

## Chem 542 Problem Set 5

1) **Math fun!** When you have to prove something like:

$$e^x = \sum_{n=0}^{\infty} \frac{1}{n!} x^n$$

we often evaluate just a few terms of the series:  $\sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2} \dots$  which seems to approach  $e^x$  if you plug in some values for  $x$ . Then we say, "good enough"! However, there is a vigorous way to solve this using the "uniqueness theorem of differential equations," which stipulates that  $e^x$  and  $\sum_{n=0}^{\infty} \frac{x^n}{n!}$  are equal if their derivatives are the same. We know that:  $\frac{\partial}{\partial x} e^x = e^x$ , so what we need to do here is to show that:

$$\frac{\partial}{\partial x} \sum_{n=0}^{\infty} \frac{1}{n!} x^n = \sum_{n=0}^{\infty} \frac{1}{n!} x^n$$

which is of course  $e^x$ . So, have at it.

**Hint:**

$$\sum_{n=0}^{\infty} n \cdot \frac{1}{n!} = \sum_{n=1}^{\infty} n \cdot \frac{1}{n!}$$

since the  $n = 0$  term of the sum doesn't contribute. Next, we can state:

$$\sum_{n=1}^{\infty} n \cdot \frac{1}{n!} = \sum_{n=1}^{\infty} \frac{1}{(n-1)!}$$

The final step of the proof requires a substitution of variables.

**Answer:** First do the derivative:

$$\frac{\partial}{\partial x} \sum_{n=0}^{\infty} \frac{x^n}{n!} = \sum_{n=0}^{\infty} n \cdot \frac{x^{n-1}}{n!}$$

and use the hint about simplifying the result:  $\sum_{n=0}^{\infty} n \cdot \frac{x^{n-1}}{n!} = \sum_{n=1}^{\infty} n \cdot \frac{x^{n-1}}{n!} = \sum_{n=1}^{\infty} \frac{x^{n-1}}{(n-1)!}$ .

Last step, we can just transform variables  $q = n - 1$ , which makes the lower limit ( $n = 1$ ):  $q = n - 1 = 1 - 1 = 0$  and changes the factorial and exponent of  $x$  as:

$$\sum_{n=1}^{\infty} \frac{x^{n-1}}{(n-1)!} = \sum_{q=0}^{\infty} \frac{x^q}{q!}$$

Since the “q” or “n” label is arbitrary, we have proved our case since  $\sum_{q=0}^{\infty} \frac{x^q}{q!} = e^x$ .

**2)** You should know about atomic units, in which  $\hbar = 1$ ,  $\frac{1}{4\pi\epsilon_0} = 1$ ,  $e^2 = 1$  (the charge of an electron), length is in Bohrs ( $a_0=0.0529$  nm), and the mass of an electron is:  $m_e = 1$ . As a result, the Hamiltonian of a multielectron system:

$$\frac{-\hbar^2}{2m} \nabla_1^2 + \frac{-\hbar^2}{2m} \nabla_2^2 - \frac{Ze^2}{4\pi\epsilon_0 r_1} - \frac{Ze^2}{4\pi\epsilon_0 r_2} + \frac{e^2}{4\pi\epsilon_0 |r_1 - r_2|}$$

becomes:

$$-\frac{1}{2} \nabla_1^2 + -\frac{1}{2} \nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{|r_1 - r_2|}$$

While this is clearly more simple, you should know that something else has to become more complex. In fact, that would be the energy and time.

**a.** Can you determine what energy is in atomic units, which is called a Hartree. Please express 1 Hartree in Joules and show your work! **Hint:** what you want to do is calculate energy *only using* the units above defined as 1 ( $\hbar$ , mass of the electron, and a Bohr for length).

For example, kinetic energy is  $\frac{p^2}{2m}$ ; although for units you scrap the “2”:  $E = \frac{p^2}{m}$ .

