PHYS3021 Quantum Mechanics I **Problem Set 3**
Due: 26 October 2017 (Thursday) **"T+2" = 30 October 2017 (Monday)**
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.

3.0 **Reading Assignment.** (Don't need to hand in everything for this item.) Chapter IV discussed operators and how to write down the Hamiltonian operator systematically. For each operator, there is an eigenvalue problem. TISE turns out to the the eigenvalue problem of $\hat{H}$. We took a detour to go through 180 years of classical mechanics, aiming at pointing out what Lagrangian mechanics does to define the conjugate momentum to a coordinate and what Hamiltonian is and how it leads to the Poisson brackets, which were taken by Dirac to "go quantum". This helps us understand Schrödinger's way of expressing the position and momentum operators is one way of fulfilling the necessary commutator $[\hat{x}, \hat{p}] = i\hbar$. In addition, Hamiltonian mechanics helps us understand why and how other classical mechanical quantities can be written into a QM operators. The eigenvalue problem of QM operator $\hat{A}$ is important in that the eigenvalues are the only possible measurement outcomes of the quantity A. In Chapter V, we solved the 1D infinite well (1D box) problem exactly. From the whole set of energy eigenfunctions, we observed the orthogonality and orthonormal properties. These are bound states, infinite many of them. Any function (same boundary conditions) can be expanded in terms of the energy eigenfunctions and the expansion coefficients have formulas to plug. This is the same for other QM operators. We explained what expectation value and uncertainty in QM means, based on measurements on identically prepared copies of system with one on a copy only. In QM, uncertainties are rigorously defined and one can calculate them. We then go further into measurement theory, pointing out the probability of getting an eigenvalue a_i of the quantity A is the $|c_i|^2$ in expansion the wavefunction under measurement in terms of the eigenfunctions ϕ_i of $\hat{A}$. We also discussed the time evolution of the energy eigenfunctions and pointed out they are stationary states. Generally, the expectation value $\langle A \rangle$ changes in time. Chapter VI will do the 1D finite well and harmonic oscillator problems.

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

3.1 **More on Angular Momentum Operators (See SQ14)**

(a) In class notes, we wrote down the operators for the components of the angular momentum $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$. TA worked out the magnitude squared $\hat{L}^2$ and its commutators in SQs. **Find** the commutator $[\hat{L}_y, \hat{L}_z]$. **Write down** the other two cyclic commutators of the components.

(b) Let's define (don't worry about what they mean for the moment) two operators

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y \ , \quad \hat{L}_- = \hat{L}_x - i\hat{L}_y \tag{1}$$

(i) **Show that** $\hat{L}_+\hat{L}_- = \hat{L}^2 - \hat{L}_z^2 + \hbar\hat{L}_z$

(ii) **Find** $[\hat{L}_z, \hat{L}_+]$ in terms of $\hat{L}_+$

(ii) **Find** $[\hat{L}_z, \hat{L}_-]$ in terms of $\hat{L}_-$

[Remark: You just did a very important exercise for QM angular momentum theory. Carry the answers with you.]

3.2 **1D Box: Orthogonality of energy eigenfunctions and $\Delta x \cdot \Delta p$ for all $\psi_n(x)$**

We solved the set of energy eigenfunctions and their eigenvalues for 1D Box.

(a) Take any two eigenfunctions and **show explicitly** (by doing integration) that they are orthogonal to each other.

(b) We did Δx and Δp for the ground state $\psi_1(x)$ in class notes. Here, you will work on all $\psi_n(x)$ by applying the formula for getting expectation values. **Evaluate**

(i) $\langle x \rangle$, $(\Delta x)^2$, and Δx for all energy eigenfunctions labelled by n.

(ii) $\langle p \rangle$, $(\Delta p)^2$, and Δp for all energy eigenfunctions labelled by n.

(iii) $\Delta x \cdot \Delta p$ for all energy eigenfunctions labelled by n.

[Remark: You knocked out all position-momentum uncertainty problems for 1D Box eigenfunctions in one shot.]

3.3 **Engineering the C1–C2 gap in a quantum well**

Particle-in-a-box can be partially realized by having the box being a thin piece of semiconductor (GaAs for example) sandwiched between two thick layers of another material.

A particular property of semiconductors is that electrons living in them have a smaller mass. Usually, the (effective) mass of electrons is about $m_{eff} \sim 0.05 m_e$ in semiconductors, where m_e is the usual electron mass. It is this property that gives us fast electronics in semiconductor devices. After all, particle of lighter mass runs faster.

A client comes to you and asks for the specification of a device that requires a 1 eV "gap" between the ground state (labelled C1) and the first excited state (labelled C2). **Estimate** the thickness of the semiconductor region (forming the 1D box) so that the C1→C2 transition is about 1 eV.

3.4 **1D Box moved to another place**

Let's move the 1D infinite well (1D Box) of width a to be **centered at** $x = 0$..

(a) We know that the ground state should be symmetric (or called even) about $x = 0$. Previously, we had the wavefunction as a sine function when the well is placed in $0 < x < a$. **Describe** how to modify (or "copy") the result when the box is shifted.

(b) Hence, **describe how** you could modify (or copy) the whole set of energy eigenfunctions when the box is shifted. **Show explicitly** that your shifted eigenfunctions indeed have the properties of bring alternating between symmetric (even) and antisymmetric (odd) functions as the energy goes up. [If you can't modify the known results, you may solve them as a new problem.]

3.5 **1D box ground state - What are its momentum components? (See Problem 2.5 and SQ17)**

This problem is slightly tedious in mathematics (Fourier transform), but you did a similar one in Problem 2.5. It is an important problem in that it is related to a common misconception about the momentum components in the energy eigenstates in a 1D box.

