PY 506 HW04

MB

25 September 2023

For this homework we start from the Time Independent Schrodinger Equation (TISE), with the radial part of the central potential given by

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\frac{\hbar^2}{2mr^2}l(l+1)+V(r)\right)u(r)=Eu(r) \tag{1}$$

Where E is the energy eigenvalue, l is the angular momentum quantum number, m is mass, and $u(r)$ is the radial wavefunction. We now define a realistic nuclear potential for a proton moving in the averaged influence of the rest of a nucleus; this potential is the Woods-Saxon potential given by

$$V_{ws}=-\frac{A_{ws}}{1+exp\left(\frac{r-R}{a}\right)} \tag{2}$$

Where A_{ws} is a constant (50 MeV), R is the nuclear radius (6 fm), and a is the skin thickness (0.6 fm). Furthermore, there exists a large part of the nuclear force that depends on whether the spin of a particle is aligned with the orbital angular momentum:

$$V_{so}(r)=-\frac{A_{so}}{2}\frac{exp\left(\frac{r-R}{a}\right)}{\left(1+exp\left(\frac{r-R}{a}\right)\right)^2}[j(j+1)-l(l+1)-s(s+1)] \tag{3}$$

For a single nucleon, $s=1/2$ and $|l-s|\leq j\leq l+s$. Thus the total potential energy in the Hamiltonian is $V(r)=V_{ws}+V_{so}$.

Given the potential described above, the problem is to find the lowest 10 eigenvalues of the Hamiltonian for $l\in 0,1,2$ assuming $A_{so}=0$. Further, for A_{so} in the range $0\leq A_{so}\leq A_{ws}/4$, we want to make a plot of how the eigenvalues evolve as a function of A_{so}.

As a starting point, we make sure our maximum radius is well outside the nuclear radius. That way we have two boundary conditions: $u(r=0)=0$ and $u(r=(\text{few}\,R))=0$. Thus only the wavefunction in between is unknown.

Solution

The total potential $V(r)$ for the Hamiltonian is the sum of the Woods-Saxon potential, the angular momentum potential, and the spin-orbit potential:

$$V(r)=V_{ws}+V_{ang}+V_{so} \tag{4}$$

$$=-\frac{A_{ws}}{1+exp\left(\frac{r-R}{a}\right)}+\frac{l(l+1)}{r^2}-\frac{A_{s}o}{2}\frac{exp\left(\frac{r-R}{a}\right)}{\left(1+exp\left(\frac{r-R}{a}\right)\right)^2}[j(j+1)-l(l+1)-s(s+1)] \tag{5}$$

Where $A_{ws}=50$ MeV and for $l\in 0,1,2$ we assume $A_{so}=0$. From TISE, we discretize the radial wavefunction $u(r)$ by cutting the r axis into small chunks i. For each (radial) position r_i we can write a wavefunction as

$$\left(-\frac{\hbar^2}{2m}\frac{du_i^2}{dr_i^2}+\frac{\hbar^2}{2mr_i^2}l(l+1)+V_i\right)u_i=Eu_i \tag{6}$$

In the method of *finite differences*, we let

$$\frac{d^2u_i}{dr_i^2} \approx \frac{1}{\Delta}(u_{i+1} - 2u_i + u_{i-1}) \tag{7}$$

Where Δ is the step size between r_i and r_{i+1}. Altogether, the fully discretized Schrodinger equation is

$$-\frac{\hbar^2}{2m\Delta}(u_{i+1} - 2u_i + u_{i-1}) + V_i u_i = Eu_i \tag{8}$$

And the full discretized potential V_i is

$$V_i = -\frac{\hbar^2}{2m}\frac{A_{ws}}{1 + exp\left(\frac{r_i - R}{a}\right)} + \frac{l(l+1)}{r_i^2} - \frac{A_{so}}{2}\frac{exp\left(\frac{r_i - R}{a}\right)}{\left(1 + exp\left(\frac{r_i - R}{a}\right)\right)^2}[j(j+1) - l(l+1) - s(s+1)] \tag{9}$$