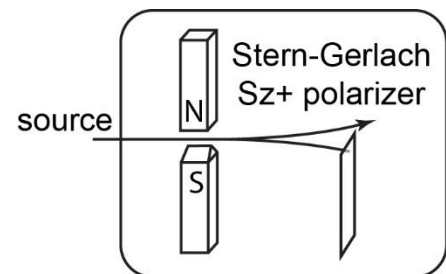
**b.** Can you determine what time is for atomic units (in seconds please)?

**Answer: a.** The correct expression is:  $\frac{\hbar^2}{m_e a_0^2} = 4.36 \times 10^{-18} J$

**b.** Since  $\hbar$  is energy times time, you can just multiply it by the inverse of a Hartree:

$$\hbar \cdot \frac{m_e a_0^2}{\hbar^2} = \frac{m_e a_0^2}{\hbar} = 2.42 \times 10^{-17} s.$$

**3)** Here we are going to develop a matrix representation  $\hat{\Omega}$  of the Stern-Gerlach device shown here:



This takes any polarized input  $\begin{bmatrix} z1 \\ z2 \end{bmatrix}$ , whether it is  $|S_z, +\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ ,  $|S_z, -\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ ,  $|S_x, +\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ ,  $|S_x, -\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$ ,  $|S_y, +\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix}$ , or  $|S_y, -\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix}$ , and outputs  $\sim |S_z, +\rangle = \begin{bmatrix} z1 \\ 0 \end{bmatrix}$ .

Here, you must determine the matrix representation of  $\hat{\Omega}$  such that:

$$\hat{\Omega} \begin{bmatrix} z1 \\ z2 \end{bmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} z1 \\ z2 \end{bmatrix} = \begin{bmatrix} z1 \\ 0 \end{bmatrix}$$

Can you use standard matrix multiplication to figure out what  $\hat{\Omega}$  is? **Hint:**  $z_1$  and  $z_2$  are independent, like vectors  $x$  and  $y$ . As a result, an equation such as:  $a \cdot x = b \cdot y$  can only have the solution  $a=b=0$ .

**Answer:** Multiply it out:

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} a \cdot z_1 + b \cdot z_2 \\ c \cdot z_1 + d \cdot z_2 \end{bmatrix} = \begin{bmatrix} z_1 \\ 0 \end{bmatrix}$$

Therefore  $a \cdot z_1 + b \cdot z_2 = z_1$ . Since  $z_2$  isn't part of the equality on the right  $b$  must be 0, leaving  $a=1$ . Next,  $c \cdot z_1 + d \cdot z_2 = 0$  and therefore  $c \cdot z_1 = -d \cdot z_2$ . Since there cannot be a relationship between  $z_1$  and  $z_2$ , the only answer to this is  $c = 0$  and  $d = 0$ . As a result, the matrix representation of the operator is:

$$\hat{\Omega} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

**4)** Now we will redo question 3 using the matrix representation of the  $\hat{\Omega}$  operator in the  $S_z$  basis:

$$\begin{aligned} \hat{\Omega} &= \sum_{i=S_z,+}^{S_z,-} \sum_{j=S_z,+}^{S_z,-} |i\rangle \langle i| \hat{\Omega} |j\rangle \langle j| \\ &= |S_z,+ \rangle \langle S_z,+ | \hat{\Omega} |S_z,+ \rangle \langle S_z,+ | + |S_z,- \rangle \langle S_z,- | \hat{\Omega} |S_z,+ \rangle \langle S_z,+ | \\ &\quad + |S_z,+ \rangle \langle S_z,+ | \hat{\Omega} |S_z,- \rangle \langle S_z,- | + |S_z,- \rangle \langle S_z,- | \hat{\Omega} |S_z,- \rangle \langle S_z,- | \end{aligned}$$

which is more easily expressed as:

$$\hat{\Omega} = \begin{bmatrix} \langle S_z,+ | \hat{\Omega} |S_z,+ \rangle & \langle S_z,+ | \hat{\Omega} |S_z,- \rangle \\ \langle S_z,- | \hat{\Omega} |S_z,+ \rangle & \langle S_z,- | \hat{\Omega} |S_z,- \rangle \end{bmatrix}$$

Please explain **in words** why you evaluate the following as either 1 or 0:

