Stellar Spectra B: AST4310 Assignment 2

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Abstract. This assignment traces and reproduces the historical analytical procedures developed by pioneers in stellar spectroscopy. This exercises and IDL based analyses describe the processes of early spectral classification, the discovery of stellar atoms and ions according to thermodynamical physical theories-especially Saha-Boltzmann distributions, and spectral radiation analysis according to Planck's law and relevant corrective terms.

Stratification of the Solar Atmosphere
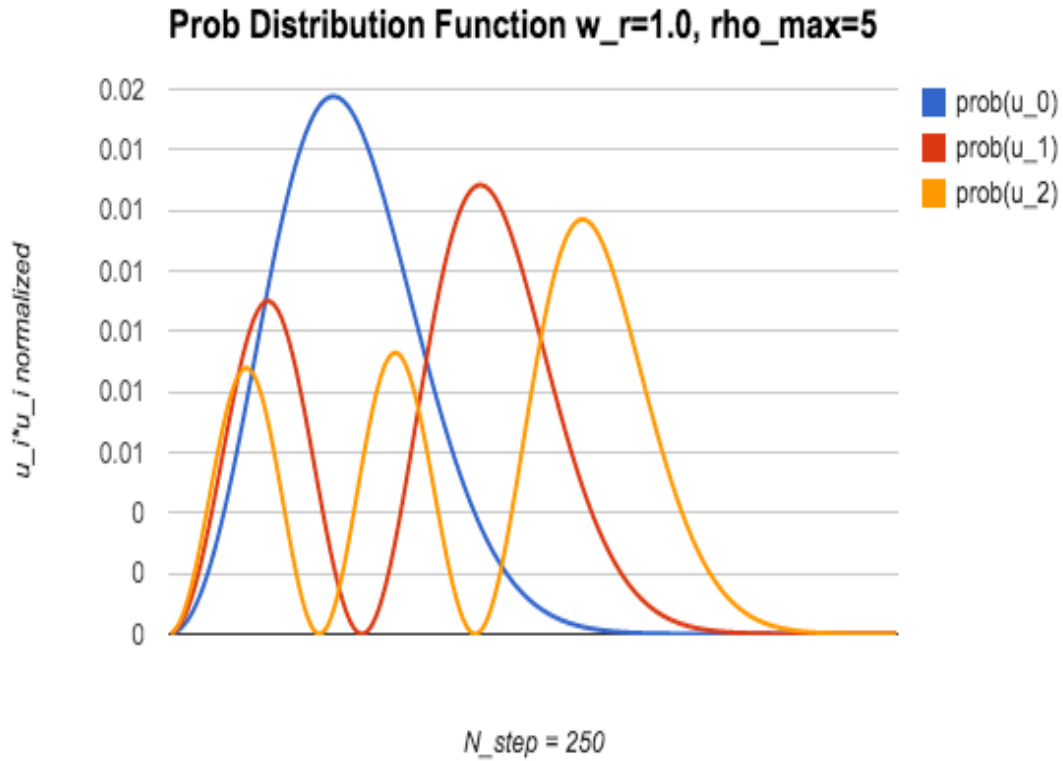
Part A test test test

Figure 1: Figure 5 (from project description) shows 3 Hydrogen I lines that are shown in the energy level diagram (figure 7) in project file.

Part B Comparing my eigenvalues with the Armadillo $eig_sym(A)$ solver yielded nearly identical results for larger values of N. The eigenvalues also correspond to the correct energy states

(3,7,11, etc) as given in the project description, so we can go on to the more complicated problem knowing the algorithm works. The numerical values are given in the table below. After running my algorithm, the parameters $N_s tep$ and ρ_{max} need to be decided upon before moving to the two electron wave equation. First, here's a table showing the number of steps given to the algorithm in order to determine four leading digits for the first 3 eigenvalues. For this case, our $\epsilon = 1e - 8$, which is the low level threshold for assigning non-diagonal matrix elements as essentially zero. Also, $\rho_{max} = 5$ for this table.

