DEPARTMENT OF PHYSICS, CHINESE UNIVERSITY OF HONG KONG
PHYS3021 QUANTUM MECHANICS I

SAMPLE QUESTIONS FOR WEEK 11 EXERCISE CLASSES (13 - 17 November 2017)

Read me: TA will discuss the **SAMPLE QUESTIONS** (SQs) and answer your questions in exercise classes every week. The SQs are designed to review what you have learnt, tell a physics story, enrich our discussions, and help you work out the upcoming Problem Set. **Your time table should allow you to attend one exercise class session. The Exercise Classes are an integrated part of the course.** You are encouraged to work out (or think about) the SQs before attending exercise class and ask the TA questions. Over the semester, you are welcome to seek help from TAs/me.

SQ27 - Most probable distance of finding electron in 3d hydrogen states
SQ28 - More on Hermitian operators [$\langle \hat{A}^2 \rangle \geq 0$ for Hermitian operator $\hat{A}$]
SQ29 - Function of operators with an important example

SQ27 *Most probable distance of finding electron in 3d hydrogen states*

For the 1s state, one can readily construct the radial probability distribution function $P(r) = r^2[R_{1s}(r)]^2$ and show that the most probable distance is at the Bohr radius a_0.

TA: Look up the $3d$ states with radial function $R_{32}(r)$. **Sketch** $R_{32}(r)$. **Construct** $P_{32}(r)$ (the 3d state) and **find** the most probable distance of finding the electron.

SQ28 *More on Hermitian operators*

(a) Is $i\frac{d^2}{dx^2}$ a Hermitian operator?

(b) Although it is intuitively obvious, **show** that the sum of two Hermitian operators $(\hat{A} + \hat{B})$ is also a Hermitian operator. [See class notes for the case of product of two Hermitian operators.]

(c) **Show** that if $\hat{A}$ is a Hermitian operator, then the expectation value of $\hat{A}^2$ for any state Ψ cannot be negative, i.e.,

$$\langle \hat{A}^2 \rangle \geq 0 \tag{1}$$

[Hint: Start with the definition of expectation value and what $\hat{A}^2$ means.]
Remark: If we use the notation $\langle f|g\rangle$ for the inner product $\int f^* g\, d\tau$, the above property of a Hermitian operator becomes

$$\langle \hat{A}^2 \rangle = \langle \Psi|\hat{A}^2\Psi\rangle = \langle \hat{A}\Psi|\hat{A}\Psi\rangle \geq 0. \tag{2}$$

There is no new physics here. But this property written as Eq. (2) is very useful in QM.

SQ29 *Function of operators (not only for Hermitian operators)*

When we proceed with the "think classical" and "go quantum" way to write down **operators**, we will encounter the situation of **a function of an operator**.

To consider a function of operator, we have two ingredients. First, we need 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 $f(x)$.] And we 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?**

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

$$f(\hat{A}) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \hat{A}^n \tag{3}$$

where $f^{(n)}(0)$ is the n-th derivative of the function $f(x)$ and evaluated at $x = 0$. The meaning is that the following steps are carried out in sequence: (i) Take a Taylor expansion of $f(x)$, (ii) replace x by the operator, (ii) the resulting expression then operators on any function that appears on the right hand side of the function of an operator.

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

$$f(\hat{H}) = \hat{\mathcal{T}} = e^{-i\hat{H}t/\hbar} \tag{4}$$

(b) The Time-independent Schrödinger equation is the eigenvalue problem of the Hamiltonian. Let the solutions be

$$\hat{H}\psi_m = E_m\psi_m \,. \tag{5}$$

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

$$\Phi = \sum_{m=0}^{\infty} c_m\psi_m \,. \tag{6}$$

TA: **Illustrate** what $\hat{\mathcal{T}}$ does on Φ, i.e. $\hat{\mathcal{T}}\Phi = ?$, and **relate** the results to the previously discussed procedure in answering **initial value problems** in QM.

[Remark: In more advanced courses/books, $\hat{\mathcal{T}}$ is the operator that propagates a wavefunction (a state) in time. From the answer of this SQ, this statement is obvious.]