**a.**  $\langle S_z,+ | \hat{\Omega} |S_z,+ \rangle$     **b.**  $\langle S_z,+ | \hat{\Omega} |S_z,- \rangle$     **c.**  $\langle S_z,- | \hat{\Omega} |S_z,+ \rangle$     **d.**  $\langle S_z,- | \hat{\Omega} |S_z,- \rangle$

**Hint:** You already know the answer from question 3, but here you have to explain in words what these matrix elements mean. For example, let's examine the second term and simplify the notation a bit:  $|+\rangle \langle +| \hat{\Omega} |-\rangle \langle -|$ ; here,  $S_z-$  polarized Ag atoms are input and  $S_z+$  Ag atoms are the output. Is it possible for the Stern Gerlach device to do this? Etc.

**Answer:** **a.** The Stern-Gerlach apparatus can easily convert  $|S_z,+ \rangle$  to  $|S_z,+ \rangle$ , since that isn't a conversion at all! **b.** This is 0 because there is no positive  $S_z+$  component in the  $S_z-$  state. Both **c.**, **d.** are 0 because the device can't output  $S_z-$  polarized Ag atoms.

5) Let's redo the question one last time. It turns out the Stern-Gerlach machine in question 3 is a manifestation of the  $S_z+$  projection operator:  $\hat{\Omega} = |S_z, +\rangle\langle S_z, +|$ . Knowing this, can you re-work question 4 entirely with Dirac Notation:

- a.  $\langle S_z, +|\hat{\Omega}|S_z, +\rangle$     b.  $\langle S_z, +|\hat{\Omega}|S_z, -\rangle$     c.  $\langle S_z, -|\hat{\Omega}|S_z, +\rangle$     d.  $\langle S_z, -|\hat{\Omega}|S_z, -\rangle$

to show that  $\hat{\Omega} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ ?

**Hint:**  $\langle S_z, +|S_z, +\rangle = 1$ ,  $\langle S_z, -|S_z, +\rangle = 0$ ,  $\langle S_z, +|S_z, -\rangle = 0$ ,  $\langle S_z, -|S_z, -\rangle = 1$

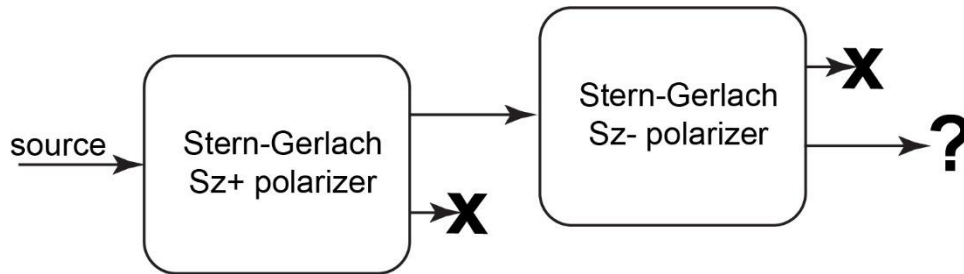
**Answer:**

- a.  $\langle S_z, +|\hat{\Omega}|S_z, +\rangle = \langle S_z, +|S_z, +\rangle\langle S_z, +|S_z, +\rangle = 1 \cdot 1 = 1$   
 b.  $\langle S_z, +|\hat{\Omega}|S_z, -\rangle = \langle S_z, +|S_z, +\rangle\langle S_z, +|S_z, -\rangle = 1 \cdot 0 = 0$   
 c.  $\langle S_z, -|\hat{\Omega}|S_z, +\rangle = \langle S_z, -|S_z, +\rangle\langle S_z, +|S_z, +\rangle = 0 \cdot 1 = 0$   
 d.  $\langle S_z, -|\hat{\Omega}|S_z, -\rangle = \langle S_z, -|S_z, +\rangle\langle S_z, +|S_z, -\rangle = 0 \cdot 0 = 0$

