Finding an Analytic Approximation for the Shape of the Excitation Cross Sections of Xenon

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Abstract

Discrepancies between the most recent set of experimental measurements of the excitation cross sections into the $5p^5 6p$ levels of xenon and the excitation cross sections currently used by Magboltz where observed. As a result of these discrepancies a better approximation of the excitation cross sections in xenon was sought using two methods. The first method was to parameterize the experimental data and use it to predict the shape of the other excitation cross sections. The second method was to parameterize the three general shapes of excitation cross sections caused by the two mechanisms of excitation and use mixing ratios to predict the shapes of each excitation level of xenon. The accuracy of the results from the two methods has yet to be tested.

1 Introduction

An understanding of the electron-impact excitation cross sections of atoms is needed in order to predict properties such as drift velocities and transfer rates when simulating physics processes. Simply knowing the magnitude of total excitation cross section; however, is not sufficient. It is important to know what the probability of having an excited atom is in a specific energy range and to do this, the shape of the excitation cross section as a function of incident electron energy is needed.

Recently Magboltz was used to find transfer rates in xenon gas mixtures by fitting experimental gas gain data from Manchanda's 1993 and 2004 papers [1,2]. Unfortunately some of the resulting transfer rates were over 100%, which indicated that the excitation cross sections for xenon in Magboltz needed adjusting. In a recent publication John T Fons and Chun C. Lin [3] attempted to experimentally determine the direct excitation cross sections from the ground state of xenon to the $5p^5 6p$ levels. To see if Magboltz had reasonable values for excitation cross sections, the excitation cross sections for the $5p^5 6p$ levels of xenon in Magboltz were compared to recent experimental measurements made by Fons and Lin and the Magboltz excitation cross sections were found to be a factor of 2-3 times lower than the experimental values in the low energy range ($\sim 0 - 50$eV). Since the transfer rates are inversely related to the excitation cross section, Magboltz would likely produce more reasonable transfer rates by updating it's excitation cross sections so that they fit the experimental data better.

2 Discrepancies Between Magboltz and Recent Experimental Data

The excitation cross sections for many of the $5p^5 6p$ in Magboltz[4] were observed to have much smaller peaks than the experimentally determined excitation cross sections from Fons and Lin[3]. Some of the excitation cross sections from both Magboltz and Fons and Lin can be seen below. To avoid repeatedly showing the same plots, only the $5p^5 6p$ excitation cross sections in worst agreement with the Magboltz data are shown below, for plots of all ten $5p^5 6p$ levels ($2p_1 - 2p_{10}$ in Paschen notation), please see the Parameterization of Experimental Data section.