N_{step}	λ_1	λ_2	λ_3	No. iterations
10	2.9338	6.6598	10.1415	139
50	2.9970	6.9850	10.963	4,039
100	2.9992	6.9962	10.991	16,474
125	2.9995	6.9975	10.994	25,826
150	2.9997	6.9983	10.996	37,443
175	2.9997	6.9987	10.997	50,991
200	2.9998	6.9990	10.998	66,827
225	2.9998	6.9992	10.998	84,775
250	2.9999	6.9994	10.999	104,290
275	2.9999	6.9996	10.999	128,507
400	3.0000	6.9998	11.000	269,020

Using $N_{steps} =250$ gives us (basically) four leading digits and the values of ϵ and ρ_{max} are good choices as well. These are the values I use throughout the project. However, just to check: when I change ρ_{max} to 10, and $N_{steps} =100$, the values are $\lambda_1 = 2.9969$, $\lambda_2 = 6.9846$, and $\lambda_3 = 10.962$. The relative error compared with the table above for n=100 are .077% for λ_1, .165% for λ_2, and .264% for λ_3. When $\rho_{max} = 100$, the results are very far off. Since this is a numerical estimation, a lower value for ρ_{max} gives a more accurate solution. However, ρ_{max} must be large enough to give us a good physical picture. Here is a graph of the N_{step} -the dimensionality of the matrix versus the number of iterations needed to get the eigenvalues. We can see that it goes$\sim O(n^2)$.

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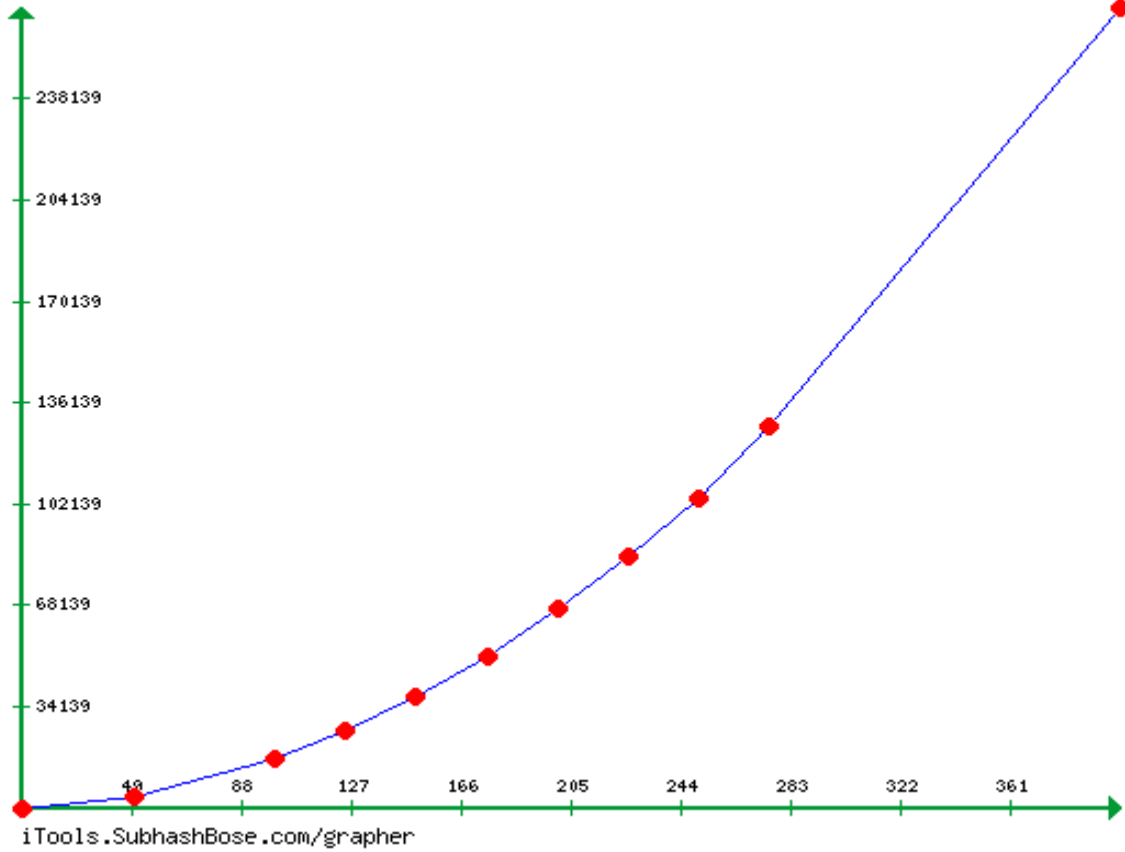
Now we'll look at the run-time of the Jacobi method versus the the armadillo solver. The values : ϵ=1e-8 and ρ_{max} =5.

