Physical Chemistry Problems and Why We Care

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1 Introduction

There are several concepts in *physical chemistry*, i.e. the physics of atoms and chemical properties, that turn out to have wide applications and we are going to explore some of them here.

First, we should acknowledge that the early history is filled with people who had the luxury to explore rather esoteric topics, while we might be learning these as a matter of our own 'development' and with a sense of what for! I'll try to make an argument that this stuff really does matter, but for now, let's start the problem set!

Second, we also need to understand that these assignments have been developed as hurtles that have almost nothing to do with the end-goal of being a health-care professional. Instead, it's better to reflect that being able to think about problem solving is actually the real goal here and we need to learn to problem solve in a systematic way.

2 Problem Sets

3 Problem #2

3.1 Background

Neutron radiation is a kind of ionizing radiation which consists of free neutrons. A result of nuclear fission or nuclear fusion, it consists of the release of free neutrons from atoms, and these free neutrons react with nuclei of other atoms to form new isotopes, which, in turn, may produce radiation.

Cold, thermal and hot neutron radiation is most commonly used for scattering and diffraction experiments in order to assess the properties and the structure of materials in crystallography, condensed matter physics, biology, solid state chemistry, materials science, geology, mineralogy and related sciences. Neutron radiation is also used in select facilities to treat cancerous tumors due to its highly penetrating and damaging nature to cellular structure. Neutrons can also be used for imaging of industrial parts termed neutron radiography when using film, neutron radioscopy when taking a digital image,

2. A particle accelerator generates neutrons at 2500K and whose speed is given by $\sqrt{(3k_B T/m)}$. Determine the de Broglie wavelength of the neutron.

3. The threshold wavelength of light required to eject electrons from the surface of the metal Lanthanum (Z = 57) is 3760 Å.
   (a) What is the work function of the metal in electron-volts and wavenumbers?
   (b) What is the maximum kinetic energy of photoelectrons emitted by this metal when it is illuminated with ultraviolet light of wavelength 2000 Å?
   (c) The work function for barium is 2.48 eV. If light of 400 nm is shined on a barium cathode, what is the maximum velocity of the ejected electrons?

4. The clean surface of Na is illuminated with monochromatic radiation of various wavelengths (λ) and the retarding (or stopping) potentials (V_s) required to stop the most energetic photoelectrons are observed as follows.

λ / Å	2536	2830	3039	3302	3663	4358
V_s / V	2.60	2.11	1.81	1.47	1.10	0.57

   Plot these data in such a way as to show that they lie along a straight line as predicted by the photoelectric equation, and obtain a numerical value for Planck's constant *h*. Note: at the stopping potential the kinetic energy of the electrons is balanced exactly by the potential energy due to the stopping potential, i.e. KE = eV_s, where e is the charge on an electron.

such as through image plates, and neutron tomography for three-dimensional images. Neutron imaging is commonly used in the nuclear industry, the space and aerospace industry, as well as the high reliability explosives industry.

The imaging is a function of the particles wavelength, λ, where higher freqencies resolve higher resolution. It's rare that one would ever have to calculate this from scratch, but the value of the exercise is ???

3.2 de Broglie Wavelenth

In 1923, Louis de Broglie, a French physicist, proposed a hypothesis to explain the theory of the atomic structure. By using a series of substitution de Broglie hypothesizes particles to hold properties of waves. Within a few years, de Broglie's hypothesis was tested by scientists shooting electrons and rays of lights through slits. What scientists discovered was the electron stream acted the same was as light proving de Broglie correct.

Thus, for this problem, we will determine the wavelength of a particle (nuetron), which also has a mass – one of the strangest scientific theories!

In this problem we are trying to determine (calculate) the 'de Brogie' wavelenth. So, let's first determine the units of a wavelength, so we have a clue where we are heading! In general, wavelength is measured as length per time, in SI units, we often see this as m/s, but for atomic particle scales, the units are often Å/second, where an Angstrom (Å) is $1 \cdot 10^{-10}$ meters, i.e very short disances! Note: an Å is not an SI unit, which is terribly lame. But let's let that go for now, I think $1 \cdot 10^{-9}$ is the SI units, which is a nanometer. Whatever!

