# Dependence of extrapolated A0 on fitting function

The Mott asymmetry extrapolated to zero foil thickness depends on the functional form of the fit of the data. In parallel with simulations, a statistical investigation of fitting functions was undertaken. Many extrapolation formulae have been used previously to approximate the data and extrapolate to the zero foil thickness for comparison with theoretical calculations with no clear consensus on the optimal function for fitting. While a χ2 value can be calculated for the goodness of data to a function, it relies on the fact that the function is truly the parent distribution for the data, so both differences between the data and the function as well as between the function tested and the true parent distribution of the data are included in the χ2 value. Therefore, merely finding a function with a good χ2 value is not sufficient to determine that that functional form is the best form for extrapolating to find the extrapolated zero foil thickness value of asymmetry, A0.

To determine an uncertainty in A0 due to the uncertainty in the optimal fitting function for extrapolation, the method of Pade approximates was applied to the experimental Mott asymmetry data. Pade approximates are a class of rational fractions which are typically well behaved and converge more rapidly than Taylor series approximations to a set of data for extrapolation. The Pade approximant take the form

Equation

for m≥0 and n≥1. To determine the Pade approximant order (Pade (m,n)) required for the zero thickness extrapolation, the statistical F-test was used. The F-test gives guidance for the validity of adding an nth term to a function is defined as: (bevington, 1st ed, p 203)

Equation

where N is the number of data points, n+1 is the number of parameters in the fit, and X(n) is defined as

Equation

where yi are the data points, f(xi) the function at that same point, σi the uncertainty in the data, and the function is summed over all data points.

Fitting was done for these studies both using the programs Root (details) and Mathematica, where the fitting was performed by defining the function and using the “NonlinearModelFit” routine with the weight option set with each point weighted by wi= 1/σi2. Data were fitted with asymmetries on the y axis and thickness on the x axis, which requires a transformation of the larger thickness uncertainties to an equivalent uncertainty in asymmetry in order to fit the data and determine uncertainty in the value A0. In mathematica, this was performed manually and the same uncertainty transformation was used for all data. In root, the dx to dy transformation was handled using the TGraphErrors protocol (ref) which provides a better function-dependent transformation of the uncertainties. Therefore, the mathematica code was used for preliminary functional form investigation, but the Root fits of the final data set have more reliable values of A0 and the associated uncertainties.

Pade(n,m) approximants were tested varying the orders of both n and m until the F-test showed that adding the latest term was not statistically justified. The Pade orders tested were the following:

Pade (1,0): A= a0+a1T

Pade (2,0): A= a0+ a1T+a2T2

Pade (3,0): A= a0+ a1T+ a2T2+ a3T3

Pade (0,1): A=1/(1+b1T)

Pade (0,2): A=1/(1+b1T+b2T2)

Pade (1,1): (a0+a1T)/(1+b1T)

Pade(1,2): A= a0+a1T /(1+b1T+b2T2)

Pade (2,1): A= (a0+ a1T+a2T2) /(1+b1T)

Since these Pade approximant orders are nested functions, the F-testing procedure described above can be used to determine if adding the next term in the series can be rejected to a given confidence level. Higher order Pade functions were also investigated, but as shown below, eliminated due to the statistical F-test results.

The functions that have been historically used (ref Dunning and Gay review 1992) for fitting Mott foil thickness extrapolations are listed here. Column two shows that each historical fit function is either equivalent to one of the Pade approximant either directly or with slight transformations, or in the case of the exponential fit, the Taylor expansion of the function is equivalent to the Pade approximant. Therefore, the fitting functions that we will address consist of the class of Pade approximants with orders as high as necessary to be excluded using the F-test.

|  |  |
| --- | --- |
| **Fit from literature** | **Similar Pade approximant** |
| A=a+bT | Pade (1,0)) |
| A=a/(1+bT) | Pade (0,1) |
| 1/A=a+bT | invert, becomes Pade (0,1) |
| 1/√A=a+bT | equivalent to Pade (0,2) |
| ln(A)=a+bT | raise both sides to e, becomes a subset of exponential fit |
| A=a+becT | Taylor expansion:  (a+b)+bcT+ 0.5bc2T2+⅙bc3T3+order(T4)  Equivalent to Pade(3,0) or higher |

Table xx shows the array of Pade fits tested for the Run 2 data, with the orders in both n and m increased until the Ftest indicates that it is statistically likely (to the 95% percent level) that the last term added was unnecessary for adequately fitting the data. The functions with too many terms according to the Ftest are noted with the red x marks in table xx and testing higher order terms is not necessary. The results of the fits are shown in table (xx+1).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Pade order | Pade(0,m) | Pade(1,m) | Pade(2,m) | Pade(3,m) |
| Pade(n,0) |  |  |  |  |
| Pade(n,1) |  |  |  |  |
| Pade(n,2) |  |  |  |  |

