Homework #4 - Solutions

Problem 1 - Photoelectric Effect

You are working in the analytical lab of a company that manufactures semiconductor processing equipment. Your equipment is manufactured from a variety of metals. One of your clients returns a piece of equipment claiming that it exhibits unacceptable levels of contamination. Your manager asks you to establish the contaminant and the base metal material used for the equipment. You decide to employ photoelectron spectroscopy with sputter depth profiling. Using this approach, you obtain the attached data set which contains measurements of the maximum kinetic energy of photo-emitted electrons versus the incident photon frequency. There are two data sets: one initial scan and a second scan after sputtering the sample with argon for 30 minutes.

a. Analyze the data and write a professional report to your manager that includes

i. A restatement of the key question to be answered.

ii. A brief discussion of the experimental design and motivation for using photoelectron spectroscopy.

iii. An analysis of the data with the relevant physical model.

iv. Be sure to include clear, descriptive captions to any figures included in your report.

v. A discussion of the statistical significance of the results, the reliability of the analysis and/or validity of the model in representing the data.

vi. A concise conclusion, based on your judgement of the data, of the metal and contaminant. You may speculate on the source of the contamination.

vii. References to any sources used in preparing your report.

Here, I'll analyze the data and create plots that will be used in the formal report. The data include measurements of KE_{max} versus photon frequency. Based on the photoelectric effect, these data should be linear with a slope equal to Planck's constant and a y-interscept equal to the negative of the material's work function, ϕ. I'll start by importing the data, fitting it to a linear model, and then plotting the results in a format suitable for a report.

```
In[•]:= TableForm[prefile = Import[
          "/Users/eltongraugnard/SkyDrive/Documents/Mse/Courses/Mse410/Homework/Mse410-
            Ece340_hmwk-04-initial-scan-data.csv", "Data"]]
```

Out[•]//TableForm=

Initial Scan

f (Hz)	KE_max (eV)
7.25×10^{14}	0.243628
7.5×10^{14}	0.36256
$8.\times10^{14}$	0.542036
8.5×10^{14}	0.773256
$9.\times10^{14}$	0.933504
$1.\times10^{15}$	1.41372
1.2×10^{15}	2.16894

```
In[•]:= TableForm[postfile = Import[
          "/Users/eltongraugnard/SkyDrive/Documents/Mse/Courses/Mse410/Homework/Mse410-
            Ece340_hmwk-04-post-sputter-scan-data.csv", "Data"]]
```

Out[•]//TableForm=

Post-Sputter Scan

f (Hz)	KE_max (eV)
$9.\times10^{14}$	0.06552
$1.\times10^{15}$	0.50932
1.2×10^{15}	1.25107
1.35×10^{15}	1.80818
1.5×10^{15}	2.62032
1.75×10^{15}	3.61378

```
In[•]:= predata = Drop[prefile, 3]; postdata = Drop[postfile, 3];
```

```
In[•]:= prelmf = LinearModelFit[predata, x, x]
```

```
Out[•]= FittedModel[ -2.69095 + 4.06177 ×10^-15 x ]
```

```
In[•]:= prelmf["ParameterErrors"]
```

```
Out[•]= {0.0749241, 8.06756 × 10^-17}
```

```
In[•]:= prelmf["AdjustedRSquared"]
```

```
Out[•]= 0.998031
```

```
In[•]:= postlmf = LinearModelFit[postdata, x, x]
```

```
Out[•]= FittedModel[ -3.7565 + 4.2037 ×10^-15 x ]
```

