PHYS3022 Applied Quantum Mechanics Problem Set 2
Due: 14 February 2020 (Friday) "T+2" = 16 February 2020 (Sunday)

Special arrangement for handing in Problem Set 2 via email. In light of the rapid development of the novel coronavirus, **don't come to campus and don't come to the Department** to hand in your work. Instead, scan a copy of your work and **submit your work via email** to **cuhkphys3022@gmail.com** by 18:00 on the due date. TA will send you a reply confirming receipt of your work.

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.

2.0 **Reading Assignment.** (Don't need to hand in everything for this item.) We discussed Hermitian operators and their properties and saw their relevance to Quantum Mechanics. We also discussed important results related to two Hermitian operators, including the generalized uncertainty relation. We also worked out the allowed eigenvalues of the angular momentum magnitude squared $\hat{J}^2$ and one component (taken to be $\hat{J}_z$), entirely based on the commutation relations among $\hat{J}^2$, $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$. This discussion on general angular momentum in QM makes the appearance of spin angular momentum unsurprising. We introduced the idea behind the Stern-Gerlach (SG) experiment. For charged particles, an angular momentum gives rise to a magnetic dipole moment. When travelling in an inhomogeneous magnetic field as in the cleverly designed magnet in SG experiments, a (nonzero) magnetic dipole moment will feel a force and the direction of the force is related to μ_z, the component along the magnetic field gradient. For example, μ_z with +ve and −ve experience forces in different directions. In SG experiment, atoms with zero orbital angular momentum (in s state so $\ell = 0$) and thus zero **orbital** magnetic dipole moment are used. The result is that the atoms emerge as two beams, one is bent upward and another is bent downward. The experiment results imply that (a) the atoms carry a nonzero magnetic dipole moment coming from a new angular momentum ($\ell = 0$ orbital angular momentum), (b) the z-component (any component) of the new angular momentum can take on only two values (because two beams emerged, no more and no less), (c) according to general results of angular momentum, the z-component must be $\pm\hbar/2$ (counting from $+\hbar/2$ to $-\hbar/2$ in step of $\hbar$, thus only two values), and the magnitude squared must be $\frac{1}{2}(\frac{1}{2}+1)\hbar^2 = 3\hbar^2/4$, (d) we call this angular momentum the SPIN ANGULAR MOMENTUM of the electron, (e) we use $s = 1/2$ for electron's spin and thus it is referred to having spin-half, and $m_s = +1/2, -1/2$ for the two z-component being $+\hbar/2$ and $-\hbar/2$, (f) by measuring the bending of the two emerging beams, the z-component of the spin magnetic dipole moment are $+\mu_B$ and $-\mu_B$, where $\mu_B = e\hbar/2m_e$ is the Bohr Magneton and it is the basic unit of magnetic dipole moment in atomic physics. These are the essential concepts on spin angular momentum. **Read class notes under Hermitian Operators and Angular Momentum in QM and Spin Angular Momentum.**

Chapters in Rae's *Quantum Mechanics* are concise and very readable, Griffiths' *An introduction to quantum mechanics*, and McQuarrie's *Quantum Chemistry* are also good places to look up more discussion.

Hermitian Operators

Read/Review class notes on Hermitian Operators (two parts)

2.1 **Hermitian Operators.** A Hermitian operator $\hat{A}$ has the properties that

$$\int f^* \hat{A} g \, d\tau = \int g \hat{A}^* f^* \, d\tau = \int g (\hat{A} f)^* \, d\tau = \int (\hat{A} f)^* g \, d\tau = \left(\int g^* \hat{A} f \, d\tau \right)^* \tag{1}$$

where $d\tau$ would mean dx in 1D, d^2r in 2D, and d^3r in 3D and the integration is over all space.

(a) **Give an example with explicit demonstration** of the following case: The operators $\hat{A}$ and $\hat{B}$ are Hermitian, but the operator formed by the product $\hat{A}\hat{B}$ is non-Hermitian.

(b) The momentum (linear momentum to be precise) operator is given by $p_x = \frac{\hbar}{i}\frac{d}{dx}$. We know that p_x, being a physical quantity, is represented by a Hermitian operator in quantum mechanics. Many students have been wondering why there is the "i" in the operator. By **contrasting** $\hbar\frac{d}{dx}$ with $\frac{\hbar}{i}\frac{d}{dx}$, **analyze or demonstrate** why we need to have the "i" in order to make p_x Hermitian.

