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Extrapolation of the Experimental Data of Electron Scattering

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EXTRAPOLATION OF THE EXPERIMENTAL DATA OF ELECTRON SCATTERING

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I Introduction

Our problem of interest is electron-atom scattering. One type of experiment is to measure the number of electrons exciting an atom from a initial s-state to a final p-state. These measurements are proportional to the differential cross section (DCS). Theoretically the DCS is given by

$$DCS = \partial\sigma/\partial\Omega = \sum_{-1}^{1} |T^{(m)}|^2 \qquad (1)$$

where $T^{(m)}$ is an complex amplitude for exciting a particular magnetic sublevel with magnetic quantum number m, and $T^{(-1)} = -T^{(1)}$.

Experimentally it is very difficult to measure absolute scattering cross sections. There is a quantity called the generalized oscillator strength (GOS) which is proportional to the DCS

$$GOS = f = \Delta E/4 \; k_i/k_f \; q^2 \sum_{-1}^{1} |T^{(m)}|^2 \qquad (2)$$

where

$$q^2 = k_i^2 + k_f^2 - 2k_ik_f \cos\theta \qquad (3)$$

Here θ is the scattering angle for the electron, and ΔE is the energy change of the atomic electron. Since $k_i \neq k_f$, it is experimentally impossible for q to be 0. However, experimentalists conjectured that for a final p- state, the GOS will extrapolate to the OOS for $q=0$, where OOS stands for the optical oscillator strength. One of the reasons this method is so attractive is that OOS is independent of the initial electron energy, and only depends on ΔE.

The purpose of this project was to investigate validity of the extrapolation procedure. We used the following mathematical basis for our extrapolation procedure. We consider f, the generalized oscillator strength, as an restriction of an analytic function on an appropriate domain, containing a closed interval with left end point 0, and right end point the physically obtainable

maximum of q^2, the square of the magnitude of the change in momentum of the outgoing and incoming electron. A well known theorem in complex analysis states that, if two analytic functions in a common domain coincide on an infinite point set with one of its cluster points inside the domain, they will be constantly equal to each other everywhere in the domain. As an result, if we could find an analytic extension function of f, it would be the only one we are after. Consequently we searched for a method to extent the function from the physically allowed interval on the q^2-axis to that appropriate domain to determine if the values of f at $q^2=0$ were the same independent of initial energy.

The simplest theoretical treatment of this problem is called the plane wave Born approximation. In this approximation, f is a fractional function with only a simple pole off the positive real line of the q^2-axis. It has the optical oscillator strength as its value at the origin.

The plane wave Born approximation is known not to be accurate enough. However Lassetre[1] claims that even if PWBA (plane wave Born approximation) is not reliable, a more accurate theory should still extrapolate to the optical oscillator strength.

The theory we are using is significantly better than the PWBA. According to Lassetre's theorem, our theory should extrapolate to the optical oscillator strength. The objective of this research project was to check this theory.

II Methodology

In our theory,

$$T^{(m)} = \sum_{l=m}^{\infty} a_l \, C(l,m) \, P_{lm}(z) \quad (m=-1, 0, 1) \qquad (4)$$

$$z \in f$$

and

$$z = \cos\theta \quad \text{while } z \in [-1, 1] \qquad (5)$$

where a_l, $C(l,m)$ are coefficients of the expansion generated by the theory, and θ stands for the scattering angle.

[1] Lassetre, Edwin N., J. Chem. Phys. 43, p.4479-4486 (1965)

We proved[2] that if any function is analytic inside and on an ellipse with foci -1 and 1, its Legendre polynomial expansion uniformly converges on that compact ellipse. $T^{(m)}$ must approach infinity at $q=0$ so that f will be finite at the origin. Since $q=0$ corresponds to a pole, there is a potential problem for large numerical errors as we approach the pole.We hoped that we could get a good result by the following method. Set up a smaller major axis such that the ellipse excludes $z_c>1$, which is such that $q(z=z_c)=0$, and keep on approaching the major axis to z_c. If the numerical result is accurate enough, we should be able to see the trend. Since this is a singularity, however, a small shift of the zero point of q and the pole of $T^{(m)}$ in the numerical calculation will possibly result in serious deviations, which is what we unfortunately found.

We generated a Fortran code to evaluate the Legendre Polynomials with recurrence functions. The coefficients we calculated for the physical region should remain valid for that enclosed by the ellipse. Consequently it is only necessary to calculate the value of f at $z=$*major axis* using equation (1) and (2).

