PHYS3021 Quantum Mechanics I Problem Set 1
Due: 20 September 2017 (Wednesday) T+2 = 22 September 2017 (Friday)
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 I served several purposes. One is to emphasize that physics is an experimental science. The classic experiments in the first 25 years of the 20th century clearly asked for a (new) quantum theory. In Planck's thermal radiation and Einstein's heat capacity theory, we stressed the implication on the discrete energies in an oscillator, which is in contrast to classical physics. Einstein's photoelectric theory and Compton's scattering experiment established the *particle nature of light.* Our discussion focused on Young's double-slit experiments using light. For dim light sources, the unusual nature of the particles (photons) becomes obvious. Photons are detected as particles and yet the two slits must be open in order to observe the interference pattern, even when only one photon is in the apparatus at a time. The results also inform us on what a wave theory (Maxwell's EM wave theory) can do and cannot do. Electrons show the same behavior in double-slit experiments. De Broglie proposed a relation $\lambda_{dB} = h/p$ to connect a particle's momentum to a wavelength. Thus, the idea of *matter waves* enters. Accepting the necessity of a wave description of particle, a wavefunction $\Psi(x,t)$ or $\Psi(\mathbf{r},t)$ is introduced. In analogous to EM wave theory, the physical meaning is attached to $|\Psi(x,t)|^2$ instead of $\Psi(x,t)$ itself, with $|\Psi(x,t)|^2$ taking on the role of a **probability density**. Thus $\Psi(x,t)$ itself is a **probability amplitude**. This sets up the stage for the next questions (next Chapter): What is the wave equation for $\Psi(x,t)$? What are the physical requirements for $\Psi(x,t)$ to be an acceptable wavefunction?

For more detail, read: PHYS1122 class notes posted in course page. The chapters on key experiments in *Modern Physics* or *Quantum Physics* books are also useful. The first chapter in McQuarrie's *Quantum Chemistry* and Rae's *Quantum Mechanics* are also good.

We left the story of the Bohr's model not discussed. We will fill it in later.

1.1 *Planck's Thermal Radiation Formula (See SQ4)*

Planck's formula of thermal radiation expressed in terms of wavelengths is

$$u(\lambda,T)\,d\lambda = \frac{8\pi hc}{\lambda^5}\frac{1}{e^{hc/k_B\lambda T}-1}\,d\lambda\ . \tag{1}$$

As $c = f\lambda$ for EM waves, the formula can be expressed in terms of frequencies as

$$u(f,T)\,df = \frac{8\pi f^2}{c^3}\frac{hf}{e^{hf/k_BT}-1}\,df \tag{2}$$

(a) Starting with Eq.(2), **show** that the Stefan-Boltzmann law follows, i.e., total energy goes like T^4.
Hint: Either you may leave an integral unattended (just a number) or use the following integral that you will see in statistical mechanics course

$$\int_0^\infty \frac{x^3}{e^x-1}\,dx = \frac{\pi^4}{15} \tag{3}$$

(b) Starting with Eq.(2), **obtain the behavior in the following situations**: (i) low frequencies for which $hf \ll k_BT$ and (ii) high frequencies for which $hf \gg k_BT$.
[Remarks on underlying physics: Classical physics only gets the results in situation (i) ($k_BT \gg hf$) and predicts the same behavior over all frequencies. It is because an oscillator can always be excited by a finite temperature T, only the extent of excitation depends on T. This breaks down in the quantum regime when an oscillator requires a minimum energy of hf to be excited. When the thermal energy k_BT is too small to excite an oscillator, that oscillator simply ceases to contribute to the total energy and gives rise to the correct drop in $u(f,T)$ at high frequencies.]

(c) (Harder) Starting with Eq.(1), **show** the Wien's law follows, i.e., λ_{max} at which the maximum of $u(\lambda,T)$ occurs scales with the temperature T as $\lambda_{max} \sim 1/T$.

(d) The Planck's constant h first appeared in the Planck's formula. It is $h = 6.626 \times 10^{-34}$ J·s (joule-second). **Show** that h has the units of an **angular momentum**.

[Remark on underlying physics: In quantum mechanics, there are many angular momenta, e.g. orbital, spin, total, etc. It so happens that they are described in terms of h or $\hbar = h/2\pi$ naturally. For example, the "spin angular momentum" of an electron has a magnitude of $\sqrt{\frac{3}{4}}\hbar$ for all the electrons in the universe, just like each electron has the same charge $-e$ regardless of where it is.]

1.2 *Basic manipulations about light (EM waves) and photons*

(a) Physics is an experimental science. But reading papers on experiments (or communicating with experimentalists) could sometimes be confusing simply because of the different "languages" in the ways that physics is taught (theory) and physics is practiced. In layman's term, they are "not talking in the same wavelength"!. This non-scientific statement is partially true in that there are common practices in what units to use in different parts of the EM spectrum. Now, let's see what people use for EM waves in UV (ultraviolet), IR (infrared), and microwave frequencies.

