ETACHA Reader

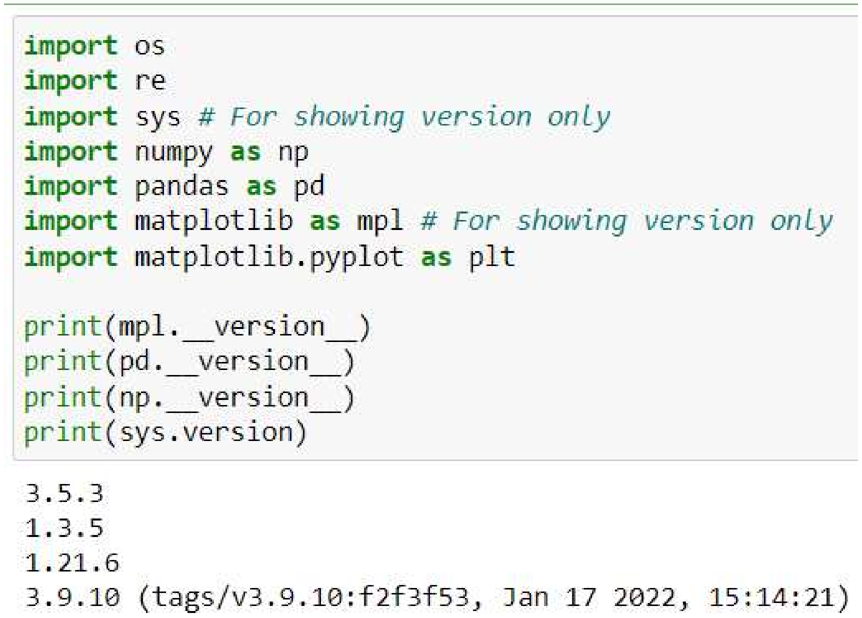
Kenny Haak

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics and used resources of the Facility for Rare Isotope Beams (FRIB) Operations, which is a DOE Office of Science User Facility under Award Number DE-SC0023633, and by the US National Science Foundation under Grants No. PHY-20-12040 and 23-10078 “Windows on the Universe: Open Quantum Systems in Atomic Nuclei at FRIB”.

Outline

Initialize

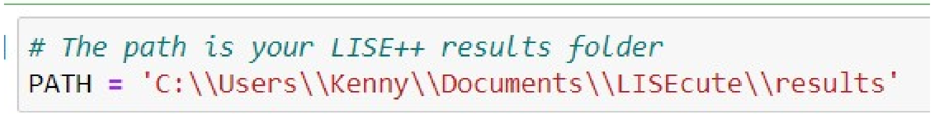
- Ensure you have these versions of packages and python



```
import os
import re
import sys # For showing version only
import numpy as np
import pandas as pd
import matplotlib as mpl # For showing version only
import matplotlib.pyplot as plt

print(mpl.__version__)
print(pd.__version__)
print(np.__version__)
print(sys.version)
```

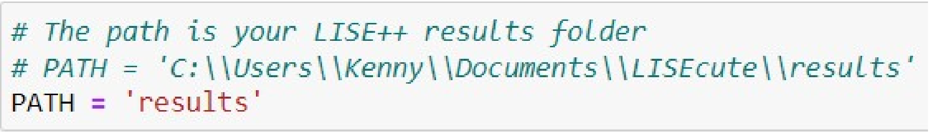
```
3.5.3
1.3.5
1.21.6
3.9.10 (tags/v3.9.10:f2f3f53, Jan 17 2022, 15:14:21)
```

Set the global PATH variable to where your LISEcute results folder is located



```
# The path is your LISE++ results folder
PATH = 'C:\\Users\\Kenny\\Documents\\LISEcute\\results'
```