(c) Let $\hat{A}$ be a Hermitian operator. **Check** whether $\hat{A} + c$, where c is a real constant, is Hermitian.

(d) Let $\hat{A}$ be a Hermitian operator. **Check** whether $\hat{A} + ic$, where c is a real constant, is Hermitian.

(e) **Show** (clearly) that $\hat{A}$ compute with $\hat{A}^2$, $\hat{A}^3$, etc.

Then we are ready to go to Problem 2.2.

2.2 **Function of an operator**

In carrying out the "think classical" and "go quantum" process, we encounter plugging in an operator into a function. Here are some examples. In harmonic oscillator, $U(x) = \frac{1}{2}m\omega^2 x^2$, which is formally a function of x (quadratic in x). In nuclear physics, the Woods-Saxon potential (confining nucleons in a nucleus) has a form of $U(x) = -U_0/(1 + \exp((x - x_0)/a))$. When we substitute the position operator for x, then we encounter a function of an operator.

To consider a function of an operator, there are two ingredients. First, there is a function. Let's call it $f(x)$. Note that the "x" here does not necessarily mean the position. It is just the variable of a function. [A single-variable function means that you give it a value of the argument "x", the function returns you a value, thus $f(x)$.] We also need an operator $\hat{A}$. When we say there is a function of the operator $\hat{A}$, then we insert the operator into the function to replace x. The question is: **What does $f(\hat{A})$ mean?** Why bother? Formally, for a harmonic oscillator, we know $f(x) = \frac{1}{2}m\omega^2 x^2$ is the potential energy function. Then, we form $f(\hat{x})$ to get the operator form of the potential energy. In doing so, actually we encounter the concept of $f(\hat{A})$.

The **definition** of a **function of an operator** is

$$f(\hat{A}) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \hat{A}^n \tag{2}$$

where $f^{(n)}(0)$ is the n-th derivative of the function $f(x)$ and evaluated at $x = 0$. **Learn this.** The meaning is to carry out the following mathematical steps in sequence: (i) Take a Taylor expansion of $f(x)$, (ii) then all the terms will have the form of x^n (see Problem 2.1(e)), and we replace x by the operator, (iii) the resulting expression then operates on any function that appears on the right hand side of the function of an operator. Based on the definition, let's practice.

(a) Based on the definition, **write down** the meaning of following function of the Hamiltonian operator $\hat{H}$:

$$f(\hat{H}) = e^{-i\hat{H}t/\hbar} \equiv \hat{\mathcal{T}} \tag{3}$$

The time-independent Schrödinger equation is the eigenvalue problem of the Hamiltonian. Let the solutions (energy eigenstates and eigenvalues) be

$$\hat{H}\psi_m = E_m\psi_m \,. \tag{4}$$

The set $\{\psi_m\}$ can be used to expand any function. Therefore, a general state (need not be an energy eigenstate) can be written as

$$\Phi = \sum_{m=0}^{\infty} c_m\psi_m \,. \tag{5}$$

Work out what $\hat{\mathcal{T}}$ does on Φ, i.e. $\hat{\mathcal{T}}\Phi = ?$ **Connect** the results to the previously discussed procedure (in PHYS 3021) in answering **initial value problems** in QM for problems with time independent $U(x)$. **The key take-home message here is: Eq. (2) is the operational meaning of a function of an operator.**

[Remarks: In more advanced courses/books, $\hat{\mathcal{T}}$ is the operator that propagates a wavefunction (a state) in time. After you work out this problem, the statement becomes obvious.]

(b) So we know what $e^{\hat{A}}$ means. In ordinary mathematics, $e^{A+B} = e^A e^B$. But we know that **operator mathematics** is in general different from ordinary mathematics. **Show that** in general $e^{\hat{A}+\hat{B}} \neq e^{\hat{A}}e^{\hat{B}}$ and **find the condition** under which $e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}$ holds.

2.3 **An alternative definition of Hermitian operators (MUST TRY)**

We defined the Hermitian operator as one that satisfies

$$\int f^* \hat{A} g \, d\tau = \int (\hat{A} f)^* g \, d\tau = \int g (\hat{A} f)^* \, d\tau = \int g \hat{A}^* f^* \, d\tau = \left(\int g^* \hat{A} f \, d\tau \right)^* \tag{6}$$

in which the definition invokes **any** two well-behaved functions f and g.

