Homework 1 (Due Jan 29th)

This first homework set is meant to remind you of the main concepts from Quantum 1. It focuses on spin, operators, diagonalization and the formalism of kets and linear algebra. We will build on all of these tools and ideas this semester, so you should make sure you have these ideas down before next week. In addition, there's a couple computational problem that are meant to introduce you to the linear algebra package for Python.

1. Spin 1/2; let's goooo

Consider a beam of spin-1/2 particles that are sent through a Stern-Gerlach device. The device measures the z-component of the spin angular momentum of the particles. After a long time, one quarter ($\frac{1}{4}$) of the particles are observed to be spin up ($|+\rangle$) and three quarters ($\frac{3}{4}$) are observed to be spin down ($|-\rangle$).

1. Sketch a histogram of the measured spin values ($+\hbar/2$; $-\hbar/2$). See Figs. 1.9, 1.10, or 1.11 in McIntyre for examples.
2. What is the expectation value of the z-component of the angular momentum ($\langle S_z \rangle$). You should be able to do this using probability theory ($\langle x \rangle = \sum_i P_i x_i$). Why does the sign of this expectation value make sense?
3. In the S_z basis, the general state vector for any particle in the beam is given by $|\Psi\rangle = a\,|+\rangle + b\,|-\rangle$. We have not yet determined the coefficients, a and b. Using the probabilities of measuring spin up and spin down for this beam, determine the normalized state vector for a particle in the beam, $|\Psi\rangle$. What are we assuming about particles in the beam when we do this?
4. Write the normalized state vector from part 3 using the linear algebra representation. That is, using $|+\rangle \doteq \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|-\rangle \doteq \begin{bmatrix} 0 \\ 1 \end{bmatrix}$.
5. Using the spin matrix for $S\_z \doteq \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$, calculate the expectation value, $\langle S_z \rangle$. How does you answer compare to part 2?
6. Now let's use the S_x spin matrix, $S\_x \doteq \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, to calculate the expectation value, $\langle S_x \rangle$. What does the sign of this expectation value tell you about the relative probabilities of the x-component of the spin angular momentum? That is, how do P_{+x} and P_{-x} compare?
7. Let's check this intuition against the calculated probabilities for observing the particles with spin up/down x-components. Calculate the probabilities of observing particles in each state: $\|_x\langle + \| \Psi \rangle\|^2$ and $\|_x\langle - \| \Psi \rangle\|^2$. Check that the probabilities sum to 1. How do these probabilities compare with your intuition from part 6?
8. We send the beam through a magnetic field that is directed in z-direction: $\mathbf{B} = B_0\hat{\mathbf{z}}$. The Hamiltonian for that interaction is: $\mu \cdot \mathbf{B} = \dfrac{qB_0}{m} S_z = \omega_o S_z$ where $\omega_0 = \dfrac{qB_0}{m}$. This Hamiltonian is diagonal in the S_z basis. Write down the energy eigenvalues and eigenstates of this Hamiltonian. Why can you simply write down the answer?
9. We let the beam time evolve in magnetic field. Using the energy eigenvalues, determine the time dependent state vector, $|\Psi(t)\rangle$.
10. Determine the probability of observing this time-evolving state vector in a spin up/down state for the z-component of the spin angular momentum. Is your answer time-dependent? Why or why not?

2. The Eigenvalue Problem; The Quantum Crux

Let's investigate a three state quantum system ($|1\rangle$, $|2\rangle$, $|3\rangle$). The Hamiltonian for this system is given by:

$$H \doteq \begin{bmatrix} E_1 & 0 & A \\ 0 & E_0 & 0 \\ A & 0 & E_1 \end{bmatrix}$$

In the $|1\rangle \doteq \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$, $|2\rangle \doteq \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$, $|3\rangle \doteq \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$ basis the Hamiltonian is NOT diagonal.

1. Are the state vectors, $|1\rangle$, $|2\rangle$, $|3\rangle$, energy eigenstates? How can you tell?
2. Diagonalize H and find the energy eigenvalues. You should find three distinct values ($E_1-?$, E_0, and $E_1+?$). What is the value of question mark?
3. Sketch an energy level diagram for this system. You can assume $E_0 < E_1$ and $A < (E_1 - E_0)$. What is the ground state, the first excited state, the second excited state? How much energy would be needed to make the transition between the ground state and the two different excited states?
4. Now that you have found the energy eigenvalues, use those eigenvalues to determine the energy eigenstates in terms of the $|1\rangle$, $|2\rangle$, $|3\rangle$ basis. Which eigenstate corresponds to the ground state? The first excited state? The second excited state?