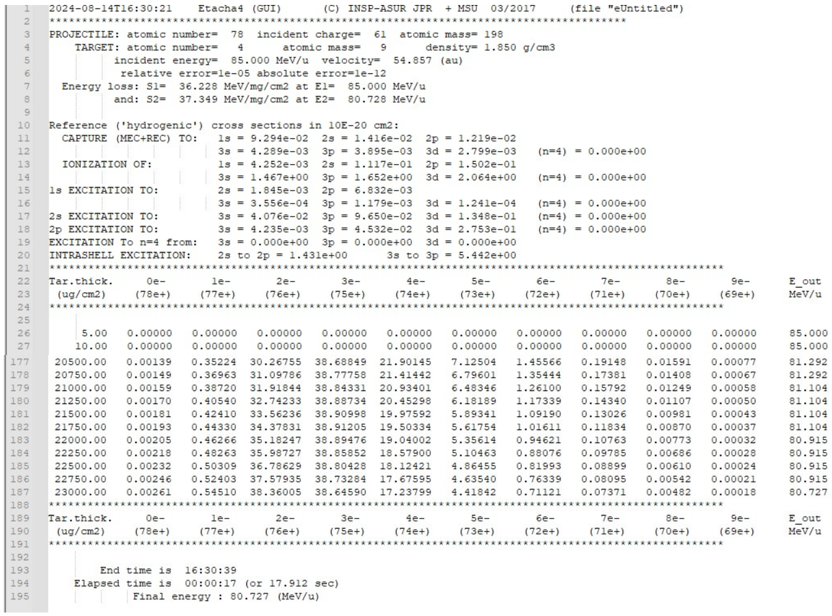
But in order for you to inspect my files I have copied this file into the home directory of this notebook



```
# The path is your LISE++ results folder
# PATH = 'C:\\Users\\Kenny\\Documents\\LISEcute\\results'
PATH = 'results'
```

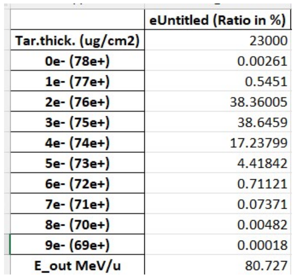
Shell Files

- ETACHA output files are divided into sets of 10 electron shells
- We usually are concerned with ions near fully stripped
- Therefore, this code has shell ‘0009’ as an example, which contains orbitals 1s through 2p
- This will report results for all 0009 ETACHA files in your LISEcute/results directory



```
2024-08-14T16:30:21    Etacha4 (GUI)      (C) INSP-ASUR JPR  + MSU  03/2017     (file "eUntitled")
*****************************************************************************************
PROJECTILE: atomic number=  78  incident charge=  61  atomic mass= 198
    TARGET: atomic number=   4      atomic mass=   9      density= 1.850 g/cm3
          incident energy=  85.000 MeV/u  velocity=  54.857 (au)
           relative error=1e-05 absolute error=1e-12
  Energy loss: S1=  36.228 MeV/mg/cm2 at E1=  85.000 MeV/u
          and: S2=  37.349 MeV/mg/cm2 at E2=  80.728 MeV/u

Reference ('hydrogenic') cross sections in 10E-20 cm2:
  CAPTURE (MEC+REC) TO:   1s = 9.294e-02  2s = 1.416e-02  2p = 1.219e-02
                          3s = 4.289e-03  3p = 3.895e-03  3d = 2.799e-03   (n=4) = 0.000e+00
  IONIZATION OF:          1s = 4.252e-03  2s = 1.117e-01  2p = 1.502e-01
                          3s = 1.467e+00  3p = 1.652e+00  3d = 2.064e+00   (n=4) = 0.000e+00
1s EXCITATION TO:         2s = 1.845e-03  2p = 6.832e-03
                          3s = 3.556e-04  3p = 1.179e-03  3d = 1.241e-04   (n=4) = 0.000e+00
2s EXCITATION TO:         3s = 4.076e-02  3p = 9.650e-02  3d = 1.348e-01   (n=4) = 0.000e+00
2p EXCITATION TO:         3s = 4.235e-03  3p = 4.532e-02  3d = 2.753e-01   (n=4) = 0.000e+00
EXCITATION To n=4 from:   3s = 0.000e+00  3p = 0.000e+00  3d = 0.000e+00
INTRASHELL EXCITATION:    2s to 2p = 1.431e+00      3s to 3p = 5.442e+00
********************************************************************************************************
Tar.thick.     0e-       1e-       2e-       3e-       4e-       5e-       6e-       7e-       8e-       9e-       E_out