Table shows a summary of the fits to the experimental data using the Pade(n,m) functions, with the red x on a graph indicating the the Ftest for the Pade order has determined, to a 95% confidence level, that the last term of the nested function was not required (the χ2 value did not increase sufficiently to justify adding the last term of the function).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Pade(n,m) order | Pade(0,m) | Pade(1,m) | Pade(2,m) | Pade(3,m) |
| Pade(n,0) |  | 43.8-0.011x  Ftest: n/a  Reduced χ2: 2.24  A=43.8463 ± 0.1447 | 44.12+0.014x+3.8e-6x2  Ftest: 12.9  Reduced χ2: 0.96  A=44.1176 ± 0.1211 | 44.35=0.019x+1.8e-5x2-1.05e-8x3  **Ftest: 5.23, DOF 7**  Reduced χ2: 0.63  A=44.3513 ± 0.1416 |
| Pade(n,1) | 44.09/(1+3e-4x)  Ftest: 12.6  Reduced χ2: 0.98  A=44.0855 ± 0.0974 | (44.2+.0052x)/(1+.00045x)  Ftest: 11.7, DOF7  Reduced χ2: 1.14  A=44.1749 ± 0.1276 | (43.8-0.031x+6e-6x2)/(1-4.5e-4x)  **Ftest: -2.4, DOF6**  Reduced χ2: 2.97  A=43.7843 ± 0.2105 |  |
| Pade(n,2) | 44.17/(1+3e-4x-3.2e-8x2)  **Ftest: 0.94 DOF7**  Reduced χ2: 0.986  A=44.1656 ± 0.1241 | (44.3+.15x)/(1+.0037x+9.4e-7x2)  **Ftest: .733, DOF6**  Reduced χ2: 1.19  A=44.2735 ± 0.06015 |  |  |

Table shows the fitted function for each Pade order, the Ftest value for comparing to a lower order Pade function with the degrees of freedom of the fit, and the value for the reduced χ2 for the fit. The final line of each has the asymmetry value extrapolated to zero thickness with standard error of the fit.

## Summary of fits

The results of the Pade approximant study of the fitting function for the Run 1 data, with the cuts of ‑0.5σ to +2σ, with the dilution subtraction as described (by Daniel) are summarized in Table 3.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Pade(n,m)**  **Run 2** | **intercept** | **dA** | **red. χ2** | **dof** | **Ftest** | **Accept/Reject** |
| (1,0) | 43.844 | 0.146 | 2.38 | 9 | n/a |  |
| (2,0) | 44.117 | 0.123 | 1.03 | 8 | 12.9 (vs Pade 1,0) |  |
| (3,0) | ~~44.353~~ | 0.143 | 0.672 | 7 | 5.21 (vs Pade 2,0) | Reject: Ftest |
| (0,1) | 44.084 | 0.0989 | 1.047 | 8 | 12.43 (vs Pade 1,0) |  |
| (0,2) | ~~44.166~~ | 0.125 | 1.05 | 7 | 0.98 (vs Pade 0,1) | Reject: Ftest |
| (1,1) | 44.176 | 0.129 | 1.21 | 7 | 11.7 (vs Pade 1,0) |  |
| (1,2) | ~~44.268~~ | 0.654 | 1.27 | 6 | 0.704 (vs Pade 1,1) | Reject: Ftest |
| (2,1) | ~~43.78~~ | 0.217 | 3.17 | 6 | -2.4 (vs Pade 1,1), constrained a0<50 | Reject: Ftest |

Table : Pade orders investigated, values of A0, dA0, Reduced χ2, Ftest and if the Ftest shows that the term is rejected.

Table 4 shows the same Pade formulation, but for the Run 1 data.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Pade(n,m)**  **Run 1** | **intercept** | **dA** | **red. χ2** | **dof** | **Ftest** | **Accept/Reject** |
| (1,0) | 43.831 | 0.124 | 1.85 | 9 | n/a |  |
| (2,0) | 44.036 | 0.116 | 0.993 | 8 | 8.8 |  |
| (3,0) | ~~44.232~~ | 0.150 | 0.79 | 7 | 2.99 | Reject: Ftest 95% conf. |
| (0,1) | 44.057 | 0.090 | 0.940 | 8 | 9.75 |  |
| (0,2) | ~~44.078~~ | 0.121 | 1.06 | 7 | 0.06 | Reject: Ftest |
| (1,1) | 44.079 | 0.122 | 1.24 | 7 | 7.44 |  |
| (1,2) | ~~44.082~~ | 0.213 | 4.49 | 6 | 0.013 | Reject: Ftest |
| (2,1) | ~~45.198~~ | 5.52 | 1.08 | 6 | 2.33 | Reject: Ftest |

Table Pade approximant results for experimental data from Run 1.

