PHYS3021 Quantum Mechanics I   Problem Set 6
Due: 4 December 2017 (Monday)   "T+2" = 6 December 2017 (Wednesday)

All problem sets should be handed in not later than 5pm on the due date. Drop your assignments into the PHYS3021 box outside Rm.213.

Please work out the steps of the calculations in detail. Discussions among students are highly encouraged, yet it is expected that we do your homework independently.

6.0 **Reading Assignment.** (Don't need to hand in everything for this item.)

Chapter X goes back to some formal QM. First, Hermitian operators, which carry real expectation values $\langle \hat{A} \rangle$ for any state, real eigenvalues, orthogonal eigenstates, non-negative $\langle \hat{A}^2 \rangle$ for any state, and many more useful properties are introduced. Obviously, the properties are perfect for physical quantities in QM. Thus, all physical quantities in QM are represented by Hermitian operators. This statement is a postulate of QM. Chapter X explores the properties that are most relevant to QM, including simultaneous eigenstates of two commuting operators. A **general uncertain relation** concerning two operators will be derived. Operator method can also give us general results for **general QM angular momentum eigenvalue problems**. The results cover the orbital angular momentum already discussed and also the spin angular momentum to be covered in the next chapter. Chapter XI discussed spin angular momentum or simply spin. It is another example of general angular momentum with $s = 1/2$, and thus only two values for its component at any direction. The Stern-Gerlach experiment, nearly 100 years old, remains a useful set up for learning and investigating QM. A matrix representation is convenient, because the size is only 2×2. Matrices representing $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$ are introduced. Using their eigenvectors and eigenvalues, the general mathematical structure of QM and the measurement theory can be illustrated. After spin, we will go back to Chapter X to summarize the course with a few QM postulates.

Chapters in Rae's *Quantum Mechanics*, Griffiths' *An introduction to quantum mechanics*, McQuarrie's *Quantum Chemistry*, Engels' *Quantum Chemistry and Spectroscopy*, and Bransden and Joachain's —e, Quantum Mechanics are good places to look up more discussion. The chemistry books are better illustrations of the hydrogen atomic orbitals.

6.1 **Having fun with the Pauli Matrices**

We introduced the matrices for $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$. It turns out that they are closely related to the Pauli matrices σ_x, σ_y, and σ_z, only off by a factor of $\hbar/2$. The Pauli matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{1}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{2}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3}$$

Here, you will explore some properties of the Pauli matrices.

(a) **Find** the commutator $[\sigma_x, \sigma_y]$ by playing with the matrices.

(b) **Find** the commutator $[\sigma_x, \sigma_y]$ without playing with the matrices, but simply using the commutators between the spin components (the definition of angular momentum in QM).

(c) **Find** σ_x^2 by playing with the matrices.

(d) Realizing that a general spin-half state χ can be written in the form of

$$\chi = c_1 \alpha_x + c_2 \beta_x$$

where α_x (β_x) is the eigenstate of $\hat{S}_x$ with eigenvalue $+\hbar/2$ ($-\hbar/2$). By operating $\hat{S}_x^2$ on χ, **find** $\hat{S}_x^2$ and hence **identify** σ_x^2. [Remark: Compare result with part (c).

(e) **Find** the product $\sigma_x \sigma_y$ and relate the result to σ_z.
[Remark: You may want to explore a cyclic pattern of this result.]

(f) While $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is the **commutator**, $\{\hat{A}, \hat{B}\} = [\hat{A}, \hat{B}]_+ \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$ is the **anti-commutator** of two operators. **Find** $\{\sigma_x, \sigma_y\}$.

(g) **What is** $\{\sigma_i, \sigma_i\}$, for $i = x$, y, and z? [Note: Answer in part (c) will be useful.]

6.2 **Eigenvalues and Eigenvectors of Pauli Matrices**

(a) **Find** the eigenvalues and eigenvectors of the three Pauli matrices.

(b) **Find** the trace of the Pauli matrices. [Hint: Very easy if you know the relation between the trace of a matrix and its eigenvalues.]

(c) **Find** the determinant of the Pauli matrices.

6.3 **The most general operator for a "component" of spin**

After we draw some axes for the x, y, and z directions, we then have S_x, S_y, and S_z for the spin angular momentum $\vec{S}$. These directions, however, are nothing special.

Therefore, one can look at the component of spin along any direction. In 3D, a direction can be specified by two angles θ and ϕ. Just think about the spherical coordinates. When θ and ϕ are given, a direction is given.

