

## q\_02\_trial

November 23, 2020

```
[1]: import numpy as np
      from matplotlib import pyplot as plt

[2]: kb = 1.38064852e-23

[3]: def poly(x,a):
      val = sum([a[j]*(x**(j)) for j in range(1,len(a))])
      return val
```

### 0.0.1 Routine for calculation of integral of a function

```
[48]: def integral(f,a_0,b_0,n,kind='simp'):
      h = (b_0-a_0)/n
      t0 = f(a_0)+f(b_0)

      if (kind=='simp'):
          t1 = sum([f(a_0+h*(2*k-1)) for k in range(1,int(n/2)+1)])
          t3 = sum([f(a_0+h*(2*k)) for k in range(1,int(n/2))])
          val = (h/3)*(t0+4*t1+2*t3)
      if (kind=='tpz'):
          t1 = sum([f(a_0+k*h) for k in range(1,n)])
          val = (h/2)*(t0+2*t1)
      return(val)
```

### 0.1 Linear regression routine

```
[4]: def linear_regression(x,y,sigma):
      '''
      Fits data(x , y) for the linear function -
      y = a1 + a2*x

      Use error propogation for calculation of
      error in a1 and a1, using given error sigma

      returns a1,a1, error(a1) , error(a1)
      '''
      s = sum([1/(sig**2) for sig in sigma])
```

```

sum_x = sum([(xi/(sigma_i**2)) for xi , sigma_i in zip(x,sigma)])
sum_y = sum([(xi/(sigma_i**2)) for xi , sigma_i in zip(y,sigma)])
sum_x_sq = sum([(xi**2/(sigma_i**2)) for xi , sigma_i in zip(x,sigma)])
sum_x_y = sum([(xi*yi/(sigma_i**2)) for xi ,yi, sigma_i in zip(x,y,sigma)])

# Parameters Calculation
denom = s*sum_x_sq - (sum_x**2)
a1 = (sum_y*sum_x_sq - sum_x*sum_x_y)/denom
a2 = ( s*sum_x_y - sum_x*sum_y ) /denom

# Error Calculation
sigma_a1_sq = sum([(((sum_x_sq-x_i*sum_x)**2)/(sigma_i**2) for x_i,sigma_i
→in zip(x,sigma)))/(denom**2)
sigma_a2_sq = sum([((s*x_i-sum_x)**2)/(sigma_i**2) for x_i , sigma_i in
→zip(x,sigma)))/(denom**2)

err_a1 = sigma_a1_sq**0.5
err_a2 = sigma_a2_sq**0.5

return (a1,a2 , err_a1 , err_a2)

```

## 0.2 Loading data

energy is converted into J

```

[11]: data = np.loadtxt('QIIdata')
data_col = np.transpose(data)

#print(data.shape)
en_kev = data[:,0]
en = np.asarray([e*1.60218e-16 for e in en_kev])
fm = data[:,1]
del_fm = data[:,2]
ft = data[:,3]
del_ft = data[:,4]

```

## 0.3 Part (I) Part(II)

taking log on both sides and linear fitting

```

[12]: log_fm = np.log(fm)
d_log_fm = np.asarray([(del_f/f) for del_f , f in zip(del_fm, fm)])

[13]: _ , a1 , _ , err_a1 = (linear_regression(en , log_fm , d_log_fm))
print(a1 , err_a1)

```

-4870625982560964.0 21382929316637.44

```
[14]: y_ft = [(1/np.log(f))**2 for f in ft]
d_y_ft = [(-2*df)/(f*((np.log(f))**3)) for df, f in zip(del_ft, ft)]
_, a2, _, err_a2 = (linear_regression(en, y_ft, d_y_ft))
print(a2, err_a2)
```

11942818631310.047 164482758744.3392

```
[104]: T = (-1/(a1*kb))
err_T = (1/(kb*a1**2))*err_a1
print('Temp estimated: {:.3e} K'.format(T))
print('error in temp estimated: {:.3e} K'.format(err_T))
```

