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.

1.0 **Reading Assignment.** (Don't need to hand in everything for this item.) Chapter II introduces the wavefunction $\Psi(x,t)$ and its necessary behavior of being an acceptable QM wavefunction. These include single-valueness and continuity. For bound states (we will do many bound state problems later), the wavefunction should also be normalizable, i.e., can be normalized. In QM there are lovely wavefunctions that cannot be normalized, e.g. the free particle $\exp(ikx)$ (plane wave) is an example. Chapter II also introduces the idea of wave packets. Wave packets are normalizable. More importantly, Fourier transform (mathematics developed more than 100 years prior to QM) implies that a wave packet can be seen as a suitable linear combination of many plane waves of different wavelengths and thus momenta. We illustrated by examples that the wider the wave packet in space x, the narrower is the range of k (thus momentum), and vice versa. This is the uncertainty relation. The point is that the uncertainty relation follows naturally from the wave description of particle. The time-dependent Schrödinger equation (TDSE) is then introduced as the proper QM wave equation for $\Psi(x,t)$. Chapter III considers $U(x,t) = U(x)$ only. In this case, TDSE can be separated into time-independent Schrödinger equation (TISE) and a temporal equation. TISE is the most important equation in QM. It gives all the states (wavefunctions) of definite energies and the allowed energies of a quantum system. Each spatial wavefunction of definite energy E evolves with its own time factor $\exp(-iEt/\hbar)$. The linear property of TDSE then allows us to solve generally the **initial value problem**, i.e., given $\Psi(x,0)$ at $t = 0$, what is $\Psi(x,t)$? A three-step recipe of solving the time evolution problem is given in Chapter III. Chapters in Griffiths' *An introduction to quantum mechanics* and Rae's *Quantum Mechanics* are good.

2.1 **Writing down Schrödinger equations** (See SQ11)

Referring to the discussion at the end of Chapter II and Chapter III, **write down** the **time-dependent** Schrödinger equation (TDSE) and the corresponding **time-independent** Schrödinger equation (TISE) for each of the following problems. In some cases, you may write a $U(x)$ or $U(\mathbf{r})$ in the equations and then define the U separately in your answer.

(a) A particle of mass m in two dimensions (2D) under the influence of an isotropic harmonic potential energy function (harmonic oscillator) characterized by a spring constant K (meaning the same spring constant K for both x-direction and y-direction). **Use Cartesian coordinates** to write down your answer.

(b) Once upon a time, you learned the plane polar coordinates using (r, θ) for specifying a position on a 2D plane. **Rewrite** your answers in (a) using plane polar coordinates.

(c) A particle of mass m_n confined in 3D by an infinite spherical wall so that it lives freely only within a sphere of a radius R centered at the origin. [Remark: This is a simple model of an neutron/proton confined in a nucleus.]

(d) Consider a hydrogen atom. The nucleus is not moving and fixed at the origin. **Write down** the equations for the electron under the influence of the nucleus in **Cartesian coordinates**, i.e., x, y, z.

(e) Repeat part (d) using the **spherical coordinates**, i.e., using (r, θ, ϕ) for specifying a position in 3D.

[Remark: What you do here is an important first step towards doing QM. Once you have the Schrödinger Equation and once you understand what it can do (TISE for the states of definite energy and the values of definite energy plus TDSE for initial value problems), then what's left is just to solve the equations. Of course there are many techniques to be picked up, but the worst (nicest) scenario will be to hire a RA or to write a program for the task.]

2.2 $|\Psi(\mathbf{r}, t)|^2$ **is probability density, Initial value problem and applying your logical thinking**

Let's consider the hydrogen atom problem in Problem 1(d) and 1(e). From high school physics, you know that a hydrogen has allowed energies given by $-13.6/n^2$ eV, where $n = 1, 2, 3, \ldots$. In QM, these are the solutions to TISE. There is a state (called $1s$) of wavefunction $\psi_{1s}(\mathbf{r})$ with energy -13.6 eV and there is another state (called $2s$) of wavefunction $\psi_{2s}(\mathbf{r})$ with energy $-13.6/4$ eV, and so on. The ψ_{1s} and ψ_{2s} are normalized.