 (ug/cm2)    (78e+)    (77e+)    (76e+)    (75e+)    (74e+)    (73e+)    (72e+)    (71e+)    (70e+)    (69e+)      MeV/u
********************************************************************************************************

     5.00   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000     85.000
    10.00   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000     85.000
 20500.00   0.00139   0.35224  30.26755  38.68849  21.90145   7.12504   1.45566   0.19148   0.01591   0.00077     81.292
 20750.00   0.00149   0.36963  31.09786  38.77758  21.41442   6.79601   1.35444   0.17381   0.01408   0.00067     81.292
 21000.00   0.00159   0.38720  31.91844  38.84331  20.93401   6.48346   1.26100   0.15792   0.01249   0.00058     81.104
 21250.00   0.00170   0.40540  32.74233  38.88734  20.45298   6.18189   1.17339   0.14340   0.01107   0.00050     81.104
 21500.00   0.00181   0.42410  33.56236  38.90998  19.97592   5.89341   1.09190   0.13026   0.00981   0.00043     81.104
 21750.00   0.00193   0.44330  34.37831  38.91205  19.50334   5.61754   1.01611   0.11834   0.00870   0.00037     81.104
 22000.00   0.00205   0.46266  35.18247  38.89476  19.04002   5.35614   0.94621   0.10763   0.00773   0.00032     80.915
 22250.00   0.00218   0.48263  35.98727  38.85852  18.57900   5.10463   0.88076   0.09785   0.00686   0.00028     80.915
 22500.00   0.00232   0.50309  36.78629  38.80428  18.12421   4.86455   0.81993   0.08899   0.00610   0.00024     80.915
 22750.00   0.00246   0.52403  37.57935  38.73284  17.67595   4.63540   0.76339   0.08095   0.00542   0.00021     80.915
 23000.00   0.00261   0.54510  38.36005  38.64590  17.23799   4.41842   0.71121   0.07371   0.00482   0.00018     80.727
********************************************************************************************************
Tar.thick.     0e-       1e-       2e-       3e-       4e-       5e-       6e-       7e-       8e-       9e-       E_out
 (ug/cm2)    (78e+)    (77e+)    (76e+)    (75e+)    (74e+)    (73e+)    (72e+)    (71e+)    (70e+)    (69e+)      MeV/u
********************************************************************************************************

        End time is  16:30:39
    Elapsed time is  00:00:17 (or 17.912 sec)
             Final energy : 80.727 (MeV/u)
```