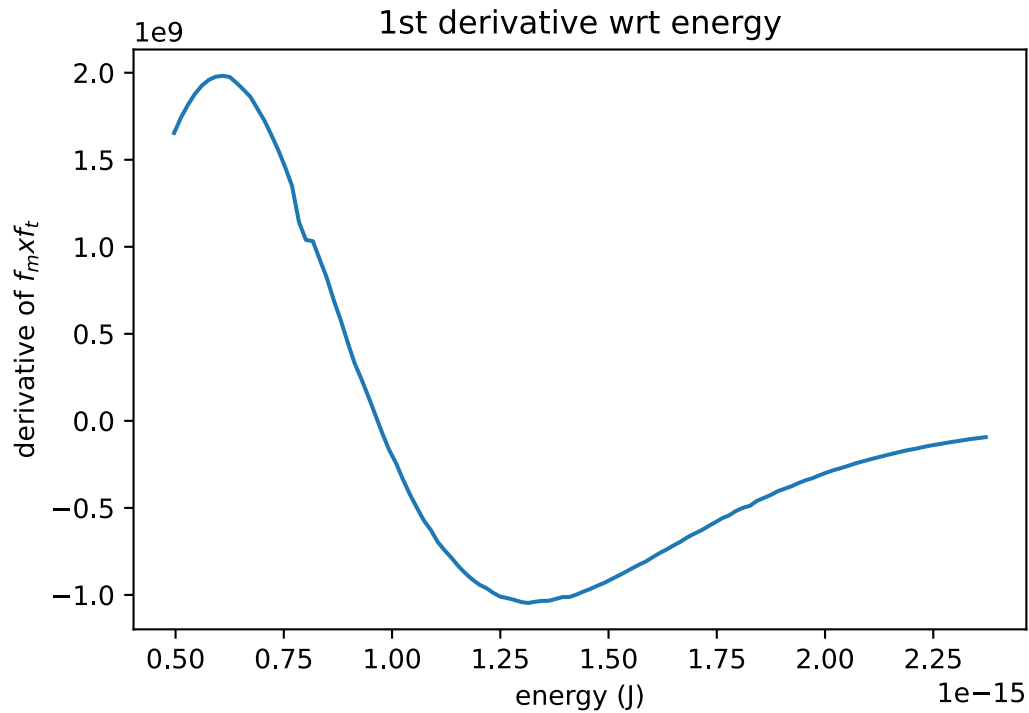
Temp estimated: 1.487e+07 K  
error in temp estimated: 6.529e+04 K

```
[105]: b = a2**(-0.5)
err_b = (-0.5)*(a2**(-(3/2)))*err_a2
print('b estimated: {:.3e} K'.format(b))
print('error in b estimated: {:.3e} K'.format(err_b))
```

b estimated: 2.894e-07 K  
error in b estimated: -1.993e-09 K

## 0.4 Part (III)

```
[80]: prod = np.asarray([f1*f2 for f1,f2 in zip(fm, ft)])
d_prod = []
for i in range(1,len(en)-1):
    del_en = (en[i+1]-en[i-1])/2
    d = (prod[i+1]-prod[i-1])/(2*del_en)
    d_prod.append(d)
en_d = en[1:-1]
plt.plot(en_d, d_prod)
plt.xlabel('energy (J)')
plt.ylabel('derivative of $f_{mxf\_t}$')
plt.title('1st derivative wrt energy')
plt.show()
```



## 0.5 Part IV

```
[81]: d2_prod = []
      for i in range(1,len(en)-1):
          num = prod[i+1]-2*prod[i]+prod[i-1]
          del_en = (en[i+1]-en[i-1])/2
          denom = (del_en)**2
          d2 = num/denom
          d2_prod.append(d2)
```

```
[87]: def find_zero(y,x):
      zeros = []
      zero_index = []
      for i in range(len(x)-1):
          sign = y[i+1]*y[i]
          if(sign<0):
              zeros.append(x[i])
              zero_index.append(i)
      return zeros , zero_index
en_zero , index_zero = (find_zero(d_prod , en_d))
print('Zero of derivative occurs at:{} J'.format(en_zero))
print('value of 2nd derivative at this point: {:.2e}'.
      ↪format(d2_prod[index_zero[0]]))
```

Zero of derivative occurs at:[9.61308e-16] J  
value of 2nd derivative at this point: -7.09e+24

## 0.6 Part V

```
[76]: fm_th = np.exp(-(1/(kb*T))*en)
      ft_th = np.exp(-b/(en**0.5))
      def calc_fm_th(en):
          fm_th = np.exp(-(1/(kb*T))*en)
          return fm_tm

      def calc_prod_th(en):
          val = np.exp(-en/(kb*T)-(b/(en**0.5)))
          return val
```

```
[95]: integ = []
      for i in range(len(en)-1):
          del_en = en[i+1]-en[i]
          val = (prod[i+1]+prod[i])*(del_en/2)
          integ.append(val)
      prod_integ = sum(integ)
      print('area under curve for given data (product of ft*fm): {:.3e}'.
            ↪format(prod_integ))
```

area under curve for given data (product of ft\*fm): 7.471e-22

using simpson for calculating theoratical integral energy range selected :energy range given in the data

```
[107]: prod_integ_th = integral(calc_prod_th , en[0],en[-1], len(en))
      print('area under curve for theoratical estimated parameters: {:.3e}'.
            ↪format(prod_integ_th))
```

area under curve for theoratical estimated parameters: 7.452e-22