N_{step}	Armasolve time	Jacobisolve time
10	.00071311	7.4863×10^{-5}
50	.00955606	.021553
100	.119834	.297856
150	.292907	1.43716
200	.543296	4.43368
250	.854114	10.6005
400	.879044	73.0668

We see that the Jacobi is actually faster for N=10 but then gets much slower as N increases into the range that we need for numerical precision.

Part C We now move on to the two electron case. The main difference here is the change in potential. The Schrödinger equation simplifies as in part a as follows:

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \frac{1}{4}\frac{mk}{\hbar^2}\alpha^4\rho^2\psi(\rho) + \frac{m\alpha\beta e^2}{\rho\hbar^2}\psi(\rho) = \frac{m\alpha^2}{\hbar^2}E_r\psi(\rho).$$

The change in potential from a goes as ρ^2 to $\omega_r^2\rho^2 + 1/\rho$. The ω_r term indicates the strength of the oscillator potential and will influence the values of the energy states of the two particle system. We look at the cases where $\omega_r = 0.01$, $\omega_r = 0.5$, $\omega_r = 1$, and
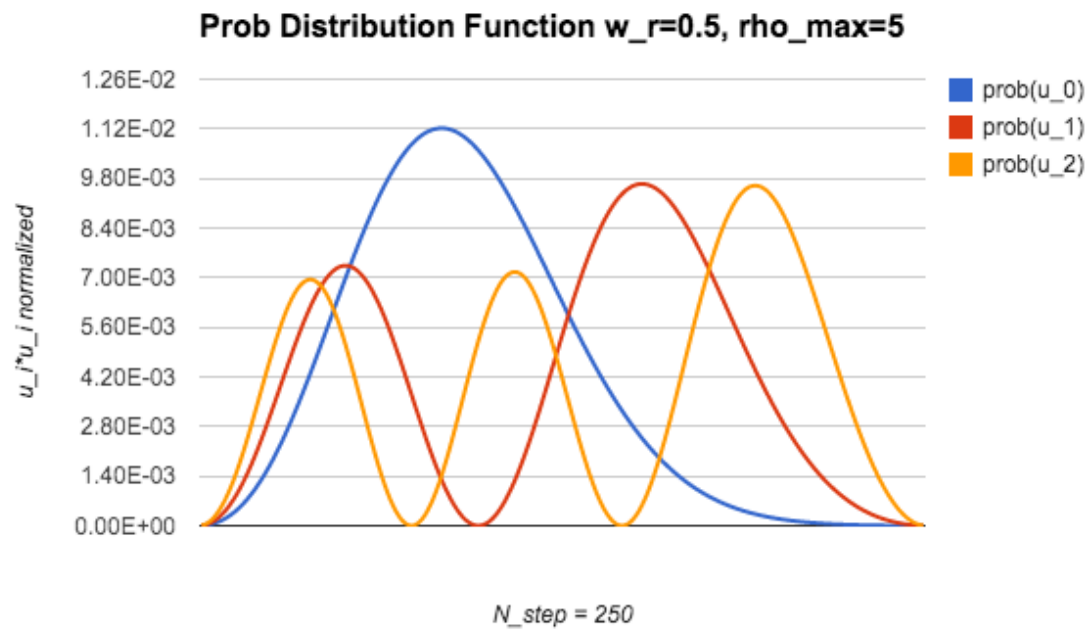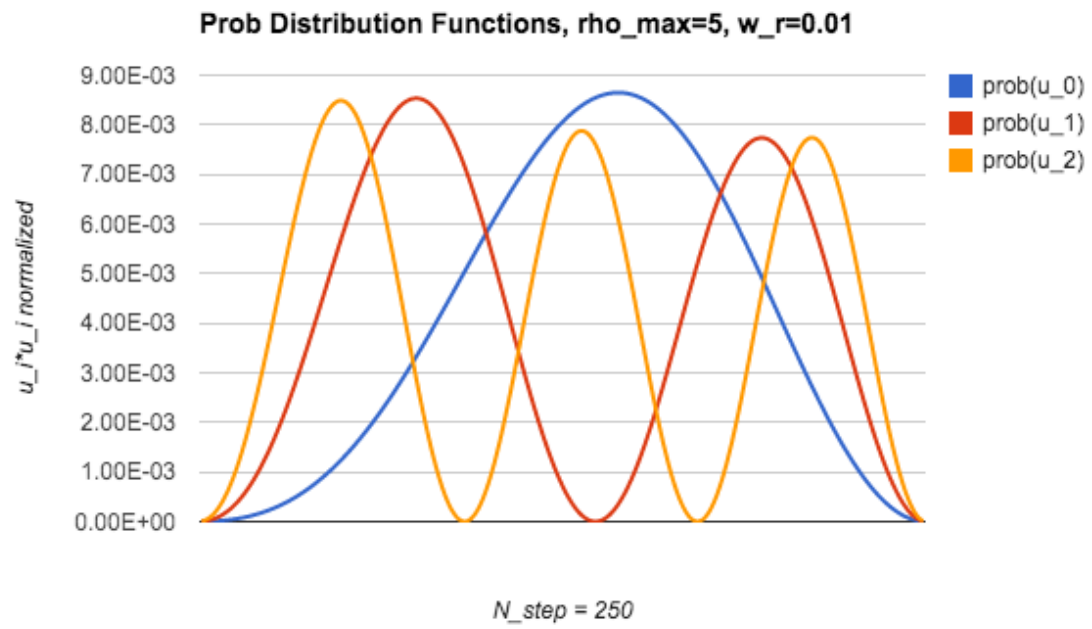
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$\omega_r = 5$. We change the potential and re-run the program for the 4 different values of ω_r. The first 3 eigenvalues are given in the table below. The results use N_{step} at 250, ρ_{max} at 5, and ϵ at 1e-8.
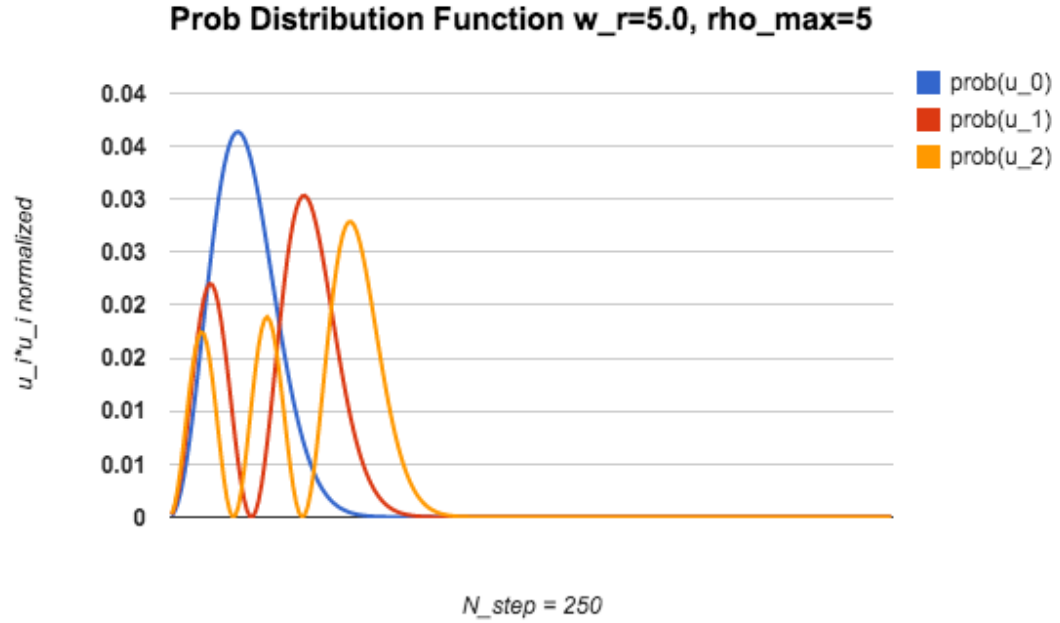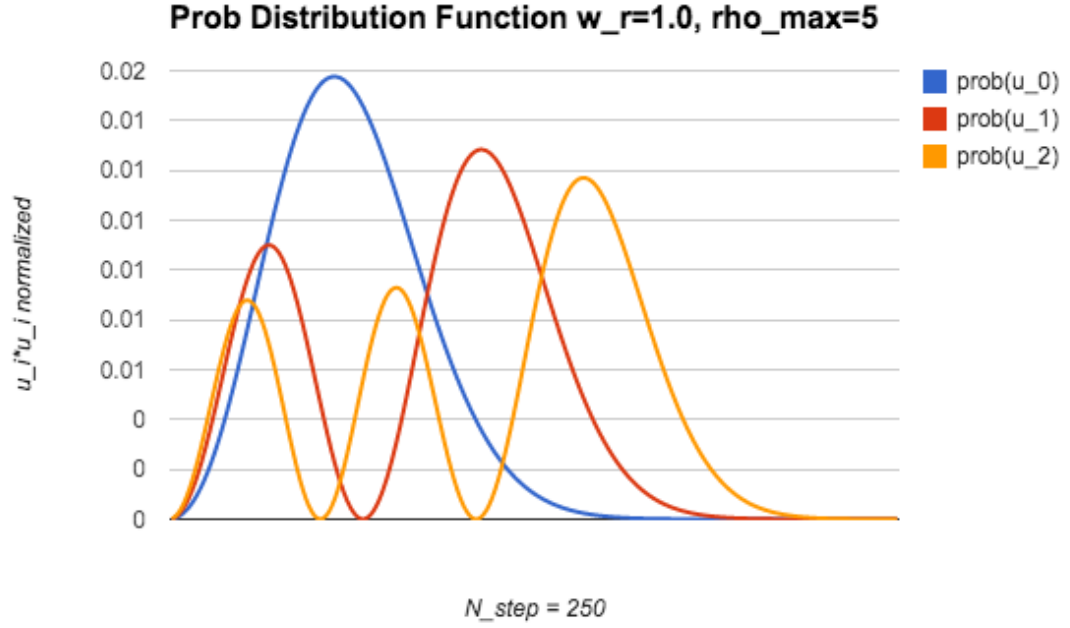
ω_r	λ_1	λ_2	λ_3
0.01	0.84075	2.1737	4.2372
0.5	2.2310	4.1691	6.3858
1.0	4.0577	7.9091	11.818
5.0	17.445	37.057	56.817