Appendix I and Appendix II show the comparisons between the analytical PWBA result and the corresponding results obtained from our numerical method. The columns labeled "Analytical" denote the result of the analytical calculation; those labeled "numerical" are of numerical calculation. We can see that the analytic results deviate from the numerical calculation significantly as z approaches closer to the critical point z_c, which is equal to 1.005219 when the initial energy $E_i=54.4$. In fact the numerical results do not ever have the proper behavior near z_c which indicates that there is a serious problem in the numerical method for calculating $T^{(m)}(z)$ and $f(z)$, when $|z|>1$.

We first suspected that there may be a problem with the accuracy of our evaluation of the Legendre polynomial $P_{lm}(z)$. We tested the subroutine used to calculate them and compared the generated value for both $|z|\leq 1$ and $|z|\geq 1$ with those on a handbook. They agreed with each other .

Finally, we checked the accuracy of the coefficients of the Legendre expansion calculated by the numerical method. We recalculated these Legendre coefficients using the conventional inversion:

$$a_{lm} = (l-m)!/(l+m)! \int_{-1}^{1} T^{(m)}(x) P_{l,m}(x)\, dx \qquad (6)$$

where a_{lm} is the coefficient of

$$T^{(m)} = \sum_l a_{lm} P_{lm}(z) \qquad (7)$$

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[2] The proof is too long to be typed and presented here.

However, from Appendix III, we can see that the cross sections for $m=0$ obtained by using eq(6) and (7) are even worse then the those generated numerically, even in the normal region $[-1, 1]$.

III Conclusion

We were not able to obtain an extrapolation procedure which was numerically stable. Evidently the Legendre series expansion is unable to produce values for the pole of $T^{(m)}$ which are sufficiently accurate numerically. As a result, we have not been able to determine whether or not the experimental extrapolation are valid.

Appendix I

The following is a comparison of the cross sections obtained from the numerical solutions and the analytical solutions for initial energy 54.4eV. Z_c is the critical point of z.

CROSS SECTIONS FOR M = 0

z	CROSS SECTION Numerical	Analytic	z	CROSS SECTION Numerical	Analytic
0.99640	1.658E+01	1.665E+01	1.00240	1.745E+02	1.505E+02
0.99680	1.817E+01	1.824E+01	1.00280	2.408E+02	2.004E+02
0.99720	2.001E+01	2.007E+01	1.00320	3.465E+02	2.800E+02
0.99760	2.215E+01	2.219E+01	1.00360	5.213E+02	4.184E+02
0.99800	2.465E+01	2.466E+01	1.00400	8.207E+02	6.918E+02
0.99840	2.761E+01	2.757E+01	1.00440	1.351E+03	1.357E+03
0.99880	3.116E+01	3.103E+01	1.00480	2.316E+03	3.773E+03
0.99920	3.546E+01	3.517E+01	Z_c=1.00520	4.118E+03	3.413E+04
0.99960	4.075E+01	4.020E+01	1.00560	7.548E+03	3.360E+04
1.00000	4.736E+01	4.639E+01	1.00600	1.418E+04	3.753E+03
1.00040	5.580E+01	5.412E+01	1.00640	2.712E+04	1.353E+03
1.00080	6.684E+01	6.396E+01	1.00680	5.258E+04	6.903E+02
1.00120	8.164E+01	7.674E+01	1.00720	1.028E+05	4.176E+02
1.00160	1.021E+02	9.377E+01	1.00760	2.020E+05	2.796E+02
1.00200	1.313E+02	1.172E+02	1.00800	3.977E+05	2.002E+02

CROSS SECTIONS FOR M = 1

z	CROSS SECTION Numerical	Analytic	z	CROSS SECTION Numerical	Analytic
0.99640	4.612E+00	4.681E+00	1.00240	3.544E+01	3.156E+01
0.99680	4.518E+00	4.592E+00	1.00280	5.717E+01	4.940E+01
0.99720	4.376E+00	4.454E+00	1.00320	9.380E+01	7.949E+01
0.99760	4.174E+00	4.252E+00	1.00360	1.575E+02	1.347E+02
0.99800	3.892E+00	3.967E+00	1.00400	2.718E+02	2.493E+02
0.99840	3.507E+00	3.574E+00	1.00440	4.821E+02	5.420E+02
0.99880	2.985E+00	3.039E+00	1.00480	8.779E+02	1.657E+03
0.99920	2.277E+00	2.314E+00	Z_c=1.00520	1.637E+03	1.637E+04
0.99960	1.316E+00	1.332E+00	1.00560	3.114E+03	1.749E+04
1.00000	0.000E+00	0.000E+00	1.00600	6.019E+03	2.110E+03
1.00040	1.827E+00	1.821E+00	1.00640	1.177E+04	8.177E+02
1.00080	4.408E+00	4.336E+00	1.00680	2.320E+04	4.469E+02
1.00120	8.136E+00	7.863E+00	1.00720	4.596E+04	2.886E+02
1.00160	1.367E+01	1.291E+01	1.00760	9.121E+04	2.056E+02
1.00200	2.211E+01	2.031E+01	1.00800	1.810E+05	1.562E+02