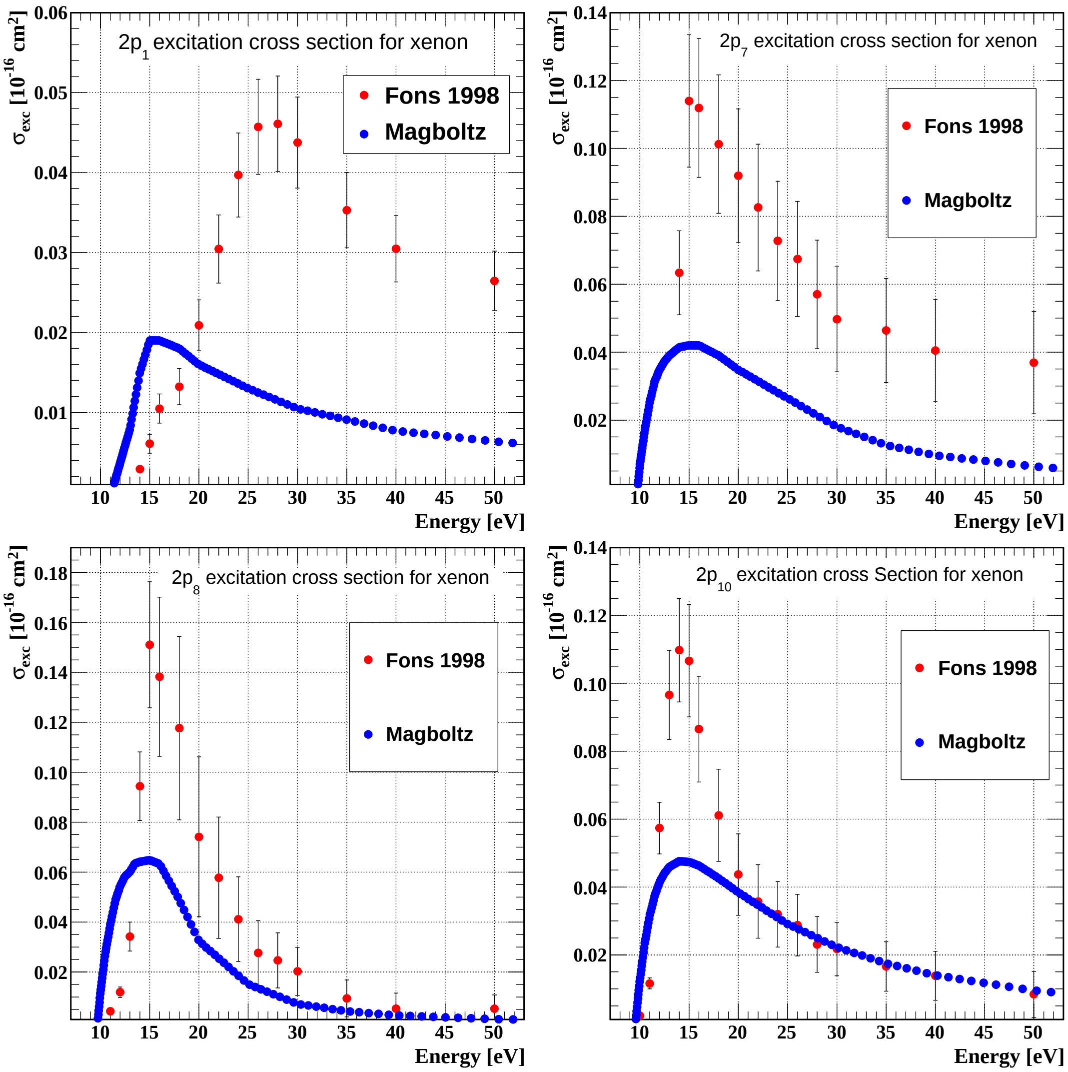

Figure 1: Excitation cross sections of the $2p_1$, $2p_7$, $2p_8$, and $2p_{10}$ levels in xenon from Magboltz and the experimental data from Fons and Lin

The experimental data taken by Fons and Lin has been called "the most recent and likely most reliable set of experimental data" [5] by Bartschat who has published many papers on theoretically calculating the excitation cross sections, and having higher excitation cross sections in the lower incident electron energy range would improve the currently unreasonable transfer rates for xenon gas mixtures. This indicated that the Fons and Lin data was likely more accurate than the current Magboltz data. In addition to the discrepancies seen between the Fons and Lin data, Magboltz did not have any data for transitions into the $5p^5 7p$ (3p in Pachen notation) states of xenon, yet excitations into the $5p^5 7p$ levels of xenon can occur and have been measured by Jung *et al.* [6]. Due to this it was justifiable to assume that the cross sections Magboltz needed to be improved.

3 Background Information on Excitation Cross Sections in Xenon

In order to properly understand the excitation cross sections of an atom it is important to understand the mechanisms by which an atom can become excited and how each excited state can be characterized. There are two mechanisms by which an atom can become excited. The first mechanism is through electromagnetic interaction and the second is through electron exchange, whereby the incident electron replaces a bound electron in the target atom. Excitations which are forbidden by the selection rules for electromagnetic interaction can occur through electron exchange, these interactions are referred to as dipole forbidden interactions. If an atom does become excited through electron exchange it is possible for the incident electron to have a different spin than the original atomic electron causing a spin forbidden excitation to occur. Electron exchange interactions also have a low probability of occurring at high energy and so they cause the excitation cross section to peak at low energy. This means that the probability of a dipole allowed, dipole forbidden spin allowed, or spin forbidden excitations occurring are all different and, as a result, the excitation cross sections of an atom can be categorized into three general shapes. One shape for dipole allowed transitions (which is dominated by electromagnetic interactions), one shape for dipole forbidden and spin allowed transitions, and one shape for spin forbidden transitions(in which only electron exchange excitation should occur)[7]. Even if the three basic shapes are known; however, the excited states of an atom still need to be characterised into the three categories of excitations so that the shape for any given excitation is known.