6) Let's call the previous projection operator  $\hat{\Omega}_{S_z+}$ , and if you had done the same question with a device that allowed the  $S_z-$  polarization to pass you would have derived:

$$\hat{\Omega}_{S_z-} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

So, what would happen if you put the two Stern-Gerlach devices side-by-side as shown here:



a. What would the output of such a device be, no matter what type of polarization is source input?

b. Use the matrix representation of  $\hat{\Omega}_{S_z+}$  and  $\hat{\Omega}_{S_z-}$  to show that your answer to pt. a is consistent with:  $\hat{\Omega}_{total} = \hat{\Omega}_{S_z-}\hat{\Omega}_{S_z+}$

c. Now redo the problem once more using  $\hat{\Omega}_{S_z+} = |S_z, +\rangle\langle S_z, +|$  and  $\hat{\Omega}_{S_z-} = |S_z, -\rangle\langle S_z, -|$  to find  $\hat{\Omega}_{total}$ .

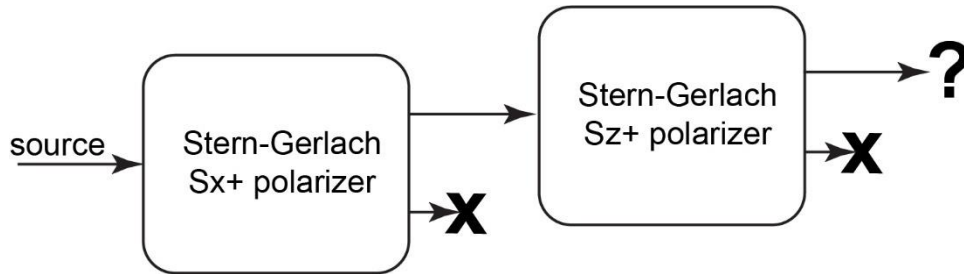
**Answer:** a. The SG device wouldn't have anything come out of it, it's basically a beam block.

b.  $\hat{\Omega}_{total} = \hat{\Omega}_{S_z-} \hat{\Omega}_{S_z+} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$

Everything is 0, yes this makes sense.

c.  $\hat{\Omega}_{total} = \hat{\Omega}_{S_z-} \hat{\Omega}_{S_z+} = |S_z, +\rangle \langle S_z, +| |S_z, -\rangle \langle S_z, -| = 0$  because  $\langle S_z, + | S_z, - \rangle = 0$ .

7) Imagine that we have the following Stern-Gerlach experiment:



a. The first device is  $\hat{\Omega}_{S_x+} = |S_x, +\rangle \langle S_x, +|$ , the projection operator into the positive x-polarized state. Using Dirac notation for the operator:

$$\hat{\Omega}_{S_x+} = \sum_{i=S_z,+}^{S_z,-} \sum_{j=S_z,+}^{S_z,-} |i\rangle \langle i| \hat{\Omega}_{S_x+} |j\rangle \langle j|$$

can you write out the matrix representation in the  $S_z$  basis set?

**Hint:**  $|S_x, +\rangle = \frac{1}{\sqrt{2}} |S_z, +\rangle + \frac{1}{\sqrt{2}} |S_z, -\rangle$ , and  $\hat{\Omega}_{S_x+} = \begin{bmatrix} \langle S_z, + | \hat{\Omega}_{S_x+} | S_z, + \rangle & \langle S_z, + | \hat{\Omega}_{S_x+} | S_z, - \rangle \\ \langle S_z, - | \hat{\Omega}_{S_x+} | S_z, + \rangle & \langle S_z, - | \hat{\Omega}_{S_x+} | S_z, - \rangle \end{bmatrix}$

b. Now, if you had  $S_z$ - polarized Ag atoms going into the  $S_z$ + Stern-Gerlach machine, there would of course be no output. However, if you were to do the same with the above machine (an  $S_x$ + polarizer followed by a  $S_z$ + polarizer, all of which can be represented as  $\hat{\Omega}_{total} = \hat{\Omega}_{S_z+} \hat{\Omega}_{S_x+}$ ) would there still be no output? Please use the matrix

representation of these operators and  $|S_z, -\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$  to solve the problem:  $\hat{\Omega}_{S_z+} \hat{\Omega}_{S_x+} |S_z, -\rangle$