(i) In experiments using UV light, the results are often given in terms of wavelength and in units of nm (nanometers or 10^{-9}m). For example, take $\lambda = 180$ nm, **calculate** the frequency f and the wave number $\tilde{\nu} = 1/\lambda$. Thinking in terms of photons, **calculate** the energy of a photon.

(ii) In experiments using IR light, the results are often given in terms of wave numbers (defined above) and in units of cm^{-1} (centimeter inverse). For example, take $\tilde{\nu} \sim 1000\ cm^{-1}$, **calculate** the frequency f and the wavelength λ. Thinking in terms of photons, **calculate** the energy of a photon.

(iii) In experiments using microwaves, the results are often given in terms of frequency and in units of MHz (megaheltz). For example, take $f = 18,000\ MHz$, **calculate** the wavelength λ and the wave number $\tilde{\nu}$. Thinking in terms of photons, **calculate** the energy of a photon.

[Remark: Thus, everybody does "talk in the same wavelength", only that different quantities/units are used. It is a fact of life. We have to live with it.]

(b) Given that the work function of chromium is 4.40 eV, **calculate** the kinetic energy of photo-emitted electrons from a chromium surface when UV radiation of wavelength 180 nm is used.

1.3 *Double-slit and Single-slit experiments*

The answer to this question **cannot be longer** than one side of an A4 page.

Double-slit and single-slit experiments using light and electrons play an important role in learning quantum mechanics as they brought out the essence of quantum behavior. They point to the need of **a wave description** of particles, thus the need of **a wavefunction** Ψ, and **interpreting** $|\Psi|^2$ as a probability density. This problem asks you to review by yourself the key results of these two experiments and how they come about using wave theory.

Students find the following results confusing, as they look similar but they are referring to different things.

For **double-slit experiments** in which the separation between the two slits is d, the condition for constructive interference and thus **seeing a maximum** on the screen is given by

$$d \sin\theta = m\lambda \tag{4}$$

where m is an integer. Thus the **first maximum** from the central maximum is observed at

$$d \sin\theta = \lambda \tag{5}$$

in a **double-slit experiment**

For a **single-slit experiment** in which the slit width is a (some authors called it w), the **first minimum** from the central maximum is observed at

$$a \sin\theta = \lambda \tag{6}$$

Eq.(5) and Eq.(6) are results that you should keep in mind. However, they look so similar and yet they are talking about different things.

Students: In less than one-side of an A4 page, **describe** how the two results Eq.(5) and Eq.(6) come about from consideration of interference.

[Remarks on underlying physics: These expressions are important for various reasons. One is that these experiments are useful in determining wavelengths, i.e. d (or a) is known from apparatus, θ can be observed, and thus λ can be found. Another is that these experiments can be used to illustrate the **Heisenberg Uncertainty Relation**, i.e., if a particle is known to pass through a single-slit (thus position in y-axis known to a range of a (slit width)), such a state necessarily contains many y-direction momentum components as required by wave mathematics (Fourier analysis). As a result, the observed fanning out pattern comes from this spread in momentum.]

1.4 *Basic manipulations in two-slit experiments*

In a two-slit experiment, light of 694.3 nm wavelength is used. On a screen that is 3 m away from the slits, the distance between neighboring maxima is observed to be 1.5 cm. **Find** the separation between the two slits.

1.5 *Matter wavelength can be controlled by temperature in experiments*

In SQ6, we saw that in the classic 1991 paper in firing helium atoms in a two-slit experiment, the matter waves of the atoms were controlled by an oven (heat atoms up and firing them out) and two temperatures (corresponding to two matter wavelengths) were used in the experiment. The point is: higher temperature, higher kinetic energy, higher momentum, and *shorter* matter wavelength.

Neutron scattering has become an important tool in studying materials. Being neutral, they can get deeper into a material than electrons. Neutrons have a magnetic dipole moment, as such they can also probe magnetic properties of a material. The matter wave wavelength of neutrons can also be controlled by temperature. Let's say the speed of a neutron is related to the temperature by $v = \sqrt{3k_BT/m_n}$, where m_n is the mass of a neutron and we want to tune the de Broglie wavelength to 5×10^{-11} m (or 50 pm (picometer)). **Calculate** the necessary temperature.

[Remark: The newly constructed "big science project" of the China Neutron Spallation Source (CNSC) in Dongguan (Guangdong, just next to us) produced the first ever pulsed neutron beam in China on 28th August 2017. The facility is due to operate for scientific research in 2018. Google "CNSC" for more detail.]

1.6 *Wave equation (string) – Illustrating the key physics (see SQ7)*

This problem is meant to bring out a few important concepts in handling wave equations. In QM, the Schrödinger equation is also a wave equation. Thus, what you do here is also applicable there, only that the wave equation will be different.

In SQ7, TA did the fundamental frequency. Here, we will work out more. The wave equation for a (guitar) string is

$$\frac{\partial^2 \psi(x,t)}{\partial x^2} = \frac{\mu}{T}\frac{\partial^2 \psi(x,t)}{\partial t^2} \tag{7}$$

where T is the tension (you tune the guitar by tightening the screw because that will alter the tension) and μ is the mass per unit length of the string (that's why the six strings in a guitar are different), and $\psi(x,t)$ is the displacement of the string from equilibrium (not vibrating).