As shown in Tables 3 and 4, many of the higher order Pade fits are rejected to a 95% confidence level by the F-test, leaving the Pade (1,0), Pade(2,0), Pade (0,1) and Pade(1,1) as viable fitting functions for the extrapolation to the asymmetry value at zero foil thickness.

The distribution of values of Ao vs. the non-excluded fitting functions is shown in Figure 1 below. There is a clear clustering of the values around 44.06, with the Pade(1,0), or linear fit the farthest outlier. A Gaussian representation of the mean and standard deviation of the full data set is shown by the blue curve, and the distribution for the mean and std dev of the data with the Pade(1,0) removed from the data set is shown by the green curve.

Figure : Distribution of the values for A0 extrapolated using the non-excluded Pade(n,m) terms.

The Pade(1,0), or linear fit, to the data appears to be a poor fit by eye. However, the fit cannot be excluded based on an F test since it has no lower order function to compare to, nor can it be rejected outright based on the χ2 value (though 2.38 and 1.85 for a 9 degree of freedom fit have 95 and 99% associated in the chart – any way to exclude based on that?). To investigate the dependence of the linear fit to the data on the number of target foils in the data set, successive target foils were removed from the fit starting with the thickest. Indeed, the Pade(1,0) fit increases with each foil removed toward a value more consistent with the other values, but when removing successive target foils from the data set, the other functions approximating the data also have deviations when, in particular, the foilset is reduced to the thinnest 5 and 6 data points

(Add images of Daniels successive fits here if we are keeping this section)

These need to be redone with corrected values

\*\*This section to be revisited with better values for dR

The alternative to using the measured foil thickness to extrapolate to zero thickness is to rather use asymmetry vs rate for the extrapolation to the asymmetry at zero rate. These have been investigated using the pade approximant formalism, and are summarized here for first run 1 then run 2.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Pade(n,m)**  **Run 1**  **A vs. Rate** | **intercept** | **dA** | **red. χ2** | **dof** | **Ftest** | **Accept/Reject** | **χ2 liklihood table** |
| (1,0) | ~~42.76~~ | .343 | 44 | 9 | n/a | Reject: χ2 |  |
| (2,0) | 43.95 | .100 | 1.59 | 8 | 241 |  |  |
| (3,0) | ~~44.05~~ | .110 | 1.30 | 7 | 2.84 | Reject: Ftest |  |
| (0,1) | ~~43.36~~ | .236 | 18.0 | 8 | 14.07 | Reject: χ2 |  |
| (0,2) | 44.07 | .090 | 1.25 | 7 | 108 |  |  |
| (0,3) | 43.96 | 0.105 | 2.02 | 6 | -1.64 | Reject Ftest |  |
| (1,1) | 44.12 | 0.100 | 1.56 | 7 | 248 |  |  |
| (1,2) | ~~44.28~~ | 0.270 | 3.16 | 6 | -2.03 | Reject Ftest |  |
| (2,1) | ~~44.04~~ | 0.118 | 1.80 | 6 | 0.21 | Reject Ftest |  |
| A=a+be^(cT) | 44.06 | 0.0355 | 1.78 | 9 | 216 |  |  |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Pade(n,m)**  **Run 2**  **A vs. Rate** | **intercept** | **dA** | **red. χ2** | **dof** | **Ftest** | **Accept/Reject** | **χ2 liklihood table** |
| (1,0) | ~~42.71~~ | .381 | 46.9 | 9 | n/a | Reject: χ2 |  |
| (2,0) | 43.96 | .205 | 5.74 | 8 | 65.5 |  |  |
| (3,0) | ~~44.20~~ | .217 | 4.36 | 7 | 3.53 | Reject: Ftest |  |
| (0,1) | ~~43.29~~ | .288 | 23.53 | 8 | 9.95 | Reject: χ2 |  |
| (0,2) | 44.11 | .193 | 5.02 | 7 | 30.5 |  |  |
| (0,3) | ~~43.97~~ | .217 | 7.53 | 6 | 0 | Reject: Ftest |  |
| (1,1) | 44.19 | .201 | 5.35 | 7 | 72.9 |  |  |
| (1,2) | ~~44.31~~ | .320 | 6.26 | 6 | 0.13 | Reject Ftest |  |
| (2,1) | ~~44.26~~ | .291 | 6.26 | 6 | 0.13 | Reject Ftest |  |
| A=a+be^(cT) | 44.12 | 0.074 | 6.94 | 9 | 61.9 |  |  |