One method of characterising the excited states of atoms is via LS-coupling. As the name suggests LS-coupling characterises atoms based on the L and S quantum numbers, where L = 0 for the s states, 1 for the p states, 2 for the d states etc. and S is the net spin. For rare gases in the ground state S = 0, since all spin up electrons are paired with a spin down electrons; furthermore, for all rare gases heavier than helium, the ground state of the atom is in the p level, meaning an excitation into a higher p level has an L_{TOT} of 2 (one from the ground state unpaired p electron and one from the excited p electron). Using the vector addition of L and S to get J gives ten possible excited states, of which seven have an S value of 1. States with an S value of 1 are referred to as triplet states since it has three degeneracies characterized by the quantum number m_s which ranges from -S to S. The remaining three excited states have an S value of 0 and are referred to as singlet states since the m_s quantum number has only one possible value, 0. Excitation into the a triplet states is spin forbidden from the ground state by the selection rule $\Delta S \neq 0$ since the initial S value is 0 and the final S value would be 1, see [8] for selection rules.

Xenon, unfortunately, is a heavy rare gas and it's excited states are not well characterized by LS coupling. The wave function of the transition states for xenon are better approximated as a superposition of singlet and triplet states, which means that each excited state in xenon is likely to have a different shape based on how much singlet and triplet component are present in the wave function.

4 Theoretical Approximations

Unfortunately solving the full Schrodinger equation for an e^- Xe collisions is not currently possible so an analytic approximation was needed. Much recent work has been done to find a good theoretical approximation for the excitation cross sections of xenon. In 1991 Puech and Mizzi published *Collision cross sections and transport parameters in neon and xenon*[9] in which they split the excitation cross sections into two categories, forbidden and allowed transitions, and used a Bethe-Born approximation with a low energy modifier in an attempt to predict the shape and magnitude of many different excitation cross sections in xenon. The low energy modifier; however, was not sufficient to adjust the shape of the low energy peaks caused by electron exchange.

K. Bartschat *et al.* published a paper in 2004 [5] attempting to use close-coupling and distorted wave calculations to determine the excitation cross sections in the $5p^5 6p$ levels of xenon and, since it was written after 1998, compared their results to the experimental results published by Fons and Lin. There was many discrepancies between the experimental data and the distorted wave and close coupling calculations and an accurate theoretical model is still needed. Since then Allan, Zatsarinny and Bartschat have done some work with B-Spline R-matrix calculations [10], but have not yet applied it to xenon in the low energy range. Since no usable theoretical approximations for predicting all the excitation levels in xenon was found the best approach for correcting the excitation cross sections in Magboltz was to parameterize the experimental data from Fons and Lin.

5 Parameterization of Experimental Data

The shape of the excitation cross section depends on the selection rules applied to a particular excited state; therefore, dipole forbidden states that have the same amount of single and triplet components in their wave function should have the same shape. This means that the data obtained by Fons and Lin at the $5p^5 6p$ (2p) level can be used to find the shape of the $5p^5 np$ levels, when n an integer above 6. For example, the shape of excitation cross section in the $2p_1$ state should be the same as the shape of excitation cross section in the $3p_1$ state, therefore once a suitable parameterization was found that correctly parameterized the 2p levels all that remained was to find a suitable scaling factor by which the excitation cross section into the higher levels reduces.

The first parameterization attempted was using Yong-Ki Kim's 1988 paper[11] where he attempted to parameterize the three different shapes of the excitation cross sections; however, the parameterizations were similar to the Bethe-Born approximations and did not fit the xenon excitation cross sections at low energy. Figure 2 below shows the spin forbidden parametrization from Kim, fit to the $2p_8$ level data from Fons. The $2p_8$ level was chosen since it is a purely triplet state in xenon and is therefore entirely spin forbidden.

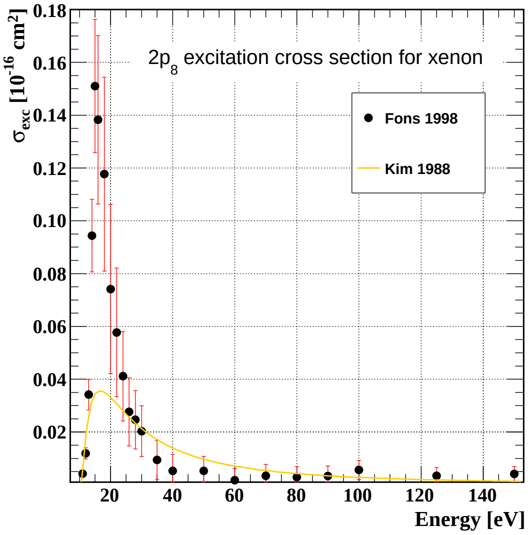

Figure 2: Parameterization from Kim fit to the experimental data of the excitation cross section of the $2p_8$ level of xenon from Fons and Lin

