## Name:

## Chem 3322 test \#1 practice questions

I want complete, detailed answers to the questions. Show all your work to get full credit.

$$
\begin{equation*}
\text { indefinite integral : } \quad \int \sin ^{2}(a x) d x=\frac{x}{2}-\frac{\sin (2 a x)}{4 a} \tag{1}
\end{equation*}
$$

The classical wave equation in one dimension is

$$
\begin{equation*}
\frac{\partial^{2} u(x, t)}{\partial x^{2}}=\frac{1}{v^{2}} \frac{\partial^{2} u(x, t)}{\partial t^{2}} \tag{2}
\end{equation*}
$$

The Schrödinger time dependent equation is, for $\psi(x, t)$

$$
\begin{equation*}
i \hbar \frac{\partial \psi(x, t)}{\partial t}=-\frac{\hbar^{2}}{2 m} \frac{\partial^{2} \psi(x, t)}{\partial x^{2}}+V(x) \psi(x, t) \tag{3}
\end{equation*}
$$

The Schrödinger time independent equation is, for $\psi(x)$

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m} \frac{d^{2} \psi(x)}{d x^{2}}+V(x) \psi(x)=E \psi(x) \tag{4}
\end{equation*}
$$

The particle in a one dimensional box (of size $L$ ) energy levels are

$$
\begin{equation*}
E_{n}=\frac{n^{2} \pi^{2} \hbar^{2}}{2 m L^{2}} \quad \mathrm{n}=1,2,3, \ldots \tag{5}
\end{equation*}
$$

energy levels of the particle on a ring of radius $R$ :

$$
\begin{equation*}
E_{n}=\frac{n^{2} \hbar^{2}}{2 m R^{2}} \quad \mathrm{n}=0,1,2, \ldots \tag{6}
\end{equation*}
$$

Speed of light $=\mathrm{c}=3.0 \times 10^{8} \mathrm{~m} / \mathrm{s}$
electron mass $=9.11 \times 10^{-31} \mathrm{~kg}$. proton mass $=1.67 \times 10^{-27} \mathrm{~kg}$.
Avogadro's constant $=\mathrm{N}_{A}=6.022 \times 10^{23} \mathrm{~mol}^{-1}$
Planck constants: $\mathrm{h}=6.6262 \times 10^{-34} \mathrm{Js}$ and $\hbar=1.05459 \times 10^{-34} \mathrm{Js}$
$\pi=3.14159$
$1 \mathrm{eV}=1.6022 \times 10^{-19} \mathrm{~J}$ (electron volt to joule conversion)
mass conversion from amu to kg: $1.66 \times 10^{-27} \mathrm{~kg} / \mathrm{amu}$
Relationship between the wavelength of a photon and its energy $\lambda=h c / E$

## Problem 1

Can a quantum mechanical particle exist in a classically forbidden region? Discuss and illustrate your answer with a sketch of a potential energy function $V(x)$ and associated wavefunction $\psi(x)$ and probability density $|\psi(x)|^{2}$ in order to support your argument.

## Problem 2

The potential energy experienced by a quantum mechanical particle, and the total energy of the particle, are illustrated below. You are to sketch a valid wavefunction that is a solution to the TISE (time independent Schroedinger equation) for this situation. Assume, as shown on the illustration, that $V_{0}<V_{1}<E<V_{2}$.

a) Is the wavelength of the particle shorter or longer in the $V_{1}$ region of space as compared to the $V_{0}$ region of space? Justify your answer mathematically and also provide a sketch.
b) Sketch a valid wavefunction that is a solution to the TISE across all of space. Don't forget to draw something in the region to the left of the $V_{0}$ region, as well as the $V_{0}, V_{1}$, and $V_{2}$ regions of space. Also, carefully sketch what happens in the regions where the potential changes. You should include some mathematical expressions to indicate what functions you have used in your sketch.

## Problem 3

Consider a particle in a one-dimensional box of length $L$.
a) Do the energy levels move up or down if the box gets longer, namely if $L$ increases? Explain your answer clearly.
b) Assume that we put this particle into its first excited state, and then cause it to undergo a transition from the first excited state to the ground state. Assume that the energy liberated in this process is carried off by a photon. If we make the box smaller ( L decreases), will the emitted photon have a longer (red-shifted) or a shorter (blue-shifted) wavelength compared to the original box? Show as much mathematical justification as you can to explain your answer.