For the code we are solving this between $r = a$ and $r = b$ ($r \in [a, b]$), and we create $N + 1$ discrete points s.t. $r_0 = a$ and $r_N = b$. For our solution, we chose $N = 100$ for raising the dimension of all the matrices in TISE. For all matrices with an $\hbar^2/2m$ factor, we chose natural units so that $\hbar = m = 1$. The kinetic energy matrix is shown below:

```
[55] ## The diagonal and off-diagonal terms
     diag = -2 * np.ones(N)
     offdiag = 1 * np.ones(N)

     T_matrix = sparse.diags([diag, offdiag, offdiag], (0,-1,1))
     print(T_matrix.todense())
```

```
[[-2.  1.  0. ...  0.  0.  0.]
 [ 1. -2.  1. ...  0.  0.  0.]
 [ 0.  1. -2. ...  0.  0.  0.]
 ...
 [ 0.  0.  0. ... -2.  1.  0.]
 [ 0.  0.  0. ...  1. -2.  1.]
 [ 0.  0.  0. ...  0.  1. -2.]]
```

Figure 1: kinetic energy matrix

Next we constructed the potential energy matrices out of the Woods-Saxon, angular-momentum, and spin-orbit potentials. Upon varying the orbital angular momentum, we see that the total potential becomes slightly less negative for increasing values of l. To show this, attached below depict 3 images of the change in potential values for $l \in 0, 1, 2$:

```
[[-9.65310905e-26  0.00000000e+00  0.00000000e+00 ...  0.00000000e+00
   0.00000000e+00  0.00000000e+00]
 [ 0.00000000e+00 -9.08544774e-26  0.00000000e+00 ...  0.00000000e+00
   0.00000000e+00  0.00000000e+00]
 [ 0.00000000e+00  0.00000000e+00 -8.55116835e-26 ...  0.00000000e+00
   0.00000000e+00  0.00000000e+00]
 ...
 [ 0.00000000e+00  0.00000000e+00  0.00000000e+00 ... -2.70110879e-28
   0.00000000e+00  0.00000000e+00]
 [ 0.00000000e+00  0.00000000e+00  0.00000000e+00 ...  0.00000000e+00
  -2.54226722e-28  0.00000000e+00]
 [ 0.00000000e+00  0.00000000e+00  0.00000000e+00 ...  0.00000000e+00
   0.00000000e+00 -2.39276651e-28]]
```

Figure 2: V matrix for $l = 0$

```
[[0.22222222 0.         0.         ... 0.         0.         0.        ]
 [0.         0.2314805  0.         ... 0.         0.         0.        ]
 [0.         0.         0.24132964 ... 0.         0.         0.        ]
 ...
 [0.         0.         0.         ... 0.24132964 0.         0.        ]
 [0.         0.         0.         ... 0.         0.2314805  0.        ]
 [0.         0.         0.         ... 0.         0.         0.22222222]]
```

Figure 3: V matrix for $l = 1$

```
[[0.66666667 0.         0.         ... 0.         0.         0.        ]
 [0.         0.69444149 0.         ... 0.         0.         0.        ]
 [0.         0.         0.72398892 ... 0.         0.         0.        ]
 ...
 [0.         0.         0.         ... 0.72398892 0.         0.        ]
 [0.         0.         0.         ... 0.         0.69444149 0.        ]
 [0.         0.         0.         ... 0.         0.         0.66666667]]
```

Figure 4: V matrix for $l = 2$

In writing the Hamiltonian matrix, we can apply the boundary conditions by setting the first element to 0 for $u(r = 0) = 0$ and the last element to 0 for $u(r = few(R)) = 0$. The Hamiltonian matrices for each l value (after the applied BCs) is provided below:

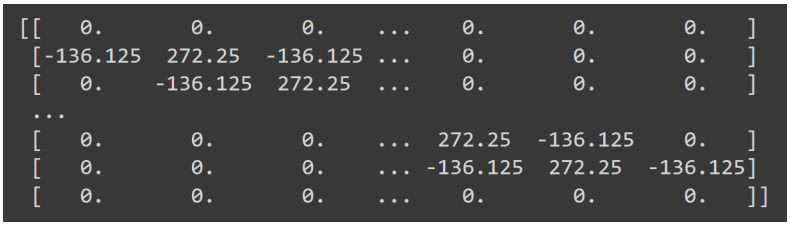

Figure 5: H matrix for $l = 0$

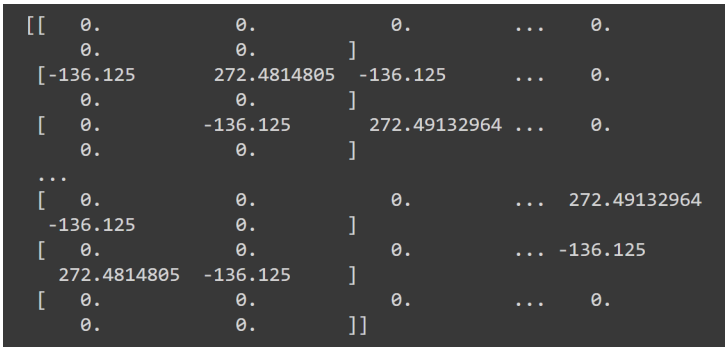

Figure 6: H matrix for $l = 1$

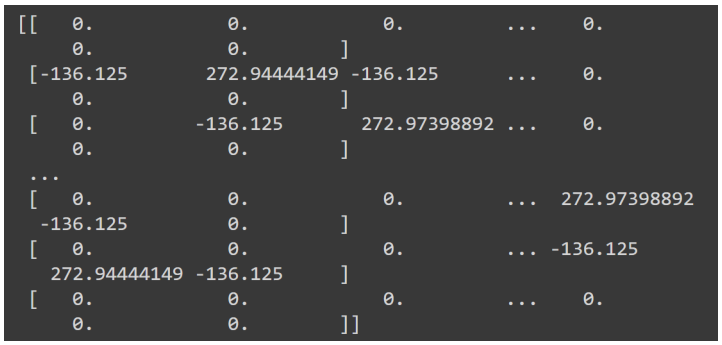

Figure 7: H matrix for $l = 2$

As expected, the Hamiltonian matrix increases slightly for small additions in l.

After solving the eigenvalue problem using numpy's *argsort*, we get a series of different eigenvalues and energies upon varying l.

```
l = 0:

Eigenvalues are:  [544.36293366+0.j 543.95187267+0.j 543.26723092+0.j 542.30969779+0.j
 541.08023744+0.j 539.58008783+0.j 537.81075948+0.j 535.77403396+0.j
 533.47196207+0.j 530.9068618 +0.j]

Energies are:  [1.         1.00483154 1.00916766 1.01300397 1.01633662 1.01916226
 1.02147803 1.02328161 1.02457119 1.02534545]

l = 1:

Eigenvalues are:  [2595.31483412+0.j 2324.41550281+0.j  613.73557012+0.j  612.98721413+0.j
  547.45149193+0.j  547.42377088+0.j  544.10086571+0.j  544.10616399+0.j
  541.52092018+0.j  541.51138584+0.j]

Energies are:  [1.         1.00001761 1.00478195 1.00479173 1.0109183  1.01096949
 1.13199321 1.13337519 4.29245915 4.7927244 ]

l = 2:

Eigenvalues are:  [6945.49224788+0.j 6673.39185752+0.j 1034.39390233+0.j 1034.53304439+0.j
  628.53942554+0.j  628.53360437+0.j  558.91933427+0.j  558.91858947+0.j
  546.84972825+0.j  546.84960925+0.j]

Energies are: [ 1.          1.00000022  1.02207002  1.02207138  1.14937195  1.1493826
  1.89155096  1.8918054  12.20334027 12.70091837]
```

Figure 8: Eigenvalues and Energies for $l \in 0, 1, 2$

According to the above, the 10 lowest possible eigenvalues of the Hamiltonian for $l \in 0, 1, 2$ are

$$\text{eigenvalues} = \{530.9068618, 533.47196207, 535.77403396, 537.81075948, \tag{10}$$

$$539.58008783, 541.08023744, 544.10086571, 544.10616399, \tag{11}$$

$$541.51138584, 541.52092018\} \tag{12}$$

Where the first 6 eigenvalues come from $l = 0$ and the last 4 eigenvalues come from $l = 1$ (note that all 10 of the eigenvalues are real). It is likely that the eigenvalues appear at their magnitude due to choosing to utilize natural units early on in solving the eigenvalue problem.