Since the fit from Kim did not seem to approximate xenon excitation cross sections very well at low energy, the analytic approximation used by Boffard *et al.* in 2007[12] to fit argon excitation cross sections and later by Jung *et al.*[13] to fit neon excitation cross sections in 2011 was used. The parameterization used in the Boffard *et al.* and Jung *et al.* was an approximation of the shape function $q_i(E)$ where $q_i(E)$ is given by the following:

$$Q_{ij}^{opt} = \frac{4\pi ekT}{hc} \frac{H\lambda_{ij} F(\lambda_{ij})}{\Omega S_{ij}^{lamp}} \frac{S_{ij}^{exc}}{IP} \tag{1}$$

where Q_{ij}^{opt} is the optical emission cross section, "λ_{ij} is the wavelength of the transition, S_{ij}^{exc} is the observed electron-excitation signal recorded by a PMT, integrated over the width of the bandpass of a monochromator, S_{ij}^{lamp} is the signal from a standard lamp which has spectral irradiance $F(\lambda_{ij}$, H is the height of an auxiliary slit used in the lamp calibration portion of the experiment, Ω is the solid angle of the collision region collected by the optical system, I is the electron beam current, P is the target gas pressure, T is the gas temperature, and e, k, h, and c are the standard atomic constants"[12].

$$q_i(E) = \frac{Q_{ij}^{opt}(E)}{Q_{ij}^{opt}(E_{ref} = 50\text{eV})} \tag{2}$$

The analytical approximation of the shape function $q_i(E)$ is:

$$q(E) = q^C(E) + q^D(E) \tag{3}$$

and finally the terms $q^C(E) + q^D(E)$ are given by:

$$q^C(E) = \frac{C1(\frac{E-E_{TH}}{E_R})^{C2}}{1 + (\frac{E-E_{TH}}{C3})^{C2+C4}} \tag{4}$$

$$q^D(E) = \frac{D1(\frac{E-E_{TH}}{E_R})^{D2}}{1 + (\frac{E-E_{TH}}{D3})^{D2+D4}} \tag{5}$$

Where E_R is the Rydberg energy (13.6eV), E_{TH} is the threshold energy of the excitation, and C1 through C4 and D1 through D4 are parameters obtained by fitting the experimental data. The following plots were obtained by using the TMinuit class in ROOT to fit function (3) to the data obtained by Fons and Lin[3].