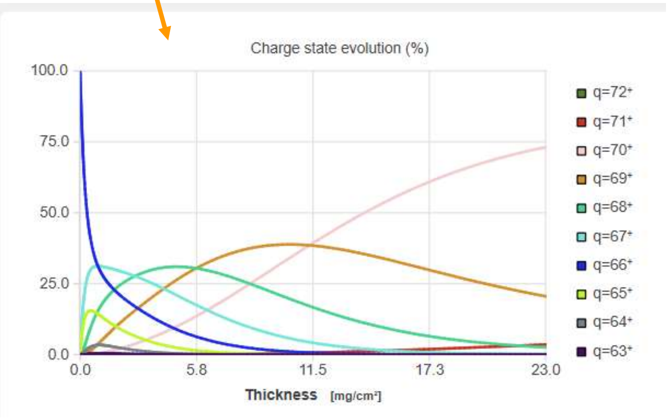
TXT to EXCEL

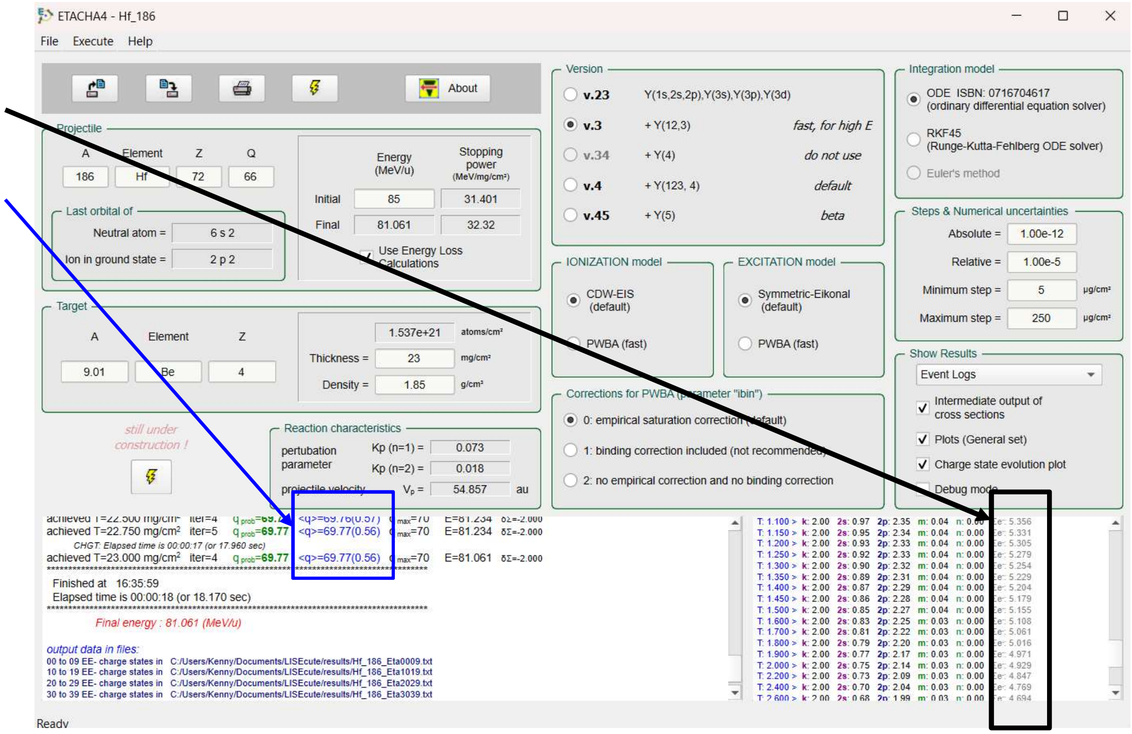


	eUntitled (Ratio in %)
Tar.thick. (ug/cm2)	23000
0e- (78e+)	0.00261
1e- (77e+)	0.5451
2e- (76e+)	38.36005
3e- (75e+)	38.6459
4e- (74e+)	17.23799
5e- (73e+)	4.41842
6e- (72e+)	0.71121
7e- (71e+)	0.07371
8e- (70e+)	0.00482
9e- (69e+)	0.00018
E_out MeV/u	80.727

Equilibrium Thickness

- There are three metrics that can help you numerically define the equilibrium thickness
  - White Chi
  - Blue Chi
  - Charge State Evolution Curve Slopes





Projectile

A	Element	Z	Q
186	Hf	72	66

Last orbital of
Neutral atom = 6 s 2
Ion in ground state = 2 p 2

	Energy (MeV/u)	Stopping power (MeV/mg/cm²)
Initial	85	31.401
Final	81.061	32.32

☑ Use Energy Loss Calculations

Target

A	Element	Z
9.01	Be	4

1.537e+21 atoms/cm²
Thickness = 23 mg/cm²
Density = 1.85 g/cm³

still under construction !

Reaction characteristics
pertubation parameter Kp (n=1) = 0.073
Kp (n=2) = 0.018
projectile velocity V_p = 54.857 au

Version
○ **v.23** Y(1s,2s,2p),Y(3s),Y(3p),Y(3d)
● **v.3** + Y(12,3) *fast, for high E*
○ **v.34** + Y(4) *do not use*
○ **v.4** + Y(123, 4) *default*
○ **v.45** + Y(5) *beta*

IONIZATION model
● CDW-EIS (default)
○ PWBA (fast)

EXCITATION model
● Symmetric-Eikonal (default)
○ PWBA (fast)

Corrections for PWBA (parameter "ibin")
● 0: empirical saturation correction (default)
○ 1: binding correction included (not recommended)
○ 2: no empirical correction and no binding correction

Integration model
● ODE ISBN: 0716704617 (ordinary differential equation solver)
○ RKF45 (Runge-Kutta-Fehlberg ODE solver)
○ Euler's method

Steps & Numerical uncertainties
Absolute = 1.00e-12
Relative = 1.00e-5
Minimum step = 5 μg/cm²
Maximum step = 250 μg/cm²