The normalized radial wavefunctions (for a harmonic oscillator) using the finite difference method is plotted below for each value of l:

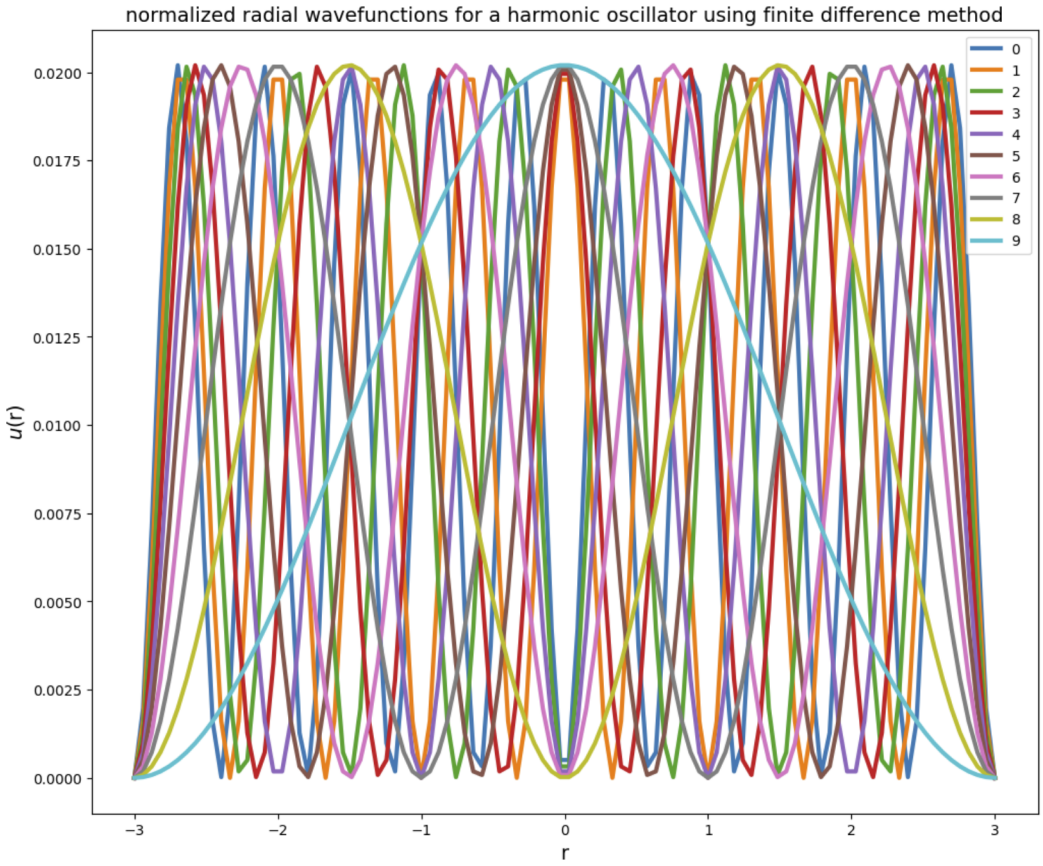

Figure 9: normalized radial wavefunctions for a harmonic oscillator using finite difference method ($l = 0$)