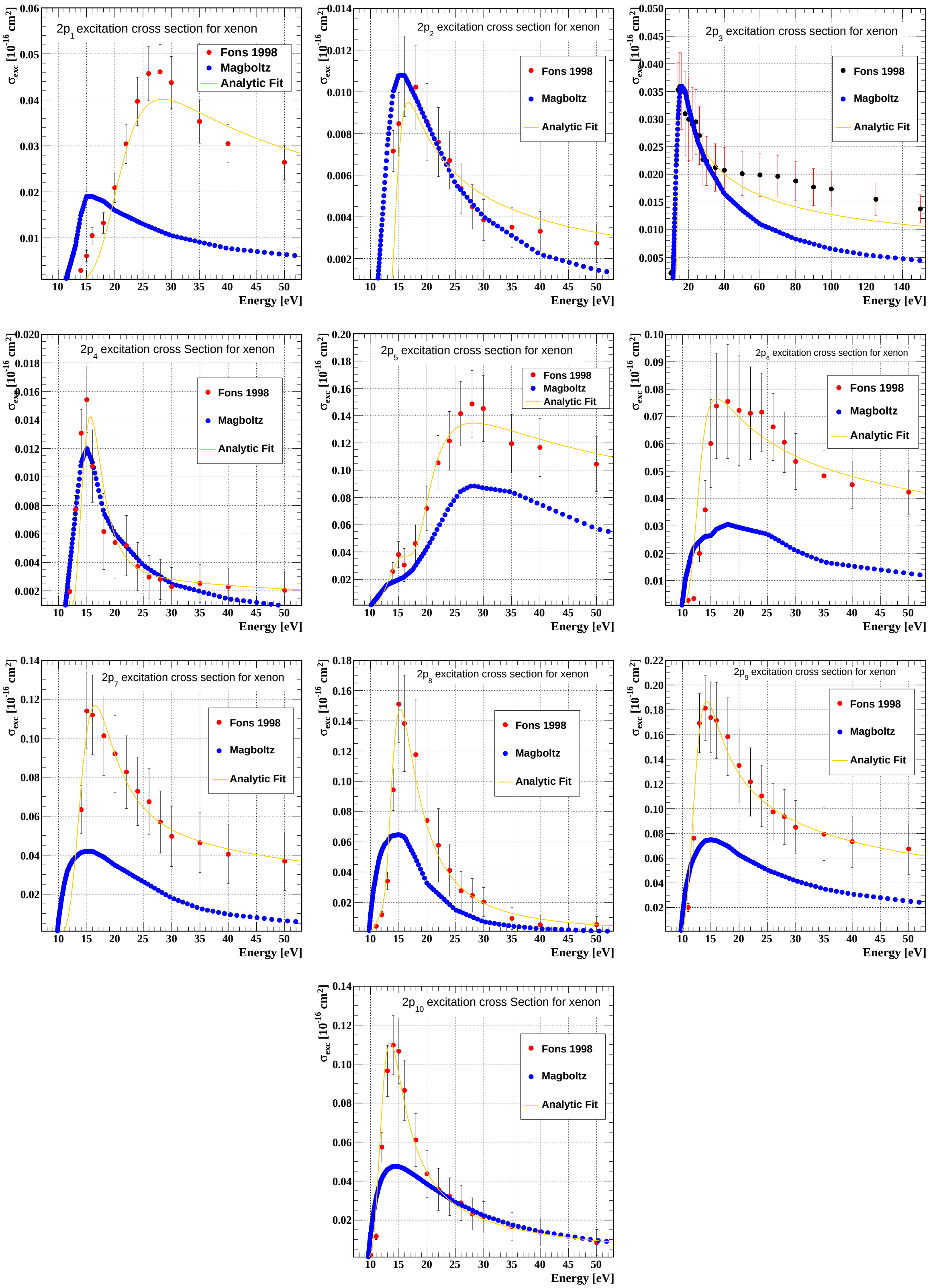

Figure 3: The analytic fit to the experimental excitation cross sections from Fons and Lin of the $2p_1 - 2p_{10}$ levels in xenon

See Table 1 in Appendix A for the resulting fit parameters C1-D4 as given by TMinuit. Figure.. above shows that the analytic fit used by Boffard *et al.* and Jung *et al.* parameterizes the xenon excitation cross sections into the $5p^5 6p$ levels well and can be used with a scaling factor to find all other p level excitations; however, in order to determine the excitation cross section for all levels of xenon, experimental data for each 6s and 5d level is needed. Fortunately, Jonh T. Fons thesis[13] contains excitation cross section measurements into the $5p^5 ns$, where n is from 7 to 11, and $5p^5 nd$ where n is from 5 to 9 which can be parameterized the same way the $5p^5 6p$ levels were. Fons also parameterized each of the three general shapes of the excitation cross section, (dipole allowed, spin allowed, and spin forbidden) and John Gastineau's Thesis[14] contains nicely tabulated LS coupling mixing ratios for xenon excitation levels. By Using the mixing ratios from Gastineau's Thesis, and the shapes of the excitation cross section from Fons thesis, it is possible to get a more general method for determining excitation cross sections.

6 Using generalized shapes and mixed state ratios to determine excitation cross sections

Fons Thesis contains a plot of the expected shapes of the excitation cross sections for the three general cases of excitation (dipole allowed, spin allowed, and spin forbidden). In order to attempt to reproduce the shapes of the $2p$ level excitation cross sections seen in the experimental data by Fons and Lin, the data points for each of the expected shapes were extracted from Fons thesis using g3data (software designed for reconstructing data points from images). Once the data points were extracted they were plotted and fit using equation (3) above; however, fitting the data using TMinuit requires error on the measurements and since all three excitation shapes were plotted on one graph the error bars were not plotted, as they would make it difficult to distinguish between the three curves. Most of the error bars in the experimental determination of excitation cross sections is statistical error, as such an error of 10% was used for the purpose of fitting the data. see Figure 4 below for the fits to the tree shapes.