Show Results
Event Logs
☑ Intermediate output of cross sections
☑ Plots (General set)
☑ Charge state evolution plot
☐ Debug mode

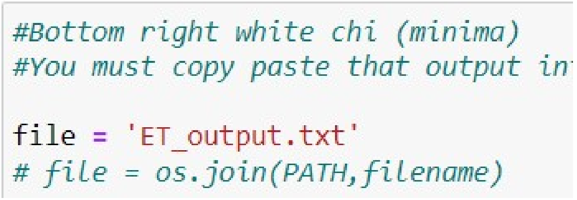
```
achieved T=22.500 mg/cm²  iter=4   q prob=69.7   <q>=69.76(0.57)  q max=70   E=81.234  δΣ=-2.000
achieved T=22.750 mg/cm²  iter=5   q prob=69.77  <q>=69.77(0.56)  q max=70   E=81.234  δΣ=-2.000
      CHGT: Elapsed time is 00:00:17 (or 17.960 sec)
achieved T=23.000 mg/cm²  iter=4   q prob=69.77  <q>=69.77(0.56)  q max=70   E=81.061  δΣ=-2.000
********************************************************************************
 Finished at   16:35:59
 Elapsed time is 00:00:18 (or 18.170 sec)
********************************************************************************
          Final energy : 81.061 (MeV/u)

output data in files:
00 to 09 EE- charge states in   C:/Users/Kenny/Documents/LISEcute/results/Hf_186_Eta0009.txt
10 to 19 EE- charge states in   C:/Users/Kenny/Documents/LISEcute/results/Hf_186_Eta1019.txt
20 to 29 EE- charge states in   C:/Users/Kenny/Documents/LISEcute/results/Hf_186_Eta2029.txt
30 to 39 EE- charge states in   C:/Users/Kenny/Documents/LISEcute/results/Hf_186_Eta3039.txt
```

```
T: 1.100 >  k: 2.00  2s: 0.97  2p: 2.35  m: 0.04  n: 0.00  Σe: 5.356
T: 1.150 >  k: 2.00  2s: 0.95  2p: 2.34  m: 0.04  n: 0.00  Σe: 5.331
T: 1.200 >  k: 2.00  2s: 0.93  2p: 2.33  m: 0.04  n: 0.00  Σe: 5.305
T: 1.250 >  k: 2.00  2s: 0.92  2p: 2.33  m: 0.04  n: 0.00  Σe: 5.279
T: 1.300 >  k: 2.00  2s: 0.90  2p: 2.32  m: 0.04  n: 0.00  Σe: 5.254
T: 1.350 >  k: 2.00  2s: 0.89  2p: 2.31  m: 0.04  n: 0.00  Σe: 5.229
T: 1.400 >  k: 2.00  2s: 0.87  2p: 2.29  m: 0.04  n: 0.00  Σe: 5.204
T: 1.450 >  k: 2.00  2s: 0.86  2p: 2.28  m: 0.04  n: 0.00  Σe: 5.179
T: 1.500 >  k: 2.00  2s: 0.85  2p: 2.27  m: 0.04  n: 0.00  Σe: 5.155
T: 1.600 >  k: 2.00  2s: 0.83  2p: 2.25  m: 0.03  n: 0.00  Σe: 5.108
T: 1.700 >  k: 2.00  2s: 0.81  2p: 2.22  m: 0.03  n: 0.00  Σe: 5.061
T: 1.800 >  k: 2.00  2s: 0.79  2p: 2.20  m: 0.03  n: 0.00  Σe: 5.016
T: 1.900 >  k: 2.00  2s: 0.77  2p: 2.17  m: 0.03  n: 0.00  Σe: 4.971
T: 2.000 >  k: 2.00  2s: 0.75  2p: 2.14  m: 0.03  n: 0.00  Σe: 4.929
T: 2.200 >  k: 2.00  2s: 0.73  2p: 2.09  m: 0.03  n: 0.00  Σe: 4.847
T: 2.400 >  k: 2.00  2s: 0.70  2p: 2.04  m: 0.03  n: 0.00  Σe: 4.769
T: 2.600 >  k: 2.00  2s: 0.68  2p: 1.99  m: 0.03  n: 0.00  Σe: 4.694
```