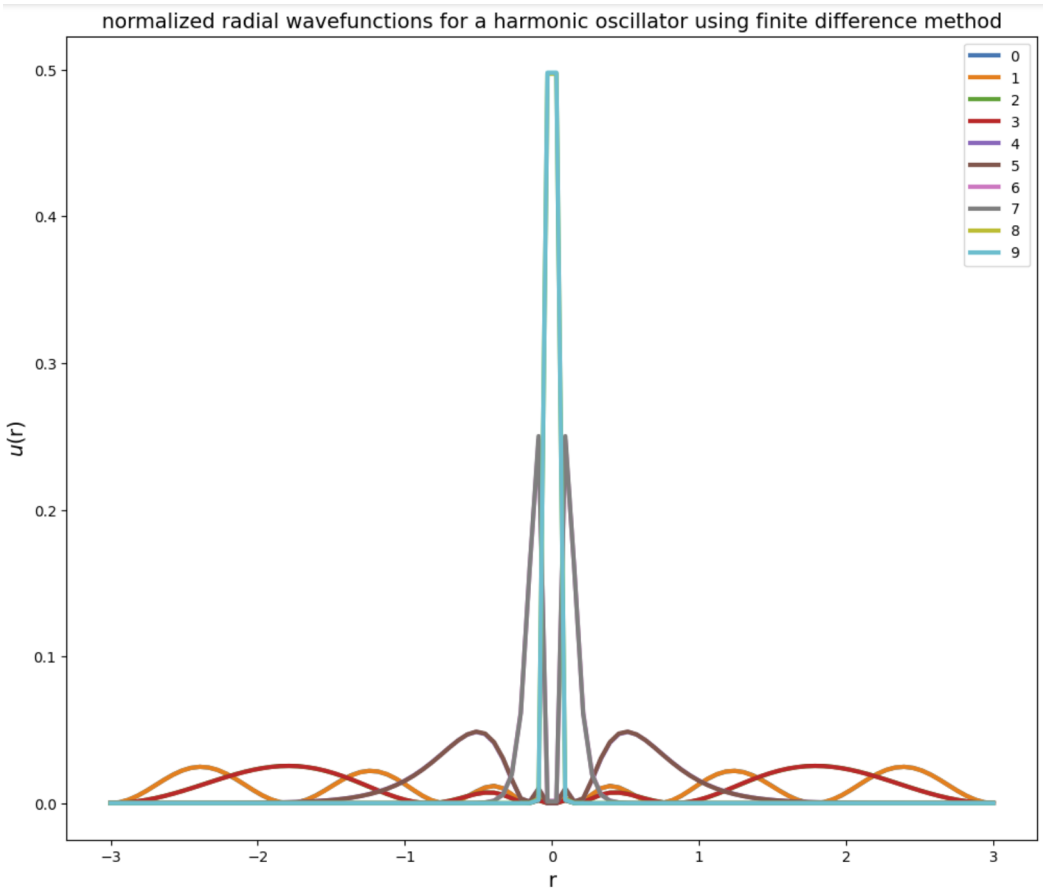

Figure 10: normalized radial wavefunctions for a harmonic oscillator using finite difference method ($l = 1$)