We are given the a number that includes temperature, as measured in Kelvin. Okay, that seems to be a weird parameter to be given! But let's back up. We are told that a particle accelartor generate nuetrons at 2500K, where K is degrees Kelvin, i.e. a temperature. By knowing temperature, we are supposed to figure out a wavelength, weird!!!

We are given the following equation to determine velocity of the nuetron

$$\nu_{rms} = \sqrt{(3k_B T/m)} \tag{1}$$

where ν_{rms} is room-mean-speed (m/s), k_B is Boltzmann's Constant ($1.38e^{-23}$ J/K or $m^2 kgs^{-2} K{-}1$) and T is temperature (degrees K) and m is the mass of the particle (kg). This equation is the root-mean square of speed (velocity) of particles – it's a kind of an average speed, see `http://www.studyphysics.ca/2007/20/ap_thermodynamics/42a_ap_kinetic_theory_gases.pdf` for a decent explanation. For now, we'll use μ_{rms} as arithmetic mean of the squares of a set of numbers). The RMS is also known as the quadratic mean and is a particular case of the generalized mean with exponent.

The mass of a nuetron, m, is 1.6750e-27 (kg) and k_B = 1.38e-23 ($m^2 kgs^{-2} K{-}1$). Using the equation above, we can do a dimensional analysis where

$$\sqrt{3m^2 \cdot kg \cdot s^{-2} \cdot K^{-1} \cdot K/kg} = \sqrt{3m^2 \cdot s^{-2}} = \sqrt{3}m/s \tag{2}$$

thus, we have units in terms of velocity!

Thus, the ν_{rms} is

```
> k_B = 1.38e-23
> T = 2500
> m = 1.6750e-27; m

[1] 1.675e-27

> nu = sqrt(3*k_B*T/m); nu

[1] 7860.728
```

Thus, we have now calculated the speed as 7860.73.[1]

3.3 Calculating λ

Next, what do we do with the velocity?

Using this site: `http://chem.libretexts.org/Core/Physical_and_Theoretical_Chemistry/Quantum_Mechanics/02._Fundamental_Concepts_of_Quantum_Mechanics/De_Broglie_Wavelength`, we might be able to evaluate the question with some sense that we understand what in the world is happening:

$$\lambda = \frac{h}{p} = \frac{h}{m\nu} \tag{3}$$

[1] However, I am not sure this is right. Did you get this as a intermediate answer with your prof? I need to figure out the units too!

where h is planck's constant, p is the particle momentum and m is the particle's mass and ν is the particles' velocity. Using a dimensional analysis we have

$$\frac{m^2 \cdot kg \cdot s^{-1}}{kg \cdot m/s} = m \tag{4}$$

and we have meters, which is how wavelengths are measured!

Based on this equation, we have velocity, ν, and we know the mass of the nuetron, which is 0. Thankfully, h, or Planck's Constant is a known quanity, altough we derive it in problem #4!

```
> h = 6.626e-34
> lambda = h /(m * nu); lambda
```

```
[1] 5.032385e-11
```

At this point, I am doing something wrong, because it's hard to belive that this wavelength is so small, 0. I suspect I didn't calculate the velocity correctly, seems way too slow!

4 On Planck's Constant

Planck's Constant is a very powerful parameter... with units as $m^2 \cdot kg \cdot s^{-1}$.

For background on Planck's constant, check out `https://en.wikipedia.org/wiki/Planck_constant`.

4.1 Stopping Voltage and Wavelength

The goals of this problem is to determine the constant using stopping voltages for various wavelengths. I am not sure how this is done, for now, let's say in a fancy machine and leave it at that.