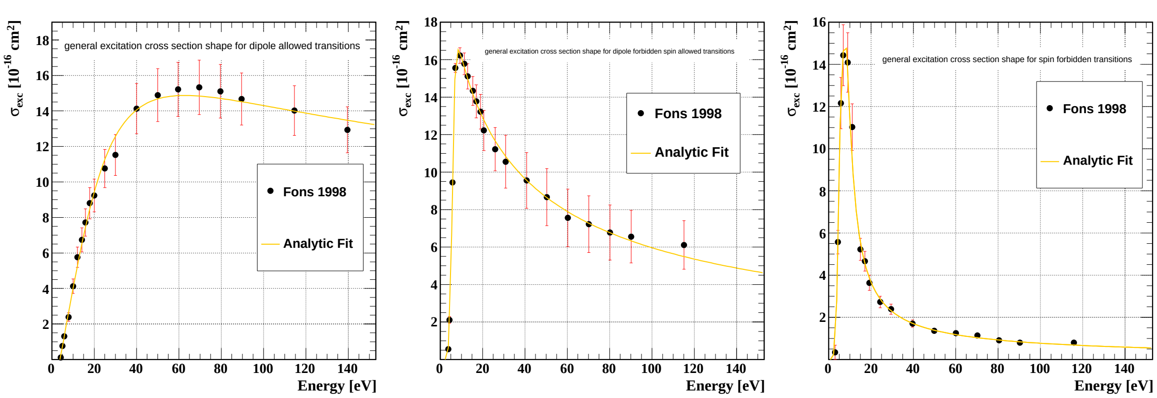

Figure 4: The analytic fit to the three general shapes of the excitation cross sections in xenon

See Appendix A Table 2 for the parameter values C1-D4 for the three general shapes of excitation cross sections. Since the general shapes in Fons thesis where given an arbitrary threshold value of $\sim$ 10eV, the starting point of the fits was set at 0eV so that they could be adjusted along the x-axis by the threshold energy of a given excitation using formula (3). Unfortunately, Since the exact starting points of each of the three shapes was difficult to determine, the spin forbidden excitation needs to be adjusted along the x-axis by the threshold energy plus 1 eV, for instance, when using the parameters seen in Table 2 to determine the shape of an excitation cross section with a spin forbidden component, the shape function of the spin forbidden component should be calculated using the formula below.

$$q(E) = q^C(E+1) + q^D(E+1) \tag{6}$$

The mixing ratios from Gastineau's theses, which describes the excited states of xenon as a mixture of LS-coupled states, were applied to the 2p levels of xenon and compared to the experimental data taken by Fons and Lin. As can be seen in Figure 5 below, the fit obtained by mixing the three general shapes and scaling them to the existing cross section data does not approximate the experimental data perfectly; however, in most cases it is extremely close and may give a more accurate cross section than what is currently used by magboltz.