In some books, Hermitian operators are motivated by requiring real expectation values. An expectation value involves one function instead of two. Thus, **an alternative definition** invoking only **one** (but any one) well-behaving function ψ is

$$\int \psi^* \hat{A} \psi \, d\tau = \int (\hat{A} \psi)^* \psi \, d\tau = \int \psi (\hat{A} \psi)^* \, d\tau = \int \psi \hat{A}^* \psi^* \, d\tau = \left(\int \psi^* \hat{A} \psi \, d\tau \right)^* , \tag{7}$$

which is obviously a statement of real expectation values.

The question is whether the definition Eq. (7) is consistent with the definition Eq. (6).

Eq. (7) involves only one function. Writing $\psi = c_1 f + c_2 g$, where c_1 and c_2 are arbitrary complex constants, f and g are two well-behaved functions, **show** that the definition in Eq. (7) as applied to ψ gives the definition Eq. (6) involving two arbitrary well-behaving functions.

Spin Angular Momentum (Learn and Practice)
Read class notes posted under Angular Momentum in QM and Spin Angular Momentum (six parts)

2.4 **Spin-1/2 Angular Momentum and the Pauli Matrices**

[In Problem 1.1, you worked on 3×3 matrices representing the $\ell = 1$ orbital momentum. It is 3×3 because $m_\ell = 1, 0, -1$ and thus the matrix representing $\hat{L}_z$ (or any component) must have 3 eigenvalues.]

The Stern-Gerlach experiment demonstrated that the spin angular momentum of an electron can only take on two possible values $+\hbar/2$ and $-\hbar/2$ for the z-component (or any component). Thus, 2×2 matrices can be used to represent spin-half angular momentum.

The following matrices for $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$ work. They are:

$$[S_x] = \frac{\hbar}{2} \sigma_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{8}$$

$$[S_y] = \frac{\hbar}{2} \sigma_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{9}$$

$$[S_z] = \frac{\hbar}{2} \sigma_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{10}$$

Without the factors of $\hbar/2$, the **Pauli matrices** σ_x, σ_y, and σ_z are explicitly given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{11}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{12}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{13}$$

Here, you will explore the properties of these matrices.

(a) **Construct** the matrix representing $[S^2]$. **Demonstrate explicitly** that $[S_x]$, $[S_y]$, $[S_z]$, and $[S^2]$ satisfy the defining commutation relations for an angular momentum in quantum mechanics. Hence, **write down** the commutation relations for σ_x, σ_y, σ_z, and σ^2.

(b) **Find** the eigenvalues and normalized eigenvectors of $[S_x]$, $[S_y]$, and $[S_z]$. [See class notes for answers, but you need to work them out explicitly.] Hence, **write down** the eigenvalues and eigenvectors of σ_x, σ_y, and σ_z.

(c) From the commutation relations among the components, we know that the eigenvector of one component cannot be the eigenvector of another component. Let's illustrate the point. **Show that** the eigenvectors α_z (for eigenvalue $+\hbar/2$) and β_z (for eigenvalue $-\hbar/2$) of $[S_z]$ are NOT eigenvectors of $[S_x]$ by operating $[S_x]$ on α_z and β_z.

(d) Then we have an interesting system to practice our knowledge of measurements in quantum mechanics. Let SGz (SGx) be a Stern-Gerlach experiment aligned for measuring the z-component (x-component) of spin-1/2 particles (electrons). Taking the beam corresponding to $S_z = +\hbar/2$ out and direct it into SGx, **analyze** the situation and **state what you can say** about the possible outcomes and the corresponding probabilities. **Hence, also find the expectation value** $\langle S_x \rangle$.

Check your value of $\langle S_x \rangle$ against plugging in the expectation value formula of $(\alpha_z^*)^T S_x \, \alpha_z$, where $(\alpha_z^*)^T$ is the transpose of α_z^*.

(e) Now, take the resulting beam in the SGx measurement corresponding to $+\hbar/2$ for S_x out and direct the beam back into a SGz experiment. **Analyze** the situation and **state what you can say** about the possible outcomes and the corresponding probabilities. **Find** the expectation value by averaging over the possibilities and by plugging formula.

[Remark: This can go on and on.]