(a) Let's say at time $t = 0$, the wavefunction is given by $\Psi(\mathbf{r}, 0) = \psi_{2s}(\mathbf{r})$. **What** is $\Psi(\mathbf{r}, t)$ at some time t later? **Evaluate** the probability densities at $t = 0$ and at time t, **compare them** and **comment** on your results. [Remark: Prior to formulation of QM, Bohr in 1913 imposed that there are states of definite energies in hydrogen for which he named them **stationary states**. "Stationary" means that something does not depend on time. I hope that at this point you see what is being stationary.]

(b) Repeat part (a) for $\Psi(\mathbf{r}, 0) = \psi_{1s}(\mathbf{r})$.

(c) Let's say at time $t = 0$, the wavefunction $\Psi(\mathbf{r}, 0)$ is given by

$$\Psi(\mathbf{r}, 0) = \sqrt{\frac{2}{3}}\, \psi_{1s}(\mathbf{r}) + \sqrt{\frac{1}{3}}\, \psi_{2s}(\mathbf{r}) \tag{1}$$

What is $\Psi(\mathbf{r}, t)$ at some time t later?

(d) **Evaluate** the probability density at time t using your $\Psi(\mathbf{r}, t)$ in part (c). **Comment** on your result in light of the probability densities in parts (a) and (b) in which the initial wavefunction is a pure ψ_{1s} and a pure ψ_{2s}.

2.3 Eigenvalue problems and TISE: An important property

(a) Let $\hat{A}$ be an operator. The eigenvalue problem of $\hat{A}$ refers to finding a special set of functions ϕ such that

$$\hat{A}\,\phi = a\,\phi \tag{2}$$

where the output after operating $\hat{A}$ is ϕ itself times an eigenvalue a. In general, it is one equation to solve for many eigenfunctions ϕ's and many eigenvalues a's. A ϕ and a value of "a" come in a pair. That is to say, $\phi_1 \leftrightarrow a_1$, $\phi_2 \leftrightarrow a_2, \ldots$, $\phi_n \leftrightarrow a_n, \ldots$

Let's consider two eigenfunctions ϕ_1 and ϕ_{13} and form a linear combination of them, i.e.,

$$f = c_1\,\phi_1 + c_{13}\,\phi_{13} \tag{3}$$

Operate $\hat{A}$ on f and **show explicitly** that f in Eq.(3) is general **NOT** an eigenfunction of $\hat{A}$. [Remark: This is an important result, but it is also a point of common misconception. CUHK Students: PLEASE carry this with you. **Linear combination of eigenfunctions of an operator is generally not an eigenfunction of the operator.** Eigenvalue problems are more stringent than solutions to a wave equation.]

(b) In part (a), after operating $\hat{A}$ on f in Eq.(3), there may be an *exceptional* scenario in which f is an eigenfunction of $\hat{A}$. **Identify** a condition for which this "accident" happens.

(c) Next, we fill in a physical context for part (a). Consider the hydrogen wavefunction in Eq.(1) in Problem 2.2. **Test explicitly** whether or not it satisfies the **time-independent** Schrödinger equation of a hydrogen atom that you wrote down in Problem 2.1. Hence, **write a statement or two** connecting the answer here for hydrogen atom and the general statement in part (a) of this problem.

[Remark: Pause. Read the whole question/your answer again. And catch the key concept that a linear combination of eigenfunctions is generally not an eigenfuction itself.]