(a) Consider shifting the box of width a to be centered at $x = 0$ (Problem 3.4(a)). For the normalized **ground state** wavefunction $\psi_1(x)$, **find** the Fourier transform $F(k)$.

(b) We again take $|F(k)|^2 dk$ as the probability of finding the wavevector k to be in the interval k to $k+dk$. (This is the same as in Problem 2.5, solutions posted.) **Sketch** $|F(k)|^2$ versus k. Hence, **evaluate** the mean $\langle k \rangle$, the variance $(\Delta k)^2$, the uncertainty Δk and hence the uncertainty in momentum $\Delta p = \hbar \Delta k$.

[Important remark: Many students (and some authors) through that with a cosine (or sine) function like $\cos(kx)$, there are only two components of k, namely $+k$ and $-k$, as they were thinking about writing cos and sin into sum or difference of exponentials. Here, you just did the Fourier transform of $\psi_1(x)$ and saw that there are many more k-components. The point is that the zero parts of $\psi_1(x)$ outside the well/box really matters. These zero parts make $\psi_1(x)$ a localized wave packet. We need many more k's (thus wavelengths) for mutual cancellations to achieve zero wavefunction outside the well.]

(c) A student asked why the operator $\hat{A}$ should be placed between two wavefunctions in calculating expectation values. The answer is that by doing so, the result makes sense and agrees with experiments. Many find it not convincing (but I do, see class notes Chapter V Part 5). Given that you just calculated Δp using a long and formal way in part (b), **re-do** the calculation for Δp by plugging into expectation value formula

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hat{A} \psi(x) dx \ , \tag{2}$$

using the state $\psi_1(x)$ without going through Fourier transform. You may copy result from Problem 3.2 into here. This part also serves to show that plugging expectation formula is **a short cut**.

(d) If part (c) is still unconvincing, **do a wrong calculation** by imposing

$$\langle A \rangle_{guess} = \int_{-\infty}^{\infty} \hat{A}\psi^*(x)\psi(x)dx \qquad \text{(this is \textbf{wrong!})} \tag{3}$$

so that $\hat{A}$ operates on the product $|\psi(x)|^2$, instead of the correct formula in Eq. (2), to **obtain** Δp for the ground state $\psi_1(x)$ and **check results** against parts (b) and (c). [Note: Not often points are given for wrong calculations.]

3.6 **Be very careful in measurements and calculations - See if this can confuse you (See SQ18)**

We stressed in class the physical meaning of the expectation value $\langle A \rangle$ and the uncertainty (ΔA) is related to measurements on identical copies of a system and each copy is measured only once. Here, we make use of the 1D box energy eigenfunctions. **Ignore any consideration on time evolution in this problem.** If you don't want to do some integrals, you may define some symbols for them.

An experimentalist prepared **a huge number of identical copies** of a state of the form

$$\Psi(x) = \sqrt{\frac{2}{3}}\,\psi_1(x) + \sqrt{\frac{1}{3}}\,\psi_2(x) \tag{4}$$

where $\psi_1(x)$ is the normalized ground state wavefunction of 1D box and $\psi_2(x)$ is the first excited state wavefunction. You may put the box wherever you like.

Case A: A student *Alice* separates the copies into three equal parts. For 1/3 of the copies, measurements on the energy E are made (system thrown away after measured once). For another 1/3 of the copies, she measures the position x (and throws copy away after a measurement). For the remaining 1/3, measurements on momentum p are made (throws away after measurement). So, she has three sets of data.

(a) **Sketch** the distribution of the data on the energy measurements. Hence, **find** the mean energy $\langle E \rangle$ and the uncertainty (ΔE)?

(b) From the two other sets of data, Alice could obtain the uncertainties in position Δx and in momentum Δp. **What** will Alice get for $\Delta x \cdot \Delta p$?

Case B: A student *Bob* first measures the energy of each copy. He **keeps the copies** after measurements. He then sorts the copies into two groups according to the energy outcomes. For Group 1 of energy E_1, he measures the position on half of the group (one measurement per copy) and the momentum on the other half of the group (one measurement per copy). He does the same for the Group 2 of energy E_2.

(c) **Find** $\Delta x \cdot \Delta p$ for Group 1.

(d) **Find** $\Delta x \cdot \Delta p$ for Group 2.

(e) But Bob's supervisor doesn't think that there should be two values of $\Delta x \cdot \Delta p$ for the samples (Eq. (4)) that s/he prepared. So Bob thought that he should take into account of the sample sizes of Group 1 and Group 2 and do some weighting/averages. **Try** a reasonable weighting scheme and **compare** result with part (b).

(f) **Write a short paragraph to point out** why $\Delta x \cdot \Delta p$'s in (b), (c), (d) are in principle different quantities and what they really refer to?

3.7 **Time evolution and possible time-dependent properties**

Consider the state $\Psi(x)$ in Eq. (4) for a 1D Box system as the initial wavefunction $\Psi(x, 0)$ at some time $t = 0$.

(a) **What** is $\Psi(x, t)$ at time t?

(b) **Find** the probability density $|\Psi(x, t)|^2$. **Sketch** $|\Psi(x, t)|^2$ as a function of x **for a few different times** t to show the key feature.

(c) **Important physics here. Evaluate** $\langle x \rangle$ using $\Psi(x, t)$ and **describe** how $\langle x \rangle$ changes in time. [Some integrals might be found in previous problems.]

(d) If the particle carries a charge q, **what would happen** when it is in the state $\Psi(x, t)$ in which its mean position $\langle x \rangle$ behaves as in part (c)? [Hint: Think along classical EM theory.]

(e) Go back to $\Psi(x, t)$ in part (a). **Find** the energy expectation value $\langle E \rangle$. Will it change with time?