Here are the values for the first 3 energy states. We see the dependence on ω_r is quite large for the values of the energy levels. For $\omega_r = .01$, the electrons are not closely coupled and the energy level of the oscillator is even lower than for the single electron case. We see when ω_r grows to 1 and 5, the values are higher. Physically, the electrons are brought closer together in the oscillator well and the repulsive force means that the energy needed for the state to exist is greater. The greater potential should lead to a higher value of the eigenvalues.

Part D Finally, we want to plot the wave functions for the first 3 energy states for the 4 ω_r values. The eigenvectors contain the constituent elements of the wave equation at the various positions along $[0, \rho_{max} = 5.0]$. The tricky part is indexing the locations of the eigenvectors within the eigenmatrix from the position of the corresponding eigenvalue. Since the Jacobi algorithm does not necessarily return the eigenvalues in sorted order, another for loop is needed to extract the first 3 eigenvectors–> corresponding to the 3 lowest energy states.

The next tricky part is determining how to normalize the eigenvectors. From quantum mechanics, we know that in an infinite potential well, the wave function should be normalized by $sqrt(2/lengthofwell)$. In our case, we have abstracted the parameters in this assignment, and therefore the normalization is a bit more abstract here. There should be an h term-or a similar term that takes into account the length of the well- included in the normalization. While this may be a concern, the probability distribution function is the square of the wave equation and must sum to 1. Therefore, any constant in front of the wave equation can be eliminated as it will not change the relative values of the wave equation when multiplied uniformly. And since we are normalizing to 1, the term can be omitted. So in my code, I've squared the eigenvectors and applied the armadillo normalise() function. I've included 4 plots for the 4 different values of ω_r. The first 3 eigenvectors are graphed on top of each other in each case to highlight the relative probability strengths.