We expect (see) that there is wave motion when we play the guitar. And what we see is real (double meaning here). Therefore, let's use a real form to describe the (standing) wave

$$\psi(x,t) = \phi(x,t) = A\sin(kx)\cos(\omega t), \tag{8}$$

where $k = 2\pi/\lambda$ is the wave vector and $\omega = 2\pi f$ is the angular frequency. Note that a more general form of the time part includes a phase in it, but $\cos(\omega t)$ suffices for our purpose of introducing the key concepts.

(a) Up to here, we only invoke the wave equation and the wave form (although the form considered something related to a guitar string, e.g. standing waves). Substituting $\phi(x,t)$ as in Eq.(8) into Eq.(7), **find** a relation between ω and k.

[Remark: An important physics concept here is that the wave equation relates (or governs) the time and spatial variations of a wave, i.e., for a particular wavelength (thus k), there is a particular frequency (thus ω).]

(b) *Boundary conditions selects certain allowed wavelengths and thus certain allowed frequencies.* Now consider a guitar string. It is not just a string lying there. It has a certain length L and it is fixed at the two ends **all the time**. At this point, it is important to note that what we have is a string with its properties and two boundary conditions, i.e. fixed at the end ends at the time. **We have not plucked the string yet.**

To satisfy the boundary conditions (B.C.) (all the time), we need to enforce it on the spatial part $A\sin(kx)$. It so happens that at $\psi = 0$ and $x = 0$, thus the no motion there and thus the B.C. at $x = 0$ is taken care of. Now is your turn to consider the B.C. at $x = L$. Imposing the condition that the string is fixed at $x = L$, **find the values of the allowed wavelengths** λ_n of the string, with $n = 1$ labelling the longest wavelength. Hence, **find the corresponding values of the allowed angular frequencies** ω_n of the string.

[Remarks: What you did here is a big part of QM problems. You have found the normal mode frequencies of the string and the corresponding wave forms (normal mode wavefunctions). Note that (ω_n, k_n) comes in a pair. In addition, you also know how each mode will evolve in time, simply with a time factor as $A_n \sin(k_n x)\cos(\omega_n t)$ or $A_n \sin(\frac{2\pi x}{\lambda_n})\cos(\omega_n t)$, with ω_n specific to the mode n.]

(c) *Superposition of modes: illustration*

Let $k_4 = 2\pi/\lambda_3$ and $k_{13} = 2\pi/\lambda_{13}$ be two allowed wavevectors obtained from two allowed wavelengths. Let's say at time $t = 0$, a wave form is created (you hold the string in a funny way at $t = 0$ to give the form) so that

$$\psi(x, t = 0) = A_4 \sin(k_4 x) + A_{13} \sin(k_{13} x) \ , \tag{9}$$

with A_4 and A_{13} being two coefficients specifying the weighting of the two components in $\psi(x, t = 0)$. Now, we claim that as time evolves (you release the string from the funny looking $t = 0$ form), **each component evolves with its own time factor with its own** ω_n, thus

$$\psi(x, t) = A_4 \sin(k_4 x)\cos(\omega_4 t) + A_{13} \sin(k_{13} x)\cos(\omega_{13} t) \ . \tag{10}$$

Show explicitly that Eq.(10) satisfies the time-dependent wave equation Eq.(7).

(d) *Superposition of modes: general*

This extends the idea in (c). Let's say at $t = 0$, the string is held in a funny form given by

$$\psi(x, t = 0) = \sum_{n=1}^{\infty} A_n \sin(k_n x) \tag{11}$$

Learning from (c), **write down** $\psi(x, t)$ at any time $t > 0$ and **show** that $\psi(x, t)$ satisfies the wave equation Eq.(7).

[Important Remarks: (i) For any form of $\psi(x, t = 0)$, Eq.(11) can always be written down, thanks to Fourier. (ii) The instant that you pluck the string ($t = 0$), you create something like a tilted tent (e.g. straight line going up from $x = 0$ to about $x = 3L/4$ and then straight line going down from there to $x = L$). This is $\psi(x, t = 0)$ in Eq.(11). The Fourier coefficients A_n can be calculated from the given $\psi(x, t = 0)$. This is a formula to plug. (iii) After knowing A_n, you know how the string vibrates at any time t, by allowing each Fourier component to evolve by **its own time part** based on its ω_n. (iv) For a free string (i.e., not pressed at any point, the whole string vibrates), the tent looks most like the fundamental (both of them have no nodes) and therefore the dominating component is the fundamental and the fundamental frequency dominates what you hear (the E sound of the first string). But it is mixed with the harmonics (A_n with $n = 2, 3, ...$) so that you realize immediately it is the sound of a guitar. (v) For our course, the key point is that all these concepts carry over to QM, only that the wavefunction in QM is in general complex and the time evolving factor is $e^{-i\omega_n t}$ instead.]