Ready

White Chi Method

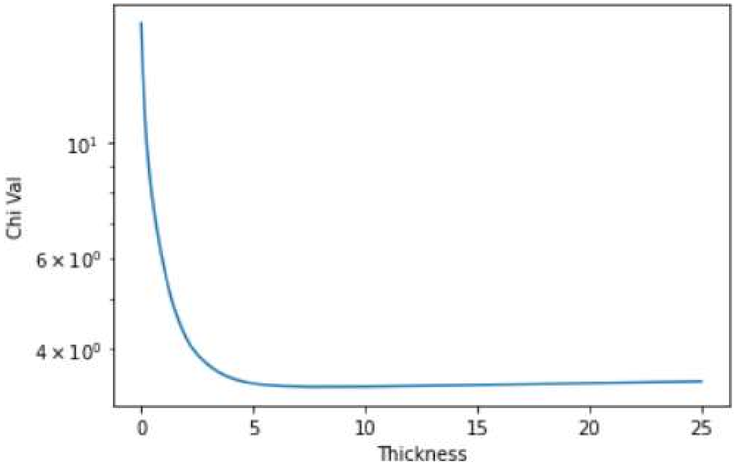
- To use the white chi method you actually have to copy and paste the text from the diagnostic output in ETACHA and store it in a file called ‘ET_output.txt’ in the same directory as the Jupyter Notebook to extract the information
- The smallest white chi usually corresponds to the thickness with the least change in charge state with increasing thickness (equilibrium)
- If confused, consult Oleg
- All data used here is
    - 85 MeV/u $^{198}Pt^{61+}$
    - Ni 25 mg/cm^2



```
#Bottom right white chi (minima)
#You must copy paste that output in

file = 'ET_output.txt'
# file = os.join(PATH,filename)
```

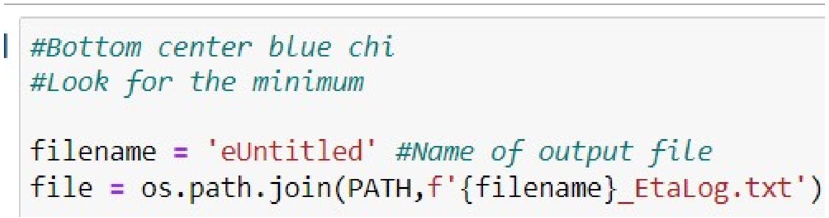
! Equilibrium

```
Minimum sigma: 3.376, Min Thick: 8.0, Max Thick: 8.5, Avg Thick: 8.25
```



Blue Chi Method

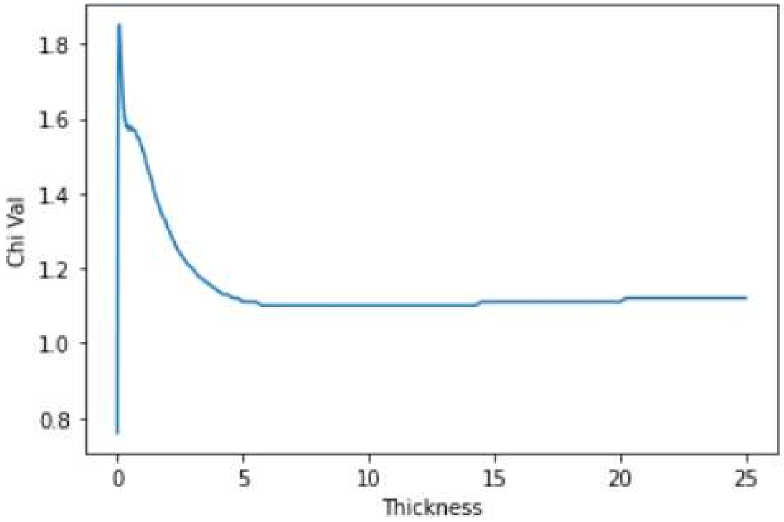
- The blue chi is the width of the charge state expectation value <q>
- This result is provided in the EtaLog.txt output file of ETACHA for LISE
- This code block will extract that value and make a plot so you can inspect for the minima
- It also prints the minima



```
#Bottom center blue chi
#Look for the minimum

filename = 'eUntitled' #Name of output file
file = os.path.join(PATH,f'{filename}_EtaLog.txt')
```