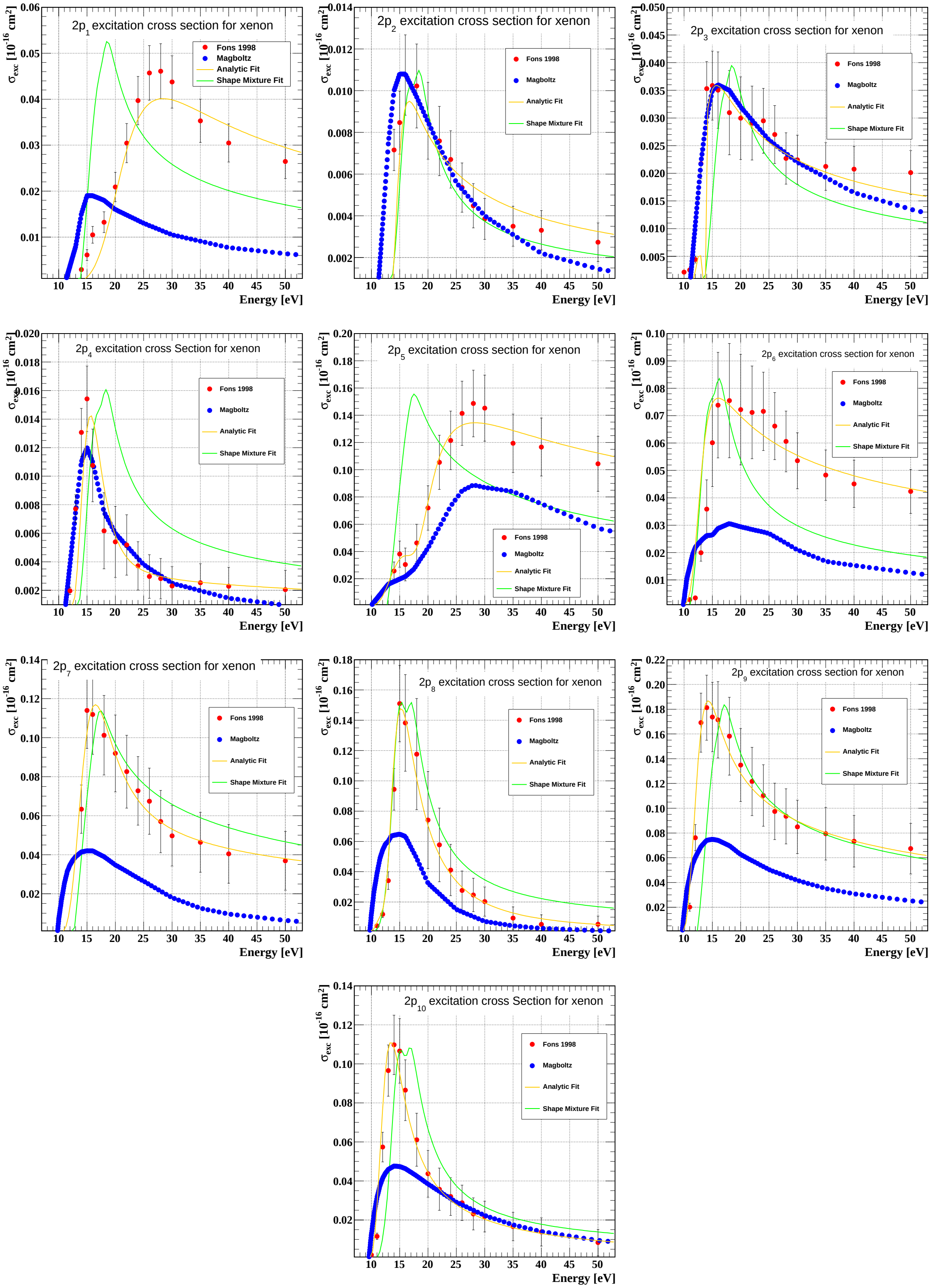

Figure 5: Mixed shape approximations for the $2p_1 - 2p_{10}$ excitation cross sections in xenon

7 Conclusion

Two methods for finding analytic formulas to describe the excitation cross sections in xenon were discussed for the purpose of updating Magboltz. Unfortunately, there is currently no theoretical approximations accurate enough to approximate the shape and magnitude of the excitation cross sections in xenon, instead the experimental data from Fons and Lin[3] and Fons Thesis[14] were parameterized in a way that they could be used to determine the shapes of the excitation cross sections for all excited states in xenon.

8 Future Work

In order for Magboltz to be updated with the cross sections proposed in this report the data for the s and d states in xenon must first be parameterized. Once all the xenon excitations have been parameterized (or predicted by the mixing ratios and three general shapes) the excitation cross sections need to be tested to ensure that they give reasonable results for total cross section, electron drift velocity, transfer rates etc. All that remains to be done in order to determine the cross sections of the s and d levels using the mixing ratio method is to apply the mixing ratio's for the d levels of xenon from Gastineau's theses to the already parameterized general shapes, to find and apply mixing ratios for the s levels, and to find a scaling factor for the magnitudes of each level (If the coefficients from this paper are used for the analytic approximations of the three general shapes, equation (6) must be used for spin forbidden transitions). In order to determine the excitation levels through parameterization of the experimental data in Fons thesis the g3data program could be used to extract the shapes of the s and d excited states of xenon. The s and d excited state data could then be parameterized in the same manner as the p states in this report. Once the s, p, and d states are parameterized they could be used in conjunction with a scaling factor to determine the excitation cross sections for all the excited states of xenon.

9 Acknowledgements

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Citations

[1] R.K. Sooda, Z. Yea, and R.K. Manchandab,“Ultra-high pressure proportional counters Part II. Xenon”, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Volume 344, Issue 2, 1 May 1994, Pages 384-393

[2] D. J. Grey, R. K. Sood, and R. K. Manchanda, “Resolution and spectral characteristics of ultra high pressure proportional counters using various quench gases”, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Volume 527, Issue 3, 21 July 2004, Pages 493-511

[3] J.T. Fons and C.C. Lin, “Measurement of the cross sections for electron-impact excitation into the 5p56p levels of xenon”, Phys. Rev. A 58, 4603 (1998)