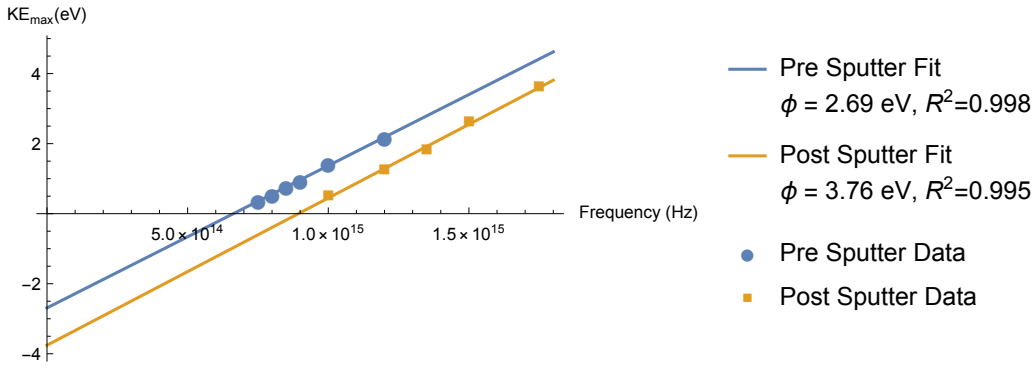
```
In[•]:= postlmf["ParameterErrors"]
```

```
Out[•]= {0.210304, 1.51972 × 10^-16}
```

```
In[•]:= postlmf["AdjustedRSquared"]
Out[•]= 0.994793

In[•]:= Show[Plot[{Legended[prelmf[x], "Pre Sputter Fit\nϕ = 2.69 eV, R^2=0.998"],
    Legended[postlmf[x], "Post Sputter Fit\nϕ = 3.76 eV, R^2=0.995"]},
   {x, 0, 1.8 × 10^15}, AxesLabel → {"Frequency (Hz)", "KE_max (eV)"}],
  ListPlot[{Legended[predata, "Pre Sputter Data"],
    Legended[postdata, "Post Sputter Data"]}, PlotMarkers → {Automatic, Medium}]]
```

Out[•]=



Problem 2 - Planck's law and photon energy distribution of radiation

Planck's law, stated in Equation 3.9, provides the spectral distribution of the black body radiation intensity in terms of wavelength through Il, intensity per unit wavelength:

```
In[•]:= FormulaData[{"PlanckRadiationLaw", "Wavelength"}]
```

Out[•]=

$$L[\lambda] == \frac{2\,h\,c^2}{\left(-1 + e^{\frac{1\,h\,c/k}{T\,\lambda}}\right)\lambda^5}$$

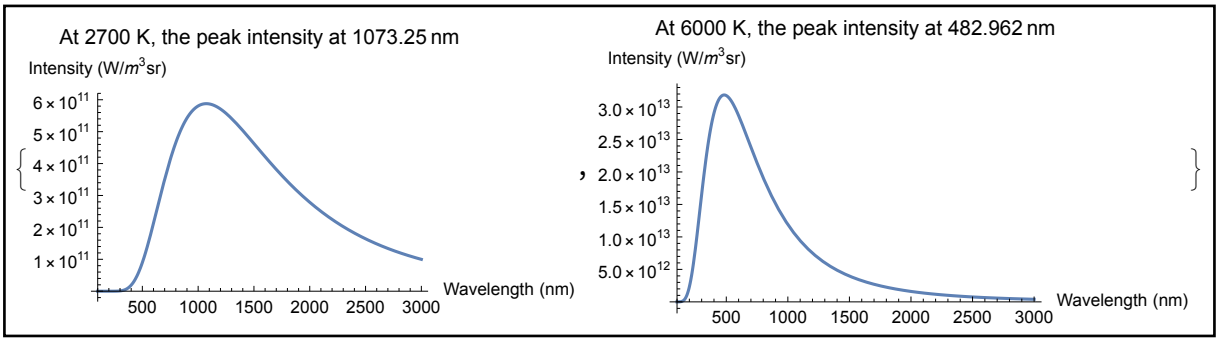
Note, this equation differs from Eqn. 3.9 in the text by a factor of π.

a. Plot Planck's radiation law for a blackbody at 2700 K and 6000 K. (Hint: you might try using Mathematica's built in "PlanckRadiationLaw.")