We given a table to measurements:

- $\lambda/\text{Å}$ is in the units of lenth and in this case is is in Å, or Angstroms. Unfortunately, the symbolism is non-standard here, where it looks like we are dividing the wavelength by the Å, but after several attempts to use the demominator, I discoverd that it was only referring to the units.
- V_s/V is the stopping voltage, but the demominator is confusing, and is again referring to the units, which are in volts!

We are told to create a line, but the predicted by the photoelectric equation:

$$E = h \cdot freq \tag{5}$$

but we don't have E or freq. This equation was proposed by Einstein – where energy is proporation to freqency and h. Now, first, there is something that is tricky about this equation, where frequency is often denoted as ν, which is also used for velocity as above. This is an annoying part of science, there just aren't enough letters for them to represent one thing. So, you have to be careful, I converted the variable to 'freq'. E might be equal to e, the energy of an electron, but I am still sorting that out.

Using a dimensional analysis, where frequency is $s{-}1$, we obtain

$$m^2 \cdot kg \cdot s^{-1} \cdot s^{-1} = kgm^2 s^{-2} = Joule \tag{6}$$

the units as espected is a joule.

Next, we can convert wavelength (m) to frequency (s) using this simple equation:

$$f = \frac{\nu}{\lambda} \tag{7}$$

, now hwaver, we need to figure out the ν, velocity! Dang! Another set of steps...But let's consider the equation given and see if can figure out it's going to be used:

$$KE = e \cdot V_s \tag{8}$$

where KE is kenetic energy (units?) and E is the charge of an electron (volts) and V_s is stopping voltage. KE is $1/2mv^2$. e is the charge of an electron.

Using dimensional analysis then we have

$$columbs \cdot volts \tag{9}$$

and then e =mc2? somehow we need to involve the speed of light? Geez, I am completely lost!

Alternatively, we can substitute E, from the photoelectric equation:

$$KE = \cdot h \cdot freq \cdot V_s \tag{10}$$

and solving for h, we get

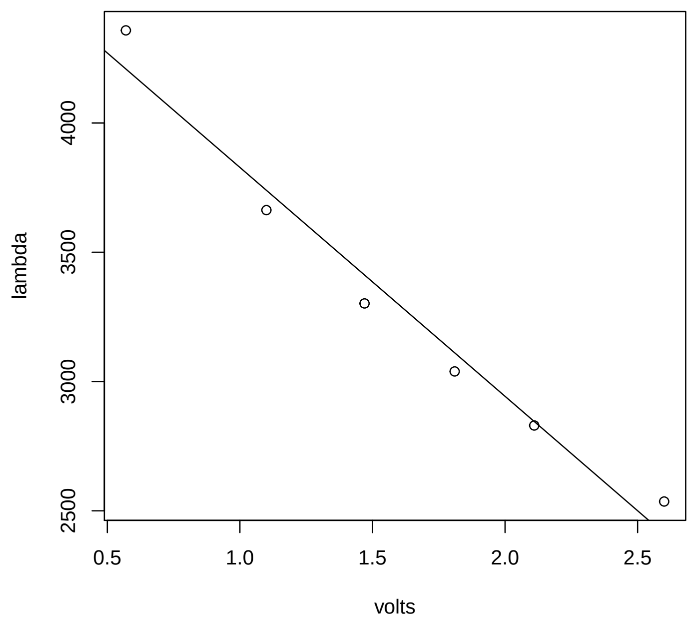
$$h = freq \cdot V_s / KE \tag{11}$$

Here, I am stuck again...

```
> lambda=c(2536, 2830, 3039, 3302, 3663, 4358)
> volts=c(2.6, 2.11, 1.81, 1.47, 1.1, .57)
> coef(lm(lambda~volts))

(Intercept)       volts
  4713.1565   -885.1904

> plot(lambda~volts)
> abline(coef(lm(lambda~volts)))
```



The the slope is not h! where h is 4713.16, based on the relationship:

$$\lambda = f(V_s) \tag{12}$$

This doesn't seem to be doing anything useful.
where E is the energy of the radiation and ν is the velocity of the particle.