[4] LXcat, ”Electron Scattering Database”, http://www.lxcat.laplace.univ-tlse.fr, accessed July 20th 2011

[5] K. Bartschat, A. Dasgupta, and D. H. Madison,“Close-coupling and distorted-wave calculations for electron impact excitation of the 5p56p states of xenon” Phys. Rev. A 69, 062706 (2004)

[6] R.O. Jung, J.B. Boffard, L. W. Anderson, and C.C. Lin, “Excitation into 5p57p levels from the ground level and the J=2 metastable level of Xe”, Phys. Rev. A 80, 062708 (2009)

[7] J.B. Boffard, R.O. Jung, L.W. Anderson, and C.C. Lin, “Electron impact excitation of rare gas atoms from the ground level and metastable levels”, Advances in Atomic, Molecular, and Optical Physics Vol. 54, 320-418 (2007)

[8] P. Ewert, “Atomic Physics”, Oxford University, http://www.physics.ox.ac.uk/users/ewart/Atomic%20Physics%20lecture%20notes%20Final.pdf, accessed on August 20 2011

[9] V. Puech and S. Miui, “Collision cross sections and transport parameters in neon and xenon”, J. Phys. D: Appl. Phys. 24 1974-1985 (1991)

[10] M. Allan, O. Zatsarinny and K. Bartschat, “Electron impact excitation of the (4p5 5s) states in krypton: high-resolution electron scattering experiments and B-spline R-matrix calculations”, J. Phys. B: At. Mol. Opt. Phys. 44 065201 (2011)

[11] Y. Kim, “Incedent-energy dependence of the electron-ion collision cross sections”, Phys. Rev. A 38, 1805-1808 (1988)

[12] J. B. Boffard, B. Chiaro, T. Weber, and C. C. Lin, “Electron-impact excitation of argon: ”, At. Nucl. Data Tables 93, 831 (2007)

[13] R.O. Jung, G.A. Piech, M.L. Keeler, J.B. Boffard, L. W. Anderson, and Chun C. Lin, “Electron-impact excitation cross sections into Ne(2p53p) levels for plasma applications”, J. Applied Phys. 109, 123303 (2011)

[14] J.T. Fons, “DETERMINATION OF XENON EMISSION CROSS SECTIONS AND THE ORIGIN OF THEIR ANOMALOUS PRESSURE DEPENDENCE”, University of Wisconson-Madison, Thesis 1998

[15] J. Gastineau, “The electron impact excitation of neon and xenon”, University of Wisconson-Madison, Thesis 1986

Appendix A: Fit Parameters

Table 1: Fit parameters for the analytic approximation of the 2p excitation levels in xenon

Excited State	C1	C2	C3	C4	D1	D2	D3	D4
$2p_1$	0.128026	3.66069	11.0079	0.546603	11.7193	8.08214	1.2661	2.82027
$2p_2$	-17172.5	-3.98918	1.32557	31.0237	9.67525	5.2604	3.88347	0.609817
$2p_3$	-11.7176	3.52909	2.99026	517.374	4.63933	2.71675	2.63721	0.443865
$2p_4$	10.592	2.82387	4.58011	0.80522	-8.64	2.74221	4.72789	0.815915
$2p_5$	12.7195	2.80567	5.88243	0.971354	-7.71186	2.5386	6.64646	1.54062
$2p_6$	3.19988e-10	-6.09689	40.8009	73.1758	14.845	4.33661	4.30147	0.374164
$2p_7$	12.0164	2.74784	5.86671	0.574707	-7.5493	2.59503	6.38656	0.592678
$2p_8$	8.56074	2.50949	4.53887	1.96126	-15.0726	2.88789	3.54246	2.0063
$2p_9$	13.85	2.30838	3.99138	0.573576	-6.50633	2.37234	4.82124	0.60728
$2p_{10}$	13.2868	2.43361	3.38805	0.606937	-4.09417	2.26301	4.34836	0.550111

Table 2: Fit parameters for the three general shapes of excitation cross section in xenon

General Shape	C1	C2	C3	C4	D1	D2	D3	D4
Dipole Allowed	8.39989	1.66578	24.4286	0.26913	-67.6927	1.35492	1.80006	1.63502
Spin Allowed	38.2219	-0.77623	25.4153	0.0341872	-9.23187	-0.59974	6.0088	10.3883
Spin Forbidden	3.0154e+06	24.5707	7.95128	0.791264	1568.38	4.97167	6.0727	2.85959