Problem Set 1
On Operators and Acceptable Wavefunctions

1. Three students are discussing what are acceptable wavefunctions. Bruce makes the suggestion that there exists a one-dimensional system for which the wave function is $\Psi(x) = N \tan(ax)$ for $a \leq x \leq \infty$ where a and N are constants.
Reena disagrees with Bruce and states that the true wavefunction for the system in question has the form $\Psi(x) = N x^{1/2}\exp(-ax)$ for $a \leq x \leq \infty$ where a and N are again constants.
Stephanie disagrees with both Bruce and Reena and suggests that $\Psi(x) = N \sin(ax)$ for $a \leq x \leq \infty$ where a and N are constants.
Which student is most likely to be correct? Justify your answer.

2. Which of the following functions are well-behaved? For those functions that are not well-behaved, indicate the reason.
(a) $u = x$, $x \geq 0$, and $u = 0$ otherwise
(b) $u = x^2$
(c) $u = e^{-|x|}$
(d) $u = e^{-x}$
(e) $u = \cos(x)$
(f) $u = \sin(\ |x|\ )$
(g) $u = \exp[-x^2]$
(h) $u = 1-x^2$, $-1 \leq x \leq +1$, $u = 0$ otherwise

3. Are the following functions normalized? If not, find the normalization constants that will complete the function.

Function	Physical space
(a) $\sin(2\pi z/b)$	one dimension, $0 \leq z \leq b$ volume element = dz
(b) $\sin(2\pi z/b) + 2\sin(3\pi z/b)$	one dimension, $0 \leq z \leq b$
(c) $\exp[-az^2]$ a is a positive constant	one dimension, $-\infty \leq z \leq +\infty$
(d) $\exp[i\, a\phi] + \exp[-i\, a\phi]$ a is a positive constant	one angular variable, $0 \leq \phi \leq 2\pi$ $d\phi$
(e) $\cos\theta \exp[-ar]$ a is a positive constant	3-D, $0 \leq r \leq \infty$, $0 \leq \theta \leq \pi$, $0 \leq \phi \leq 2\pi$ volume element = $r^2 dr \sin\theta d\theta\, d\phi$

4. The wavefunction of an electron in the lowest energy state of the hydrogen atom is the function

$\Psi(r) \propto \exp[-r/a_0]$
with a_0 = 52.9 pm and r the distance from the nucleus. Notice that this wavefunction depends only on this distance, not the angular position. This wavefunction is not normalized.

Normalize it using $d\tau = r^2 dr \sin\theta d\theta\, d\varphi$,
where θ= 0 to π, φ = 0 to 2π, r = 0 to ∞
and given the definite integral from a table of integrals,

$$\int_0^\infty x^n \exp[-ax]dx = n!/a^{n+1}.$$

Calculate the probability of finding the electron inside a small volume of magnitude 1.0 pm^3 located at the nucleus, and at a distance a_0 from the nucleus.

5. For the following physical quantities, determine the quantum mechanical operator:

(a) the potential energy of a system consisting of 1 nucleus of atomic number 2 and 2 electrons at distances r_1 and r_2 from the nucleus, given that the charge of an electron is -e.

(b) the angular momentum of a particle of mass m about the z axis. Recall from first year Physics that angular momentum about the z axis is given by $xp_y - yp_x$.

(c) the potential energy of a particle of charge q and mass m in an electric field of magnitude ε directed along the z axis

(d) the kinetic energy of two electrons [designate their position variables as (x_1,y_1,z_1) and (x_2,y_2,z_2)].

(e) the total energy of a Be^{3+} ion in the absence of any external fields.

6. Write down as explicitly as you can, the time-independent non-relativistic Schrödinger equation for the following systems:
[HINT: First you need to figure out what constitutes the physical system, then, what are the variables with which to express its kinetic energy and potential energy in classical physical terms. Then use the corresponding quantum mechanical operators to replace the classical physics variables to get the operator for the total energy, the Hamiltonian. Then write down the Schrödinger equation in terms of these operators. Be sure to define all your symbols after each equation.]

(a) a system of 4 particles each one of mass M in field-free space (V=0)

(b) the He atom

(c) a hydrogen atom in an electric field of magnitude ε directed along the z axis [Review your college physics, what is the potential energy for a charged particle in an electric field?]

(d) the HD diatomic molecule.