(a) Now we want to construct the operator $\hat{S}_{\theta,\phi}$ corresponding to the component of $\vec{S}$ in that direction. Following **think classical** and **go quantum**, **show that** the operator is given by

$$\hat{S}_{\theta,\phi} = \frac{\hbar}{2} \begin{pmatrix} \cos\theta & \sin\theta\, e^{-i\phi} \\ \sin\theta\, e^{i\phi} & -\cos\theta \end{pmatrix} \tag{4}$$

(b) As a quick check, **show** that Eq. (4) reduces to the matrices for $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$, when the corresponding angles are chosen.

(c) **Find** the eigenvalues and normalized eigenvectors of $\hat{S}_{\theta,\phi}$.
[Remark: Now you see that if you have done this part first, 6.2(a) will be trivial.]

(d) Let's have some fun with measurements. Let $\beta_{\theta,\phi}$ be the eigenvector corresponding to the eigenvalue $-\hbar/2$. If a beam of particles prepared to be in this state is sent into a Stern-Gerlach experiment measuring the x-component of spin, i.e., SGX, **what could you say** about the outcomes? Now take the exiting beam corresponding to the measured result of $+\hbar/2$ in SGX and then send the beam again into a Stern-Gerlach experiment SG(θ, ϕ). **what could you say** about the outcomes?

6.4 **The mean spin angular momentum** $\langle\hat{\vec{S}}\rangle$

Recall that an expectation value involves two ingredients: a quantity (an operator) and a state.

There is a quantity called spin, which is a vector $\hat{\vec{S}} = \hat{S}_x\hat{\imath} + \hat{S}_y\hat{\jmath} + \hat{S}_z\hat{k}$. Given a state, one can calculate the expectation value $\langle\hat{\vec{S}}\rangle$ by calculating the expectation value of each component.

(a) Warming up! Take the state to be the eigenvector β_z of $\hat{S}_z$ corresponding to the eigenvalue $-\hbar/2$. **Find** the expectation values $\langle\hat{S}_x\rangle$, $\langle\hat{S}_y\rangle$, and $\langle\hat{S}_z\rangle$. If we think about a mean spin angular momentum $\langle\hat{\vec{S}}\rangle$ as $\langle\hat{\vec{S}}\rangle = \langle\hat{S}_x\rangle\hat{\imath} + \langle\hat{S}_y\rangle\hat{\jmath} + \langle\hat{S}_z\rangle\hat{k}$, **what would you say** about the direction of $\langle\hat{\vec{S}}\rangle$?

(b) Go back to 6.3(d). Take the state to be the eigenvector of $\hat{S}_{\theta,\phi}$ corresponding to the eigenvalue $-\hbar/2$, i.e. the state is $\beta_{\theta,\phi}$ in 6.3(d) again. Take this state, **calculate** the expectation values $\langle\hat{S}_x\rangle$, $\langle\hat{S}_y\rangle$, and $\langle\hat{S}_z\rangle$. From the results, **what would you say** about the direction of $\langle\hat{\vec{S}}\rangle$?

6.5 **Matrix formulation of QM harmonic oscillator**

We discussed in class that every QM problem can be turned into a big matrix (sometimes small such as spin) problem. This problem is to illustrate that even one can do the 1D harmonic oscillator problem by matrices.

Once upon a time, some clever physicists (meaning: Heisenberg, Born) found that the momentum operator and the position operator in the 1D harmonic oscillator problem of characteristic angular frequency ω are given by an infinite by infinite matrices of the form

$$\hat{x} = \left(\frac{1}{2}\frac{\hbar}{m\omega}\right)^{1/2} \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots \\ 1 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ . & . & . & . & \cdots \end{pmatrix} \tag{5}$$

$$\hat{p} = \left(\frac{1}{2}m\hbar\omega\right)^{1/2} \begin{pmatrix} 0 & -i & 0 & 0 & \cdots \\ i & 0 & -i\sqrt{2} & 0 & \cdots \\ 0 & i\sqrt{2} & 0 & -i\sqrt{3} & \cdots \\ 0 & 0 & i\sqrt{3} & 0 & \cdots \\ . & . & . & . & \cdots \end{pmatrix} \tag{6}$$

[Don't worry how these matrices are obtained. For those really wanted to do, read optional set of class notes on the operator method in harmonic oscillator.]

(a) By multiplying matrices, **show** that the given $\hat{x}$ and $\hat{p}$ give the correct commutation relation.

(b) **Construct** the Hamiltonian, which is now an infinite by infinite matrix, and **find** the eigenvalues of a 1D harmonic oscillator.