2.5 Component of spin angular momentum in any direction

You have seen $[S_x]$, $[S_y]$, and $[S_z]$, and that they all have eigenvalues $\pm\hbar/2$. The SG experiment can be placed in any direction and there are always two beams coming out. There is nothing special about x, y, and z directions. Here, you will study the eigenvalue of the component of spin angular momentum along an arbitrary direction. An arbitrary direction is specifed by two angles via $\mathbf{r} = \sin\theta\cos\phi\,\hat{i} + \sin\theta\sin\phi\,\hat{j} + \cos\theta\,\hat{k}$, where $\mathbf{r}$ is a unit vector along the specified direction. It follows that the component $[S_{\theta,\phi}]$ can be represented by the 2×2 matrix:

$$[S_{\theta,\phi}] = \frac{\hbar}{2} \begin{pmatrix} \cos\theta & \sin\theta\, e^{-i\phi} \\ \sin\theta\, e^{i\phi} & -\cos\theta \end{pmatrix} \tag{14}$$

It is easy to see that $[S_z]$ emerges when we set $\theta = 0$ (recall spherical coordinates).

Find the eigenvalues of $[S_{\theta,\phi}]$. [Optional (no bonus points): Find the corresponding eigenvectors.]

2.6 More on the Pauli Matrices

(a) **Find the trace** of the three Pauli matrices. [Hint: You found the eigenvalues in Problem 2.4.]

(b) **Find the determinant** of the three Pauli matrices.

(c) **Find** the product $\sigma_y\sigma_z$ and relate the result to σ_x. [Reamrk: You may want to explore a cyclic pattern of this result.]

(d) The commutator of two operators $\hat{A}$ and $\hat{B}$ is defined by $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. Let's define the **anti-commutator** to be $\{\hat{A}, \hat{B}\} = [\hat{A}, \hat{B}]_+ \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$. **Find** $\{\sigma_y, \sigma_z\}$.

(e) **Find** σ_y^2 by multiplying matrices together.

(f) Here is another way to identify what the operator for $[S_y^2]$ is and then extract the operator σ_y^2. Realizing that a general spin-half state χ can be written in the form of

$$\chi = c_1\alpha_y + c_2\beta_y$$

where α_y (β_y) is the eigenstate of $\hat{S}_y$ with eigenvalue $+\hbar/2$ ($-\hbar/2$). By operating $\hat{S}_y^2$ directly on χ and realizing χ is a general state, **find** $\hat{S}_y^2$ and hence **identify** σ_y^2. [The answer of course should be the same as that in (e).]

(g) Hence, **find** $\{\sigma_i, \sigma_i\}$, for $i = x$, y, and z.

[Remark: At this point, you have worked out all the properties of the Pauli matrices. You will need them if you go into quantum-X, where X can be computing or information.]

2.7 **Pauli matrices - they help factorize** $(p_x^2 + p_y^2 + p_z^2)$

When you were in primary school, you knew that $p_x^2 - p_y^2 = (p_x + p_y)(p_x - p_y)$. When you were in secondary school, you knew that $p_x^2 + p_y^2 = (p_x + ip_y)(p_x - ip_y)$. It was a big step forward with the non-trivial idea of i. Now you are studying physics in university, what's next? Naturally, the question is to simplify $p_x^2 + p_y^2 + p_z^2$, which is the magnitude squared of a 3-component vector $\vec{p} = p_x\hat{i} + p_y\hat{j} + p_z\hat{k}$. A related question is whether we can write $E^2 - c^2(p_x^2 + p_y^2 + p_z^2)$ into a product of two terms.

Let's form a vector $\vec{\sigma} = \sigma_x\hat{i} + \sigma_y\hat{j} + \sigma_z\hat{k}$, where σ_i are the Pauli matrices. That is to say, each component is a 2×2 matrix. Following what you know about dot product of two vectors and matrix manipulations, **evaluate** $\vec{\sigma} \cdot \vec{p}$ and $(\vec{\sigma} \cdot \vec{p})^2$. [Reamrk: Inspect and appreciate the result and the beauty of mathematics. Now at the university level, even i is not sufficient, you need to use matrices.]

Hence, **express** $E^2 - c^2(p_x^2 + p_y^2 + p_z^2)$ as a product of two factors.

[Remarks: You may recognize $E^2 - c^2(p_x^2 + p_y^2 + p_z^2) = 0$ as a relativistic relation between energy and the momentum for a massless particle (no m^2c^4 term), if $\vec{p}$ is taken to be the momentum. Hence, you showed that $(E + something)(E - something) = 0$, and that something is a matrix. In going quantum, we would get $(E - something)\psi = 0$, which is a relativistic QM equation. In fact, it is the Dirac equation for massless fermions. It sounds useless. Not so! It is now a popular topic due to the fact that electrons in graphene (one layer of graphite) behave like massless fermions! The equation is more complicated for massive fermions. We need to invoke 4×4 matrices called the Dirac matrices, which are formed by stacking up the Pauli matrices. The resulting equation is the famous Dirac equation.]