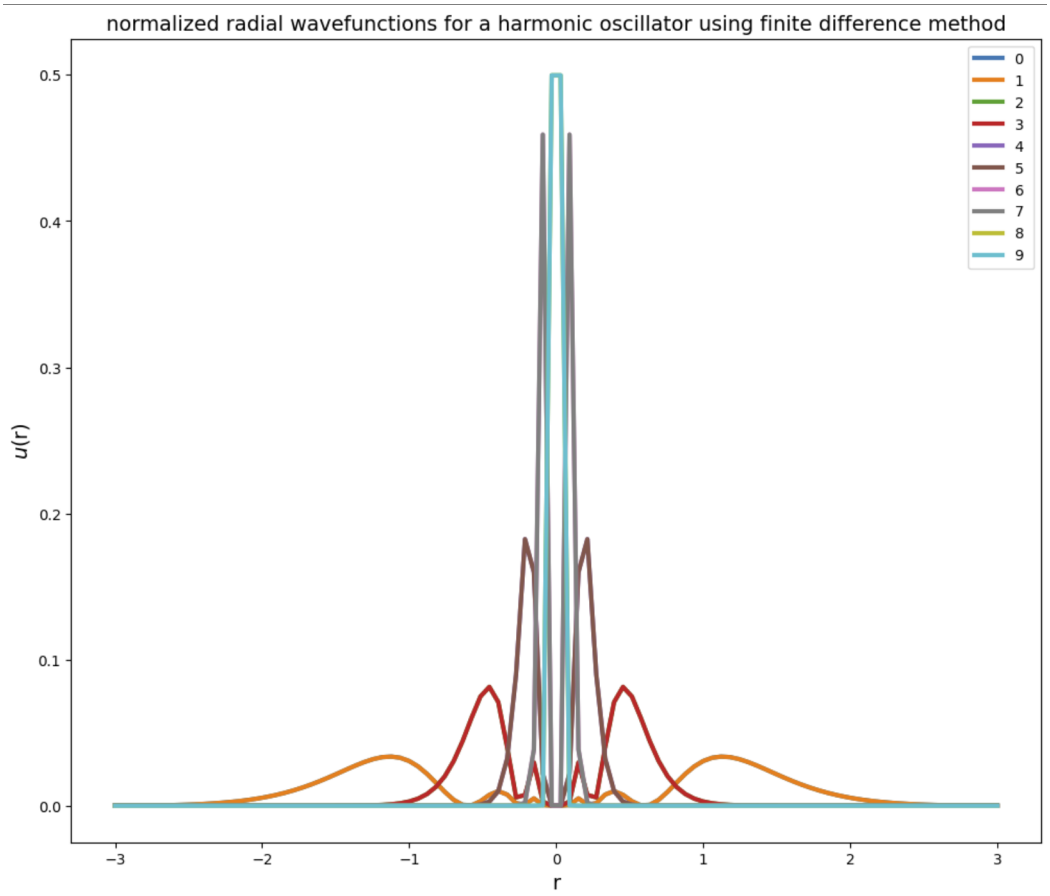

Figure 11: normalized radial wavefunctions for a harmonic oscillator using finite difference method ($l = 2$)

As we can see, the most noise occurs in $l = 0$ and becomes more well defined for higher values of l. Here depicts the eigenvalue evolutions over A_{so} for each l value, where we let $0 \leq A_{so} \leq A_{ws}/4$:

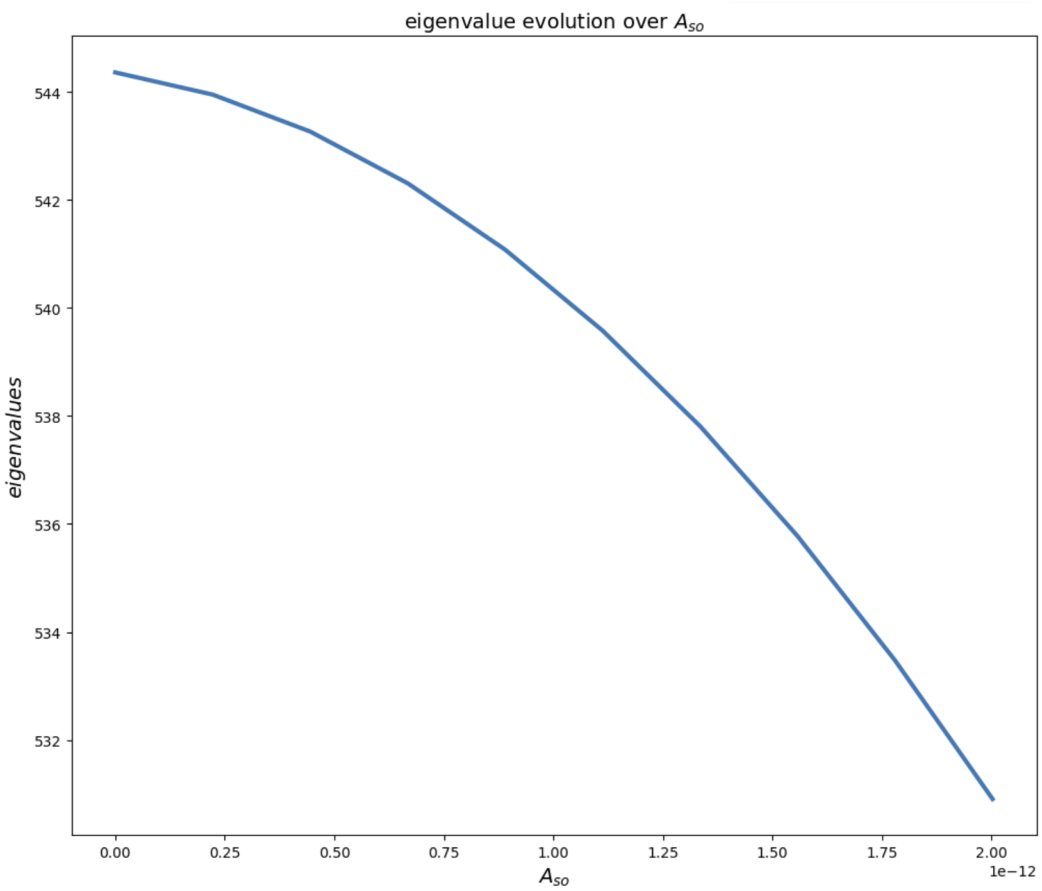

Figure 12: eigenvalue evolution over A_{so} ($l = 0$)

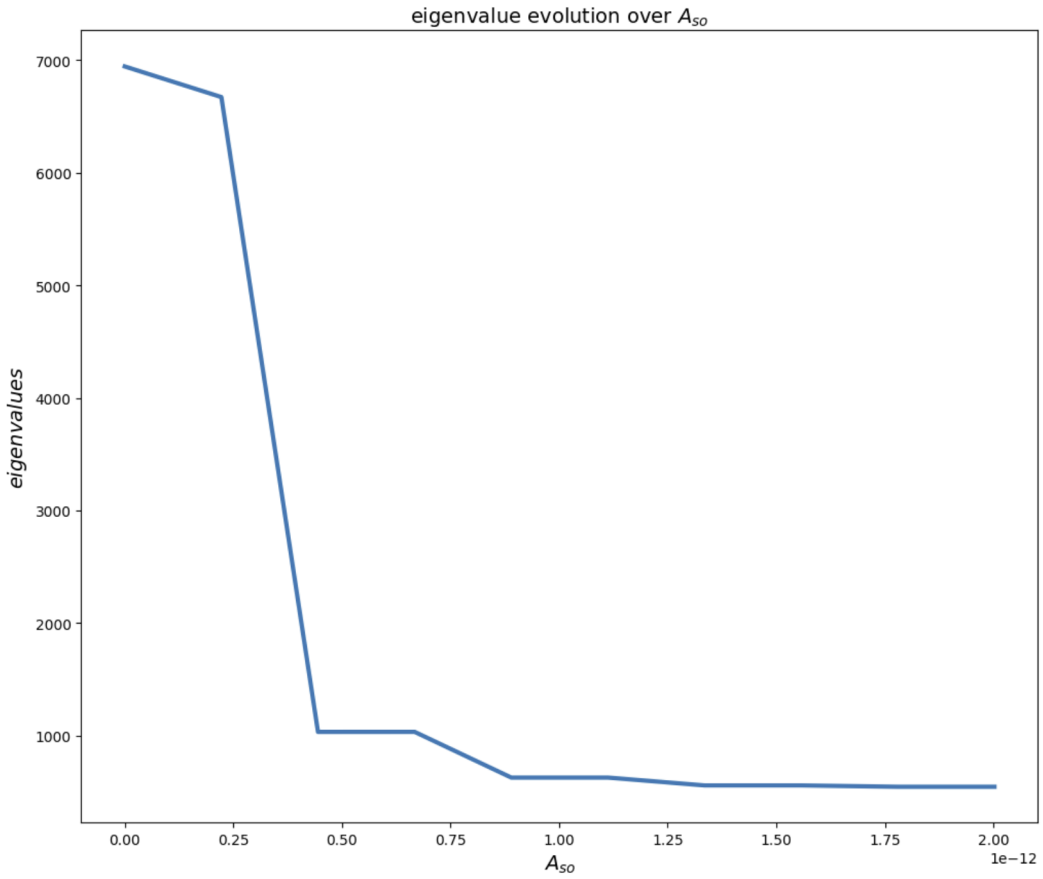

Figure 13: eigenvalue evolution over A_{so} ($l = 1$)