Using *Mathematica*'s built in PlanckRaditationFormula, we have:

In[•]:=
```
Framed[
 {Plot[PlanckRadiationLaw[Quantity[2700, "Kelvins"], Quantity[x, "Nanometers"]],
   {x, 100, 3000}, AxesLabel → {"Wavelength (nm)", "Intensity (W/m^3sr)"},
   PlotLabel → Row[{"At 2700 K, the peak intensity at ",
      N[PlanckRadiationLaw[Quantity[2700, "Kelvins"], "MaxWavelength"]]}]],
  Plot[PlanckRadiationLaw[Quantity[6000, "Kelvins"], Quantity[x, "Nanometers"]],
   {x, 100, 3000}, AxesLabel → {"Wavelength (nm)", "Intensity (W/m^3sr)"},
   PlotLabel → Row[{"At 6000 K, the peak intensity at ",
      N[PlanckRadiationLaw[Quantity[6000, "Kelvins"], "MaxWavelength"]]}]]}]
```

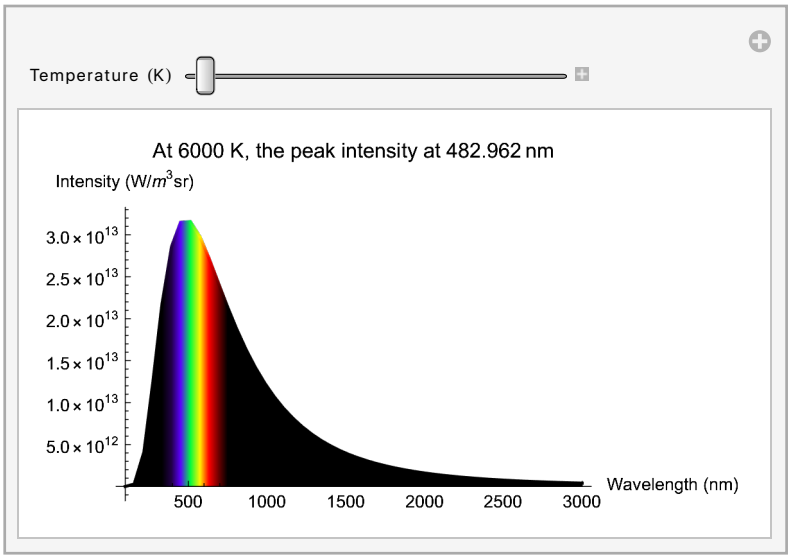
Out[•]=



Above, I used two separate plots since the intensities are different by a few orders of magnitude.
Below, I used the Manipulate function and some fancy filling to plot at input temperatures.

In[•]:=
```
Manipulate[
 Plot[PlanckRadiationLaw[Quantity[T, "Kelvins"], Quantity[x, "Nanometers"]],
  {x, 100, 3000}, MaxRecursion → 0,
  ColorFunction → (ColorData["VisibleSpectrum"][#] &), ColorFunctionScaling → False,
  Filling → Axis, AxesLabel → {"Wavelength (nm)", "Intensity (W/m^3sr)"},
  PlotLabel → Row[{"At ", T, " K, the peak intensity at ",
     N[PlanckRadiationLaw[Quantity[T, "Kelvins"], "MaxWavelength"]]}]],
 {{T, 6000, "Temperature (K)"}, 273, 10^6, 100}]
```

Out[•]=



b. At what wavelength does the peak intensity occur for the above two temperatures?

From the built-in *Mathematica* function, we can find the wavelength for the peak intensity, which was used in the plots above.

Thus, the wavelengths for peak intensity are 1073 nm at 2700 *K* and 483 nm at 6000 *K*.

c. Compare the peak wavelengths from part (b) to those computed using Wien's displacement law, $\lambda_{max} \approx (2.89\times10^{-3}\ \text{m K})/\text{T(in K)}$.

I create a function for Wien's displacement law, but convert to nanometers, since those were the units from the PlanckRadiationLaw

In[•]:=
```
λmax[T_] := 2.89 × 10^-3 / T 10^9 nm K
```

In[•]:=
```
{λmax[2700 K], λmax[6000 K]}
```

Out[•]=
```
{1070.37 nm, 481.667 nm}
```

In[•]:=
```
{2 (λmax[2700 K] - 1073.249 nm) / (λmax[2700 K] + 1073.249 nm) 100 "%",
 2 (λmax[6000 K] - 482.962 nm) / (λmax[6000 K] + 482.962 nm) 100 "%"}
```

Out[•]=
```
{-0.268577 %, -0.268566 %}
```

We see that for each temperature, the wavelength of peak intensity predicted by Wien's displacement law is within 0.5 % from the value found using Planck's radiation law.