Appendix II

The following is a comparison of the generalized oscillator strength obtained from the numerical and analytic solution for 54.4 eV. Z_c is the critical point of z.

Generalized Oscilator Strength
FOR AN ENERGY OF 54.40 EV

z	CROSS SECTION		z	CROSS SECTION	
	Numerical	Analytic		Numerical	Analytic
0.99640	3.482E-01	3.509E-01	1.00240	4.660E-01	3.930E-01
0.99680	3.508E-01	3.536E-01	1.00280	4.930E-01	3.960E-01
0.99720	3.536E-01	3.562E-01	1.00320	5.240E-01	3.990E-01
0.99760	3.566E-01	3.589E-01	1.00360	5.562E-01	4.021E-01
0.99800	3.598E-01	3.616E-01	1.00400	5.812E-01	4.052E-01
0.99840	3.634E-01	3.644E-01	1.00440	5.789E-01	4.083E-01
0.99880	3.674E-01	3.671E-01	1.00480	5.031E-01	4.114E-01
0.99920	3.719E-01	3.699E-01	Z_c=1.00520	2.519E-01	4.146E-01
0.99960	3.772E-01	3.727E-01	1.00560	-3.972E-01	4.178E-01
1.00000	3.834E-01	3.755E-01	1.00600	-1.927E+00	4.210E-01
1.00040	3.909E-01	3.784E-01	1.00640	-5.376E+00	4.243E-01
1.00080	4.001E-01	3.812E-01	1.00680	-1.297E+01	4.276E-01
1.00120	4.115E-01	3.841E-01	1.00720	-2.943E+01	4.309E-01
1.00160	4.259E-01	3.871E-01	1.00760	-6.470E+01	4.342E-01
1.00200	4.438E-01	3.900E-01	1.00800	-1.396E+02	4.376E-01

Appendix III

The following is the comparison of the cross sections for m=0 calculated using the coefficients from eq(6) (by numerical calculation), the numerical and analyti solutions. Z_c is the critical point of z.

	CROSS SECTION		
z	eq(6)	numerical	analytic
0.9964000	17.59354	1.658E+01	1.665E+01
0.9968000	19.30448	1.817E+01	1.824E+01
0.9972000	21.27625	2.001E+01	2.007E+01
0.9976000	23.56468	2.215E+01	2.219E+01
0.9980000	26.24119	2.465E+01	2.466E+01
0.9984000	29.39923	2.761E+01	2.757E+01
0.9988000	33.16152	3.116E+01	3.103E+01
0.9992000	37.69249	3.546E+01	3.517E+01
0.9996001	43.21677	4.075E+01	4.020E+01
1.000000	50.04342	4.736E+01	4.639E+01
1.000400	58.61216	5.580E+01	5.412E+01
1.000800	69.55167	6.684E+01	6.396E+01
1.001200	83.78282	8.164E+01	7.674E+01
1.001600	102.6775	1.021E+02	9.377E+01
1.002000	128.3184	1.313E+02	1.172E+02
1.002400	163.9262	1.745E+02	1.505E+02
1.002800	214.5656	2.408E+02	2.004E+02
1.003200	288.3530	3.465E+02	2.800E+02
1.003600	398.4980	5.213E+02	4.184E+02
1.003999	566.8372	8.207E+02	6.918E+02
1.004399	829.9591	1.351E+03	1.357E+03
1.004799	1249.917	2.316E+03	3.773E+03
Z_c=1.005199	1932.939	4.118E+03	3.413E+04
1.005599	3062.533	7.548E+03	3.360E+04
1.005999	4957.213	1.418E+04	3.753E+03
1.006399	8172.682	2.712E+04	1.353E+03
1.006799	13680.27	5.258E+04	6.903E+02
1.007199	23179.92	1.028E+05	4.176E+02
1.007599	39644.59	2.020E+05	2.796E+02
1.007999	68271.29	3.977E+05	2.002E+02