Prob Distribution Functions, rho_max=5, w_r=0.01

N_step = 250

Prob Distribution Function w_r=0.5, rho_max=5

N_step = 250

Prob Distribution Function w_r=1.0, rho_max=5

N_step = 250

Prob Distribution Function w_r=5.0, rho_max=5

N_step = 250

We can see the coupling effect of the oscillator strength. The electron can spread out more freely with lower ω_r values and is more tightly bound for higher ones. The shape of the distribution functions seems correct and the strong and weak particle interactions due to the strength of the harmonic oscillator as ω_r are also apparent from the plots. The area under the curve for each of the 3 energy states sum to 1. The peaks for the energy states 2 and 3 have higher probabilities closer to zero for $\omega_r = .01$ and this is reversed for $\omega_r = 0.5, 1.0,$ and 5.0. I have some reservations about the correctness of the

eigenvector plots, but here's my hand-waving attempt: I imagine the probability of the smaller relative radius would be greater for a weaker harmonic oscillator coupling than for a stronger one. Based on these plots, I conjecture that the higher ω_r means a more tightly bound nucleus with the electrons pushing more towards the outside of the well (Coulomb repulsion) which is a result of the higher potential energy of that system. The lower ω_r strength has a higher entropy and lower energy than the higher ω_r strengths. We can also see this higher cost energy effect in the relative growth of the first 6 eigenvalues as plotted below in a stacked area chart divided by the four oscillator strengths:

Rho_max = 5.0, takes N=250 steps to get there
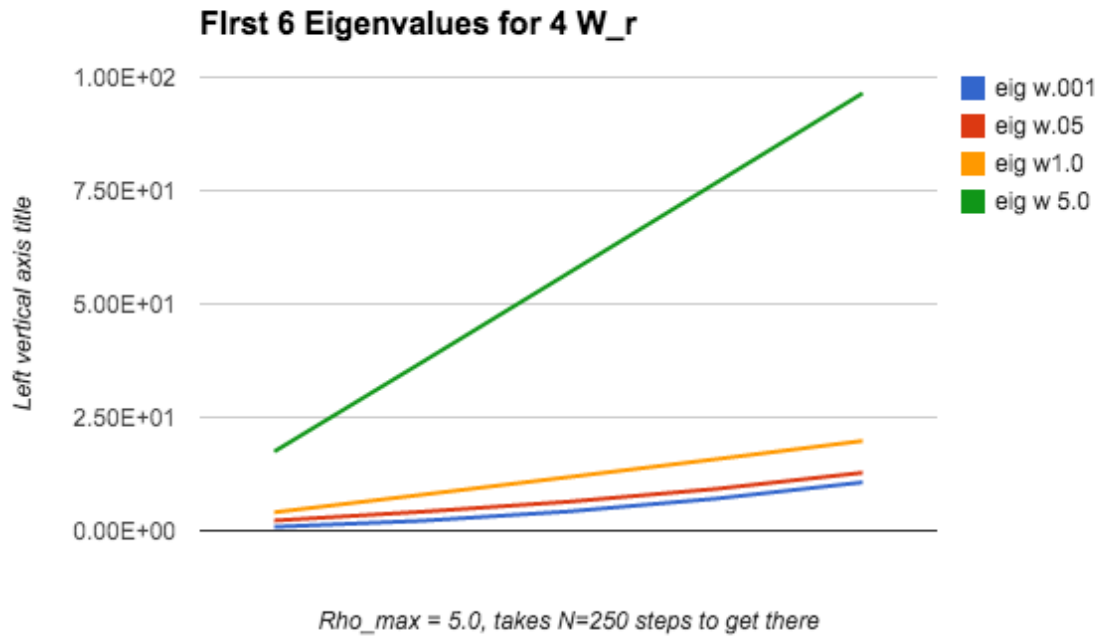
Conclusion This project has interesting physical takeaways and demonstrates how some simple algorithms can aid a great deal toward solving problems where there is no easy analytical solution.