3. Spin Games

Diagonalization is one of the key processes for quantum mechanics; it is needed to find the eigenvalues and eigenvectors of operators. Two by two matrices are relatively easy to diagonalize analytically as you typically solve quadratic questions. Higher order operators are more challenging to diagonalize because with each new dimension you introduce an additional term in the polynomial you attempt to solve. In this problem, you will diagonalize the S_x operator for a spin 1 system.

$$S_x \doteq \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

1. Diagonalize S_x to find the eigenvalues of the operator. What is the order of the polynomial you have to solve? Why does that make sense?
2. Using these eigenvalues, find the eigenvectors of the S_x operator.
3. Can you measure S_x and S_z at the same time? Why or why not?
4. Compute the commutator $[S_x, S_z]$. What does that result tell you about the uncertainty principle as it relates to a spin-1 system?

4. Time Evolution

General time evolution of states is hard, but when the Hamiltonian is time independent and we know the energy eigenstates, time evolution is pretty much a procedural calculation (just multiply by $e^{\frac{-iE_n t}{\hbar}}$). However, we have to have the appropriate energy eigenstates, which can be tricky. Let's explore how we get there with a system where the energy eigenstates are not as straightforward.

Consider a spin-1/2 particle that is allowed to evolve in a uniform magnetic field. The particle is initially in the state $|\psi(0)\rangle = |+\rangle_n$ where $\hat{n} = (\hat{x} + \hat{y})/\sqrt{2}$. The magnetic field that the particle is placed in is given by $\mathbf{B} = B_0(\hat{x} + \hat{z})/\sqrt{2}$.

1. In this situation, the state vector is not an energy eigenvector; the state vector is not aligned to the magnetic field. We first need to write $|\psi(0)\rangle$ in the usual $|+\rangle, |-\rangle$ basis. In general, $|n\rangle_+ = \cos\frac{\theta}{2}|+\rangle + e^{i\phi}\sin\frac{\theta}{2}|-\rangle$. Sketch the initial state vector in 3D space and determine θ and ϕ. Write down $|\psi(0)\rangle$ in the usual $|+\rangle, |-\rangle$ basis.

2. As the particle has a magnetic moment, it will tend to align with the magnetic field, which does not point in the direction of the initial state vector. So, we also need to determine the initial state in terms of the basis of the magnetic field direction. This is the energy basis for this problem, so we can use our simple expansion with exponential terms (with $\pm\hbar\omega/2$). (Recall: finding the state in the energy basis of the problem makes it easy for us to use this expansion.). In general, the energy basis states are given by:
$$|+\rangle_{n'} = \cos\frac{\theta}{2}\,|+\rangle + e^{i\phi}\sin\frac{\theta}{2}\,|-\rangle$$
and
$$|-\rangle_{n'} = \cos\frac{\theta}{2}\,|+\rangle - e^{i\phi}\sin\frac{\theta}{2}\,|-\rangle$$
where $\hat{n}' = (\hat{x} + \hat{z})/\sqrt{2}$. Sketch the magnetic field field vector in 3D space and determine θ and ϕ. Write down $|\psi(0)\rangle$ in the $|+\rangle_{n'}, |-\rangle_{n'}$ basis; you will need to use projection operators and/or the closure relationship.
3. Now that you have $|\psi(0)\rangle$ in the energy ($|+\rangle_{n'}, |-\rangle_{n'}$) basis, use the exponential expansion to find $|\psi(t)\rangle$.
4. Finally, compute the time dependent probability of measuring $S_y = +\hbar/2$. You should find that it is proportional to: $2 + \sqrt{2}\cos\omega t + \sin\omega t$. Given that it is time dependent, what does that tell you about the state (re: stationary states)?

5. Jupyter and Linear Algebra

You will turn in this question using a Dropbox file request. Turn in the notebook, not a PDF of it.

Python is a powerful and flexible programming language that can be used to solve many kinds of scientific problems. The wide variety of modules and libraries that are available for Python have specific uses for particular kinds of problems. In this problem, you will learn to use the `numpy` module and the associated `linalg` library to do common linear algebra manipulations that readily appear in quantum mechanics problems. In so doing, you will solve homework problem 1 again, but this time using Python. The idea is that while most of the homework problems you work are analytically tractable and not terribly cumbersome, other problems you might encounter will not be and using something like `numpy.linalg` will be very useful. I recommend using Anaconda Python as it has all the libraries and modules we need.

For this assignment, download this Jupyter notebook and work through the notebook. All the instructions appear in the notebook. The design is such that you are shown how to do some calculation, and then asked to translate that calculation to the problem at hand.