2.4 Mean, variance and standard deviation, Gaussian wavefunction, normalization, Fourier transform, and uncertainty relation (See SQ9 and SQ13)

Introduction to mean and variance: Here is a practical introduction to the mean and variance. Let's say there are k possible discrete results (outcomes) of measurements of a quantity x (discrete variable) and the values are given by $\{x_1, x_2, \ldots, x_k\}$. One could make a large number N of measurements. At the

end, n_1 measurements give x_1,...,n_k measurements give x_k. Obviously, $\sum_{i=1}^{k} n_k = N$. Operationally, the mean (or arithmetic mean) is simply

$$\overline{x} = \frac{1}{N}\sum_{i=1}^{N} x_i = \frac{1}{N}\sum_{i=1}^{k} n_i\, x_i = \sum_{i=1}^{k} \frac{n_i}{N}\, x_i \qquad (4)$$

The variance is

$$\sigma_x^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \overline{x})^2 = \frac{1}{N}\sum_{i=1}^{k} n_i\,(x_i - \overline{x})^2 = \sum_{i=1}^{k} \frac{n_i}{N}\,(x_i - \overline{x})^2 \qquad (5)$$

Here, you see the ratios n_i/N, which is called the relative frequency of the outcome x_i. These are the practical approaches (definitely not mathematical approach). These are also what you can do for experimental data.

Now, if a **long run** of measurements are taken or a rigorous way to calculate the value n_i/N in a long run, the value we expect of the relative frequency of an outcome is the **probability of the outcome** $P(x_i)$. For a discrete variable x, the set of probabilities $P(x_1)$, $P(x_2)$,...,$P(x_k)$, forms a **probability distribution**. Obviously, $\sum_{i=1}^{k} P(x_i) = 1$, which is related to normalization in QM. Similar to Eqs. (4) and (5), the mean or **expectation value** or *expected value* of x and the variance are

$$\langle x \rangle \;=\; E(x) = \mu = \sum_{i=1}^{k} x_i P(x_i) \qquad (6)$$

$$\sigma_x^2 \;=\; V(x) = \sum_{i=1}^{k}(x_i - \mu)^2 P(x_i) \qquad (7)$$

Finally, in QM, we encounter continuous variable x for which the probability distribution function is $P(x)$ with $P(x)dx$ being the probability of finding measurement results to be in the range x to $x+dx$. Obviously, we have $\int P(x)dx = 1$. In this case, the mean and the variance become

$$\langle x \rangle \;=\; \int x P(x)dx \qquad (8)$$

$$\sigma_x^2 \;=\; \int (x - \langle x \rangle)^2 P(x)dx \qquad (9)$$

where the integration is over the range of possible outcomes. The standard deviation σ or SD follows from the square root of the variance. This ends a poorman's introduction to the mean and the variance.

(a) Starting from either Eq. (7) or Eq. (9), **show that** the variance can be calculated by the following equation

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 \qquad (10)$$

[Remark: In QM, Eq. (10) is used to evaluate the (uncertainly)^2 of a quantity.]

(b) For a fair (unbiased) dice with outcomes one to six, **find** the mean, variance, and SD.

(c) For two fair dices together, the outcomes range from 2 to 12. **Find** the mean, variance, and SD.

(d) Now, we do a bit of QM. Let's say someone gives you a Gaussian wavefunction $\psi(x)$ of the form

$$\psi(x) = A^{1/2} e^{\frac{-x^2}{4\sigma^2}} = A^{1/2}\exp\left(-\frac{x^2}{4\sigma^2}\right) \qquad (11)$$

In QM, $|\psi(x)|^2$ is the probability density and thus plays the role of $P(x)$. By normalizing $P(x)$, **find** the prefactor A. Hence, **find** the mean position $\langle x \rangle$ and the variance (call it $(\Delta x)^2$).

(e) Next, take $\psi(x)$ in Eq. (11) (A is now known) and see it as a wavepacket. **Using Fourier transform**, **find** $F(k)$.

(f) Stretch your imagination a bit. Let's treat $F(k)$ as another QM wavefunction but it is in k-space (just like x). Hence, $|F(k)|^2 dk$ is the probability of finding the wavevector k in the Fourier decomposition to be in the interval k to $k + dk$. **Check** whether the $F(k)$ you obtained is properly normalized or not. If not, normalize it.

(g) Hence, using $|F(k)|^2$ to **find** the mean k ($\langle k \rangle$) and variance $(\Delta k)^2$. [Hint: Here, $|F(k)|^2$ plays the role of $P(x)$ in the Introduction.]