Problem 3 - Wave Function

Consider an electron in a 1-dimensional box of length a. The wave function for an electron in this box is given by:

$$\psi(x) = A\,i\,\mathrm{Sin}\left[\frac{n\pi}{a}x\right]$$

a. Normalize the wave function. Show all work in a step-by-step manner.

To normalize teh wave function is to determine the coefficient, A. For an electron confined to a 1D box of width a, we know that the probability density integrated over the width of the box must be unity: $\int_0^a |\psi(x)|^2 dx = 1$, where $|\psi(x)|^2 = \psi^*(x)\psi(x)$. Thus, for our wavefunction, we have

$$\int_0^a |\psi(x)|^2 dx = \int_0^a \left(A^*(-i)\,\mathrm{Sin}\left[\frac{n\pi}{a}x\right]\right)\left(A\,(i)\,\mathrm{Sin}\left[\frac{n\pi}{a}x\right]\right)dx$$
$$= |A|^2(-i)(i)\int_0^a \mathrm{Sin}^2\left[\frac{n\pi}{a}x\right]dx = |A|^2\int_0^a \mathrm{Sin}^2\left[\frac{n\pi}{a}x\right]dx$$

At this point, we can ask *Mathematica* to compute the integral:

```
In[•]:= Integrate[(Sin[n π / a x])^2, {x, 0, a}]
```

$$\text{Out[•]=}\ \frac{1}{4}a\left(2 - \frac{\mathrm{Sin}[2n\pi]}{n\pi}\right)$$

Since n is an integer, we know the Sin[2nπ] term will be zero. Thus the integral simplifies to $\frac{a}{2}$. We can assume that the coefficient A is real to find

$$|A|^2\left(\frac{a}{2}\right) = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$$

Thus, our wave function is

$$\boxed{\psi(x) = \sqrt{\frac{2}{a}}\,i\,\mathrm{Sin}\left[\frac{n\pi}{a}x\right]}$$

Problem 4 - Operators

The momentum operator in quantum mechanics, $\hat{p}_x$, in one dimension is given by:

$$\hat{p}_x = -i\hbar\nabla_x = -i\hbar\frac{d}{dx}$$

a. Show that the momentum operator can be written as: $\hat{p}_x = \frac{\hbar}{i}\nabla_x$

From the equation above, we can write

$$\hat{p}_x = -i\hbar\nabla_x = -i\hbar\nabla_x\left(\frac{i}{i}\right) = -\frac{i^2}{i}\hbar\nabla_x \Rightarrow \boxed{\hat{p}_x = \frac{\hbar}{i}\nabla_x}$$

b. Given the wave function:

$$\Psi(x, t) = Ae^{-ikx}e^{i\omega t}$$

find the eigenvalue for momentum. Show all work in a step-by-step manner.

The eigenfunction/eigenvalue relationship for momentum is

$$\hat{p}_x\Psi(x, t) = p\Psi(x, t)$$

Solving this equation, we have

$$\hat{p}_x\Psi(x, t) = -i\hbar\nabla_x\Psi(x, t) = -i\hbar\frac{d}{dx}\left(Ae^{-ikx}e^{i\omega t}\right) = -i\hbar A(-ik)e^{-ikx}e^{i\omega t}$$

$$= i^2\hbar k Ae^{-ikx}e^{i\omega t} = -\hbar k Ae^{-ikx}e^{i\omega t} = -\hbar k\Psi(x, t) = p\Psi(x, t)$$

$$\Rightarrow \boxed{p = -\hbar k}$$

Upon inspection of the wave function, we recognize it as describing a wave traveling in the -x direction, which is consistent with the momentum eigenvalue.