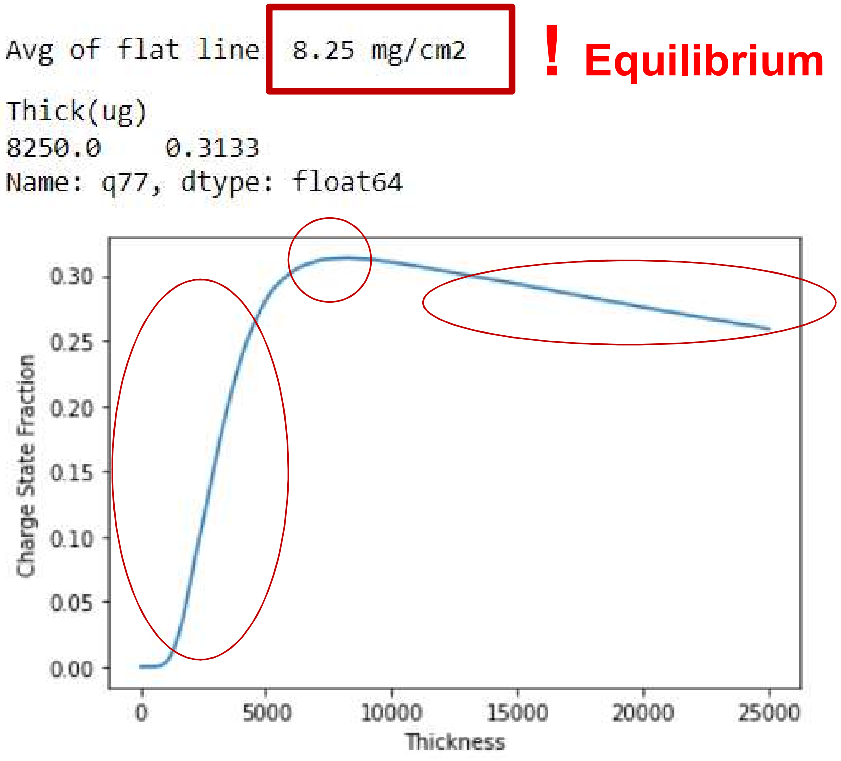
! Equilibrium

```
10.0 mg/cm^2
```



Charge State Evolution Curve Slope

- Here we simply inspect the charge state fractions and their evolution curves
- You need to set the specific charge state you are inspecting, I recommend He-like or something close to fully stripped
- When the slope approaches zero, this means the electron loss and capture cross sections for that orbital has balanced each other out
- This code is designed to handle fine grain resolution charge state evolution curves, and will take the center of the “highest flat zone”



```
Avg of flat line 8.25 mg/cm2
Thick(ug)
8250.0    0.3133
Name: q77, dtype: float64
```

! Equilibrium

Afterword – Highest Flat Zone

- Why the "Highest Flat Zone" for the charge state evolution curve?
- In nuclear experiments, a heavy ion beam with high Z will enter the target most likely not at its "most-stripped" or at equilibrium
- Therefore these lower lying orbitals like the 1s get populated quickly (sharp rise)
- After this process slows down and equilibrium is approached, the beam is always continuously losing energy
- The stripping power of the material is dependent on beam energy, so the lower lying orbital begins to slowly deplete (slow fall)
- That's why we want the highest flattest point, it is the point where you have reach optimal stripping from the material and are beginning to fall backwards to a lower energy equilibrium

Afterword – Comparing Methods

- You can see all methods don’t necessarily agree. The first real minima of blue chi is much further than the white chi and evolution curve methods
- The white chi and evolution curve methods actually agree in this case, we could conclude that this concurrence gives us confidence in the value of 8.25 mg/cm^2 eq. thickness for Ni target
- It makes you wonder… That 17 mg/cm^2 target for the 198Pt exp at NSCL was PRETTY EQUILIBRATED huh?
- THAT is why we didn’t use the MC NeR method… You can check my thesis if you are curious about what all this nonsense is about