remark actually makes sense for plane-polarized light, but we will see that all this makes sense from a more profound level. The one aspect that becomes clear from the analogy to polarized light is that *vectors* have a required property to describe these states. (Note: The electric field directions are vectors. See Eq. (2.4.10) and also see Figure (13).) For this reason we consider it important to embark into a discussion of vector spaces.

Homework:

Circularly polarized light: In this homework, we will: (a) first present an expression for circularly polarized (Eq. (2.4.15) below), (b) simplify this expression using an identity from complex numbers, (c) convince ourselves (pictorially) that the expression we presented is indeed circularly polarized, (d) construct an analogy between SG_y^+ with circularly polarized light.

In Equation (2.4.10) we talked about how plane-polarized light can be represented using a moving wave. But note here that the plane of polarization remains x-z forever. (How do we know that? The electric field remains along the x-axis for all time.) Consider, now, a wave that looks like:

$$E = E_0 \left[\frac{1}{\sqrt{2}} \hat{x} \cos\left(kz - \omega t\right) + \frac{1}{\sqrt{2}} \hat{y} \cos\left(kz - \omega t + \frac{\pi}{2}\right) \right] \tag{2.4.15}$$

Note the first term in Eq. (2.4.15) is the same as Eq. (2.4.10). But the second term is out-of-phase by $\frac{\pi}{2}$. (Do you understand this last statement? If not come see me.)

1. I will now help you show that the plane-of-polarization of the wave in Eq. (2.4.15) rotates as a function of time (as opposed to remaining fixed along $\hat{x}$, as Eq. (2.4.10) does).

(a) Show that Eq. (2.4.15) is identical to (there is a hint below):

$$E = E_0 \; Re\left[\frac{1}{\sqrt{2}}\hat{x}e^{\imath(kz-\omega t)} + \frac{\imath}{\sqrt{2}}\hat{y}e^{\imath(kz-\omega t)}\right] \tag{2.4.16}$$

Where $Re\left[\cdots\right]$ stands for the real part of the bracketed term. Hint:

i. Take Eq. (2.4.16), and substitute $e^{\imath(kz-\omega t)} = \cos(kz-\omega t) + \imath\sin(kz-\omega t)$. (Do your remember this identity? It is from complex numbers: $e^{\imath\theta} = \cos(\theta) + \imath\sin(\theta)$, we have used $\theta = (kz-\omega t)$ in this identity.)

ii. Take only the real part (as is required by the operation $Re\left[\cdots\right]$. You will obtain Eq. (2.4.15)

(b) Consider the following for values of time, $t = \frac{kz}{\omega}$, $t = \frac{kz}{\omega} + \frac{\pi}{4\omega}$, $t = \frac{kz}{\omega} + 2\frac{\pi}{4\omega}$, $t = \frac{kz}{\omega} + 3\frac{\pi}{4\omega}$, $t = \frac{kz}{\omega} + 4\frac{\pi}{4\omega}$. At each value of t, draw the direction of the vector in Eq. (2.4.16). Do you notice anythings special? Does this direction change with time? Can you comment on what you see? [2].

(c) Like for the case of plane-polarized light, we propose $SG_y^+ \leftrightarrow$ Eq. (2.4.15) which we call right circularly polarized due to the positive sign. You must have noticed in the previous problem that the rotation occurs in a fashion similar to a right hand screw which is why it is called right circularly polarized light. If you flip the sign in Eq. (2.4.15) you will see that the rotation is similar to that due to a left hand screw and hence the equation with the flipped sign is called left circularly polarized light.

(d) We then construct the analogy $SG_y^- \leftrightarrow$ Eq. (2.4.15) with the sign flipped. This analogy gives us the relations

$$SG_y^+ = \frac{1}{\sqrt{2}}\left[SG_z^+ + \imath SG_z^-\right] \tag{2.4.17}$$

and

$$SG_y^- = \frac{1}{\sqrt{2}}\left[SG_z^+ - \imath SG_z^-\right] \tag{2.4.18}$$

Notice that the $\imath$ makes its appearance here through Eq. (2.4.16)

(e) *Complex numbers already !!*

(f) Show that the choice in Eqs. (2.4.17) and (2.4.18) makes the states $SG_z^\pm$, $SG_x^\pm$ and $SG_y^\pm$ symmetric. Hint: To answer this question, think about the angle between $SG_z^\pm$ and $SG_x^\pm$. Utilize the connection to x and x/ vectors and try to obtain the angle using "dot" products. Now, what are the angles between $SG_z^\pm$ and $SG_y^\pm$?

(g) Importantly, from Eqs. (2.4.13), (2.4.14), (2.4.17) and (2.4.18) we note that the states corresponding to SG_z^+ and SG_z^- must form a complete set!! Can you explain why?

So this is a two-dimensional space that can have complex coefficients. Hence, in essence SG experiments are explained by invoking a *four-dimensional real linear vector space*!!

[2]For reasons you see in this example, Eq. (2.4.16) is called *circularly polarized light*

2. The quantity $[a \times SG_z^+ + b \times SG_z^-]$ which is now an arbitrary linear combination of the two vectors with (possibly) complex values for "a" and "b" is called a "spinor", since it is an object associated with the spin of a particle.

3. Spinors form the basis of much what exists now-a-days in the quantum information and quantum computing literatures.

2.5 A brief summary of Stern-Gerlach experiments

- The physical picture of the experiment gets translated mathematically to the set of vectors: $\mathbf{S_z^+}$, $\mathbf{S_z^-}$, $\mathbf{S_x^+}$, $\mathbf{S_x^-}$, etc.
- The space represented by these vectors is *an abstract two-dimensional space*. Note: the axes in this abstract space: $\mathbf{S_z^+}$, $\mathbf{S_z^-}$, for example, are not the same axes where the magnetic fields are aligned.
- This abstract space is a portion of what we will later begin to describe as the Hilbert space.
- It appears that the "projection" process we discussed in this space completely describes what happens in the measurements involved during Stern-Gerlach experiments.
- But, this space is complex. Hence, it is difficult to properly draw it on a board (because it is two-dimensional *and* complex). However, we may be able to visualize it in our minds.
- Certain words are now limiting because of the presence of complex numbers. The words, angle, or dot product were originally developed for real-space vectors and we will need to generalize these definitions.
- We find that the following represents a mathematically consistent description of what is happening in these experiments:

  Stern-Gerlach spin states $\rightarrow$ vectors (in a complex space).
  Measurement $\rightarrow$ projection
  Note also that the projection appears to occur onto special directions!!
  Projected components $\rightarrow$ complex numbers in general
  Measured quantities $\rightarrow$ absolute values of projected components.

  Hence, although the projected components may be complex, the measured values are generally real.
- While we have based our study thus far on the Stern Gerlach experiments, which deal with spin, we will find later that the above description is appropriate for *all kinds of measurable quantities*.
  - For example, we will late introduce an arbitrary vector that describes the electronic properties of a system and even that vector resides in the complex Hilbert space we described above.
  - An experiment conducted on that vector is a projection similar to what we have introduced above.
- The above ideas will, in a few classes, translate to "the postulates of quantum mechanics".