**Answer: a.** If you evaluate the matrix elements you find:

$$\langle S_z, + | \hat{\Omega}_{S_x+} | S_z, + \rangle = \langle S_z, + | \left\{ \frac{1}{\sqrt{2}} |S_z, +\rangle + \frac{1}{\sqrt{2}} |S_z, -\rangle \right\} \left\{ \frac{1}{\sqrt{2}} \langle S_z, +| + \frac{1}{\sqrt{2}} \langle S_z, -| \right\} |S_z, +\rangle = \frac{1}{2}$$

Once you run through them all you find that  $\hat{\Omega}_{S_x+} = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ .

**b.** The result of matrix multiplication is:

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$$

If you input  $S_z$ - polarized Ag atoms, you get some  $S_z$ + output:

$$\frac{1}{2} \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

8) Using the following descriptors:  $|S_y, +\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{i}{\sqrt{2}}|-\rangle$  and  $|S_y, -\rangle = \frac{1}{\sqrt{2}}|+\rangle - \frac{i}{\sqrt{2}}|-\rangle$

can you demonstrate that  $\hat{S}_y = \frac{\hbar}{2} \{-i \cdot |+\rangle\langle -| + i \cdot |-\rangle\langle +|\}$ ?

**Hint:** recall how to use complex conjugates when dealing with kets vs. bras.

**Answer:** Using the convention:  $\hat{S}_y = \frac{\hbar}{2} |S_y, +\rangle\langle S_y, +| - \frac{\hbar}{2} |S_y, -\rangle\langle S_y, -|$

Next you plug in the definitions above:

$$\hat{S}_y = \frac{\hbar}{2} \left\{ \left( \frac{1}{\sqrt{2}}|+\rangle + \frac{i}{\sqrt{2}}|-\rangle \right) \left( \frac{1}{\sqrt{2}}\langle +| - \frac{i}{\sqrt{2}}\langle -| \right) - \left( \frac{1}{\sqrt{2}}|+\rangle - \frac{i}{\sqrt{2}}|-\rangle \right) \left( \frac{1}{\sqrt{2}}\langle +| + \frac{i}{\sqrt{2}}\langle -| \right) \right\}$$

Now FOIL out the insides:

$$\begin{aligned} \frac{\hbar}{2} \left\{ \left( \frac{1}{2}|+\rangle\langle +| + \frac{i}{2}|-\rangle\langle +| - \frac{i}{2}|+\rangle\langle -| + \frac{1}{2}|-\rangle\langle -| \right) \right. \\ \left. - \left( \frac{1}{2}|+\rangle\langle +| + \frac{i}{2}|+\rangle\langle -| - \frac{i}{\sqrt{2}}|-\rangle\langle +| + \frac{1}{2}|-\rangle\langle -| \right) \right\} \end{aligned}$$

You can see that several factors cancel out:

$$\begin{aligned} \frac{\hbar}{2} \left\{ \left( \frac{1}{2}|+\rangle\langle +| - \frac{1}{2}|+\rangle\langle +| \right) + \left( \frac{i}{2}|-\rangle\langle +| + \frac{i}{2}|-\rangle\langle +| \right) - \left( \frac{i}{2}|+\rangle\langle -| - \frac{i}{2}|+\rangle\langle -| \right) \right. \\ \left. + \left( \frac{1}{2}|-\rangle\langle -| - \frac{1}{2}|-\rangle\langle -| \right) \right\} \end{aligned}$$

Which leaves  $\hat{S}_y = \frac{\hbar}{2} \{i|-\rangle\langle +| - i|+\rangle\langle -|\}$

9) For this question we will use a matrix representation to demonstrate:

$$[\hat{S}_i, \hat{S}_j] = i\hbar \cdot \epsilon_{i,j,k} \cdot \hat{S}_k$$

You need to know that:  $\hat{S}_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ ,  $\hat{S}_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ , and  $\hat{S}_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