(h) Finally, **evaluate** the product $\Delta x \cdot \Delta k$. We know that $\hbar k = p$, hence **write down the answer** for $\Delta x \cdot \Delta p$ for the Gaussian wavefunction given in part (d).

[Remarks: If you follow through parts (d)-(h), you did for yourself many things, including a type of integrals called the **Gaussian integrals**, properties of Gaussian or normal distribution, and the physics of the ground state of harmonic oscillator and its uncertainty relation. See Problem 2.5.]

2.5 **1D harmonic oscillator: ground state, and copying results ain't that easy** (See Problem 2.4 and SQ12)

For a particle of mass m living in 1D and under the influence of a harmonic oscillator, $U(x) = \frac{1}{2}Kx^2 = \frac{1}{2}m\omega^2 x^2$, where ω is the angular frequency that characterizes the harmonic (or parabolic) potential energy function. The time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}m\omega^2 x^2\,\psi(x) = E\,\psi(x) \tag{12}$$

which is an equation to solve for many ψ's and many E's.

Let's take on a humble task. Someone solved the TISE and claimed that one particular solution (eigenfunction) has the following Guassian (also called normal) form (here $B^{1/2}$ is the normalization constant):

$$\psi(x) = B^{1/2}e^{\frac{-m\omega x^2}{2\hbar}} = B^{1/2}\exp\left(-\frac{m\omega x^2}{2\hbar}\right) \tag{13}$$

You may re-calculate all the things below or "copy" with skills (care) results from Problem 2.4.

(a) **Show explicitly** that $\psi(x)$ satisfies the TISE in Eq. (12) and **find** the corresponding energy E.

(b) **Normalize** $\psi(x)$ in Eq. (13), hence **write down** the properly normalized $\psi(x)$.

(c) Using the probabilistic interpretation of $|\psi(x)|^2$, **find** the mean position $\langle x \rangle$, variance $(\Delta x)^2$, and uncertainty in position Δx.

(d) Take $\psi(x)$ and **find** its Fourier transform $F(k)$. Again, take $|F(k)|^2 dk$ as a probability, **find** the mean k ($\langle k \rangle$), variance $(\Delta k)^2$, and uncertainty in k (Δk).

(e) Hence, **find** $\Delta x \cdot \Delta k$ and $\Delta x \cdot \Delta p$.

[Remarks: Here, you see a procedure in evaluating $(\Delta x)^2$ and $(\Delta k)^2$ (thus $(\Delta p)^2$) for a given $\psi(x)$, through a Fourier transform. This is a formal procedure. We will soon develop a **short cut** for obtaining $(\Delta p)^2$ using the momentum operator $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$. The calculation becomes shorter. The result of course will be the same.]

2.6 **Operators**

(a) **Determine** whether each of the following operators is linear or nonlinear. (i) $\hat{A}f(x) = [f(x)]^2$, i.e., take in $f(x)$ and square it. (ii) $\hat{A}f(x) = f^*(x)$, i.e., take in $f(x)$ and "complex it" (turn i to $-i$). (iii) $\hat{A}f(x) = [lnf(x)]$, i.e. take the natural log of $f(x)$.

(b) **Find** the commutators $[\hat{A}, \hat{B}]$ for the following cases. (i) $\hat{A} = \frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$. [Note: What is the general function to take in?] (ii) $\hat{A}f(x) = [f(x)]^2$ and $\hat{B}f(x) = \sqrt{f(x)}$.

(c) Consider three operators $\hat{A}$, $\hat{B}$, $\hat{C}$. **Show** that $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$ by operating on a general $f(x)$, where $[\hat{A}, \hbar B]$ is the commutator.

(d) You learned in primary school that $(A+B)(A-B) = A^2 - B^2$. This is ordinary algebra. For operator algebra, **What is** $(\hat{A} + \hat{B})(\hat{A} - \hat{B})$ (recall that the ordering of operators is a serious matter). Hence, **state the condition** under which the result becomes the same as in ordinary algebra?