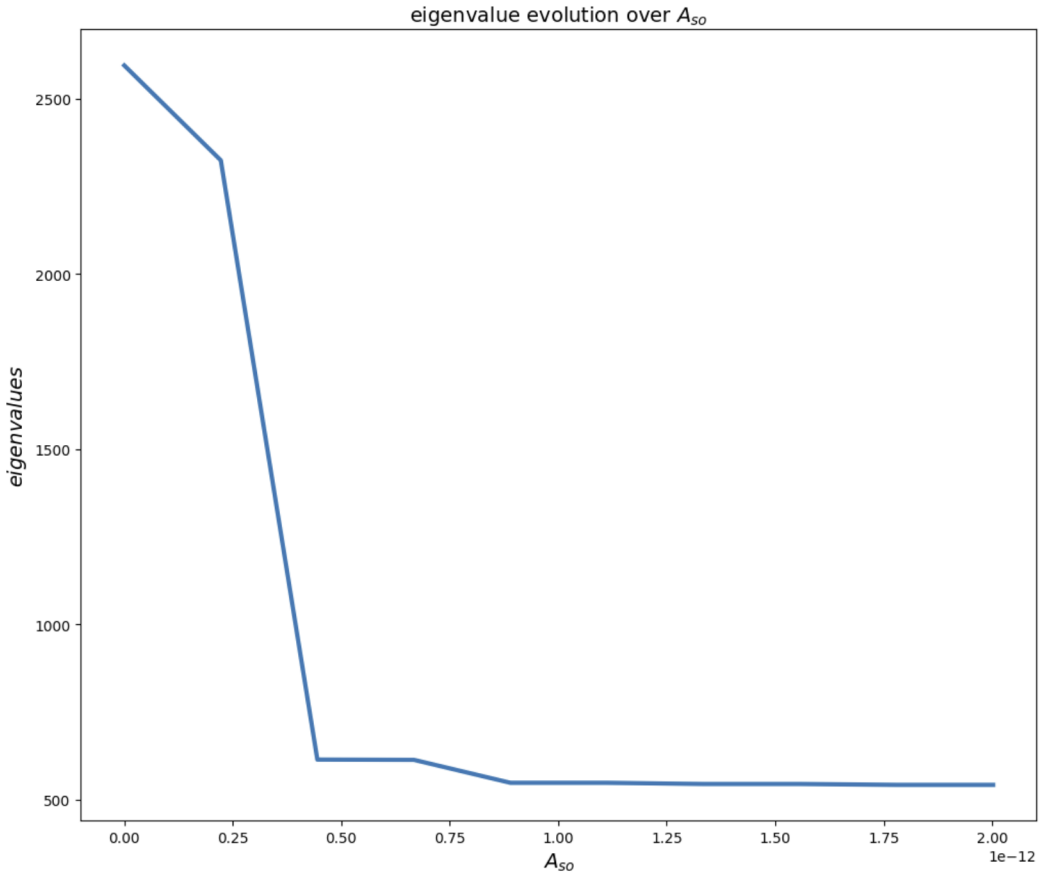

Figure 14: eigenvalue evolution over A_{so} ($l = 2$)

As we can see, the eigenvalues evolve the slowest for $l = 0$ and the fastest for $l = 2$.

Q: Should we expect graphs of these shapes?

A: Yes. For $l \in 0, 1, 2$ the first radial wavefunction graph displays noise because there is no involvement of an angular momentum potential. The 2 other radial wavefunction graphs are most close to one another because they both are shaped under a nonzero angular momentum potential. Clearly, the angular momentum potential plays a dominant role in the eigenvalue evolution for $0 \leq A_{so} \leq A_{ws}/4$ and the probability to locate nucleons in intervals of our choosing.