Please use the following approach:

a) Demonstrate  $\hat{S}_x \hat{S}_y = \frac{i\hbar}{2} \hat{S}_z$

b) Demonstrate  $\hat{S}_y \hat{S}_x = -\frac{i\hbar}{2} \hat{S}_z$  and thus  $[\hat{S}_x, \hat{S}_y] = i\hbar \cdot \hat{S}_z$

c) Now use the same approach to show:  $[\hat{S}_x, \hat{S}_z] = -i\hbar \cdot \hat{S}_y$

**Answer: a)**  $\hat{S}_x \hat{S}_y = \frac{\hbar^2}{4} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \frac{\hbar^2}{4} \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}$

Some factoring yields  $\hat{S}_x \hat{S}_y = \frac{i\hbar}{2} \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \frac{i\hbar}{2} \hat{S}_z$

**b)**  $\hat{S}_y \hat{S}_x = \frac{\hbar^2}{4} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \frac{\hbar^2}{4} \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix} = -\frac{i\hbar}{2} \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = -\frac{i\hbar}{2} \hat{S}_z$

Thus,  $\hat{S}_x \hat{S}_y - \hat{S}_y \hat{S}_x = \frac{i\hbar}{2} \hat{S}_z - \left(-\frac{i\hbar}{2} \hat{S}_z\right) = i\hbar \cdot \hat{S}_z$

**c)** First,  $[\hat{S}_x, \hat{S}_z] = \hat{S}_x \hat{S}_z - \hat{S}_z \hat{S}_x$ . We will evaluate  $\hat{S}_x \hat{S}_z$  first:

$$\hat{S}_x \hat{S}_z = \frac{\hbar^2}{4} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \frac{\hbar^2}{4} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

This is a bit tricky- you make progress by factoring out an “i”:  $\hat{S}_x \hat{S}_z = \frac{\hbar^2}{4} i \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}$ . Now try

factoring out a “-i”:  $\hat{S}_x \hat{S}_z = \frac{\hbar^2}{4} (-i) \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$  and upon further rearrangement you find:

$$\hat{S}_x \hat{S}_z = -\frac{i\hbar}{2} \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = -\frac{i\hbar}{2} \hat{S}_y$$

Next:

$$\hat{S}_z \hat{S}_x = \frac{\hbar^2}{4} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \frac{\hbar^2}{4} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

Like before you factor out an “i” to find:

$$\hat{S}_z \hat{S}_x = i \frac{\hbar^2}{4} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \text{ which we see is } \hat{S}_z \hat{S}_x = \frac{i\hbar}{2} \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \frac{i\hbar}{2} \hat{S}_y$$

Consequently,  $[\hat{S}_x, \hat{S}_z] = \hat{S}_x \hat{S}_z - \hat{S}_z \hat{S}_x = -\frac{i\hbar}{2} \hat{S}_y - \frac{i\hbar}{2} \hat{S}_y = -i\hbar \hat{S}_y$

**10)** Now let’s work with some anti-commutators:

**a)** Please show that  $\{\hat{S}_x, \hat{S}_x\} = \hat{S}_x \hat{S}_x + \hat{S}_x \hat{S}_x = \frac{\hbar^2}{2}$  using the matrix representation.

**b)** And that  $\{\hat{S}_y, \hat{S}_z\} = \hat{S}_y \hat{S}_z + \hat{S}_z \hat{S}_y = 0$ .

**Answer: a)**  $\hat{S}_x \hat{S}_x = \frac{\hbar^2}{4} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \frac{\hbar^2}{4} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ . Hence  $\hat{S}_x \hat{S}_x + \hat{S}_x \hat{S}_x = 2 \frac{\hbar^2}{4} \mathbf{I} = \frac{\hbar^2}{2}$ , where  $\mathbf{I}$  is the identity matrix.

**b)**  $\hat{S}_y \hat{S}_z = \frac{\hbar^2}{4} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \frac{\hbar^2}{4} \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix}$ . Likewise  $\hat{S}_z \hat{S}_y = \frac{\hbar^2}{4} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} =$

$$\frac{\hbar^2}{4} \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix}.$$

It is clear that the two matrices are the negative of each other, so when added you get 0.