Chem 5314 homework #1 – due Sept. 6, 2018

Problem 1 – classical wave equation

a) Show that \( u(x,t) = \sin(kx - \omega t) \) satisfies the classical wave equation by using the trigonometric identity \( \sin(A - B) = \sin A \cos B - \cos A \sin B \).

b) Show that \( u(x,t) = \sin(kx - \omega t) \) satisfies the classical wave equation by directly using the function \( \sin(kx - \omega t) \) in the wave equation.

c) Show that \( u(x,t) = \cos(kx - \omega t) \) satisfies the classical wave equation (do not use Euler’s formula).

Problem 2 – linearity

An operator \( \hat{B} \) is said to be linear if, for every pair of functions \( f \) and \( g \) and scalar \( c \), \( \hat{B}(f + g) = \hat{B}f + \hat{B}g \) and \( \hat{B}(cf) = c\hat{B}f \).

a) Prove that the operator \( \hat{A} = \frac{d}{dx} \) is a linear operator by using the definition of a derivative:

\[
\frac{d}{dx} f(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}
\]

Problem 3 – Taylor series

For (a), (b), and (c) you can look up the answers using any resource.

a) Write down, up to (and including) 7th powers of \( x \), the Taylor series for \( \sin x \).

b) Write down, up to 7th powers of \( x \), the Taylor series for \( \cos x \).

c) Write down, up to 7th powers of \( x \), the Taylor series for \( e^x \).

d) Write down, up to 7th powers of \( x \), the Taylor series for \( e^{ix} \) by using your answer (c).

e) By comparing your answer (d) to the Euler formula \( e^{i\theta} = \cos \theta + i \sin \theta \) show how you could identify the \( \sin x \) and \( \cos x \) Taylor series (assuming you didn’t know them).
Problem 4 – time dependence

Suppose we have a wavefunction

$$\psi(x, t) = \psi_1(x)e^{-iE_1 t/\hbar} + \psi_2(x)e^{-iE_2 t/\hbar}$$

(3)

with $E_1 \neq E_2$. Write down an expression for the probability density corresponding to this wavefunction and reduce it to an explicitly real form containing only trigonometric functions (i.e. get rid of all $i$’s). Based on this expression, describe the time dependence (i.e. find the frequency) of the probability density.

Problem 5 – operators

Consider the operator

$$\hat{A} = x \frac{d}{dx} - \frac{d}{dx} x$$

(4)

What does this operator do to a function $f(x)$? Based on your answer, express this operator in a simpler form.

Problem 6 – total derivative

What is wrong with the following math:

With $\mathbf{r} = (x, y, z)$ and $V$ the potential energy,

$$\nabla V \cdot d\mathbf{r} = \left( \frac{\partial V}{\partial x}, \frac{\partial V}{\partial y}, \frac{\partial V}{\partial z} \right) \cdot (dx, dy, dz) = 3 \, dV$$

(5)

Problem 7 – heat equation

In a metal rod of length $L$ with non-uniform temperature, heat (thermal energy) is transferred from regions of higher temperature to regions of lower temperature. The heat equation, which describes this behavior, is given by

$$\frac{\partial u}{\partial t} = k \frac{\partial^2 u}{\partial x^2}$$

(6)

where $u(x,t)$ is the temperature of the rod at location $x$ and time $t$ and where $k$ is the thermal diffusivity. We will assume that the initial $(t = 0)$ temperature distribution in the
rod is given by \( u(x, 0) = f(x) \) and that the ends of the rod are kept cold: \( u(0, t) = u(L, t) = 0 \)
on the Celcius scale (note: negative temperatures are allowed since we are using the Celcius scale).

a) Apply the separation of variables procedure to the heat equation to obtain two ordinary
differential equations, one in time and one in space. As part of your procedure, call the
constant \(-\lambda\) and assume, for what follows, that \( \lambda > 0 \) (so that you can take a square root
of \( \lambda \) without having to worry about imaginary numbers).

b) We will now work towards solving the ordinary differential equation with respect to
space. Since this is a second order equation (namely, the highest derivative that appears is
of second order) we need to find two linearly independent solutions and then combine them
with linear combination coefficients \( c_1 \) and \( c_2 \) to arrive at the most general solution. Do
this (hint: your two linearly independent solutions should be a sin function and a cosine
function).

c) From the general solution to the spatial ordinary differential equation of part (b), we
now need to make it satisfy the end-conditions \( u(0, t) = u(L, t) = 0 \), which means that the
solution of part (b) must be zero at \( x = 0 \) and also at \( x = L \). Do this (hint: the \( x = 0 \)
boundary condition will eliminate the cosine part of the solution and the \( x = L \) boundary
condition will impose some restrictions on the possible values of \( \lambda \)).

d) Now that you know something about the possible values of \( \lambda \), go ahead and solve the
ordinary differential equation with respect to time (hint: its just a decaying exponential).
e) Write the product solution \( u(x, t) \) from your time and space pieces.
f) Solve the heat equation for the initial condition

\[
f(x) = 6 \sin\left(\frac{\pi x}{L}\right)
\]

Verify that your solution satisfies all of the criteria (the heat equation, the initial temperature
distribution, and the end-conditions).

g) Plot your solution to (f) at three different time values: the initial time \( (t = 0) \), a time
close to the initial value, and a time close to the final temperature profile in the rod but
still small enough that the profile is clearly non-zero. Describe these heat profiles in words.
Note: you will have to assign values to some of the constants \((k, L)\).

h) Solve the heat equation for the initial condition

\[
f(x) = 12 \sin\left(\frac{9\pi x}{L}\right) - 7 \sin\left(\frac{4\pi x}{L}\right)
\]
Verify that your solution satisfies all of the criteria (the heat equation, the initial temperature distribution, and the end-conditions).

i) Plot your solution to (h) at three different time values: the initial time \( t = 0 \), a time close to the initial value, and a time close to the final temperature profile in the rod but still small enough that the profile is clearly non-zero. Describe these heat profiles in words: there is something striking that happens with respect to the two different wavelengths present that you should highlight.

j) Solve the heat equation for the initial condition \( f(x) = 1 \) and plot your solution for three different time values as you have done previously. Note: this is a much more difficult problem; you should look at, for example, http://web.mit.edu/18.06/www/Spring09/sines.pdf

**Problem 8 – two-dimensional function**

Give an example of a function of two variables, \( f(x, y) \), that cannot be written as the product of two single-variable functions, \( g(x) \) and \( h(y) \).