

Time of Flight Data Analysis

This is a brief discussion of how to analyze the TOF data for thermal neutrons. For information about the experiment and equipment see <http://norbert.mit.edu/reactor/>.

The flux of neutrons with speeds between v and $v + dv$ will be proportional to

$$j(v) dv = n \sqrt{\frac{2}{\pi}} \left(\frac{v}{v_0} \right)^3 e^{-(v/v_0)^2} dv$$

where

$$v_0 = \sqrt{2k_B T/m} \approx 2300 \text{ ms}^{-1}.$$

If the detector efficiency is proportional to $1/v$ we might expect a neutron counting rate for neutrons with speeds between v and $v + dv$ to be proportional to

$$\left(\frac{v}{v_0} \right)^2 e^{-(v/v_0)^2} dv$$

However, the chopper passes neutrons for a finite period of time every time it opens. Thus the time of flight of the neutrons from the chopper to the detector varies and the counts in each channel of the MCS represent neutrons that have a range of speeds. When the detector is close to the chopper, that does not matter much as neutrons of all speeds present in the beam will arrive at the detector at the same time (on the scale of the time resolution for the chopper) and the counts in the MCS will just measure the transmission of the chopper as a function of time. That function will be the convolution of two slits each 1.0 mm wide and will therefore be triangular in shape. The chopper wheel spins at 1800 rpm and the slits are at a radius of 54.5 mm. From this, it is easy to calculate that the triangular transmission function of the chopper should have a half-width at the base of $95 \mu\text{s}$. This was verified by fitting the TOF spectrum obtained when the BF_3 detector was 3.25 m from the chopper. I will use the variable t_H to represent the $95 \mu\text{s}$ half-width of the chopper transmission. I will also use ℓ to be the distance from the chopper to the BF_3 detector and consider the neutrons counted into channel m of the MCS. The sweep of the MCS is triggered by a light pulse some time before the chopper opens. I assume that the MCS is counting into channel n_0 when the chopper transmission is maximum.

Now let's consider channel m of the MCS. It will represent a time $t_m = t_D(m - n_0)$ with respect to the time the chopper was maximally open. Note that t_m may be negative. If $t_m \leq -t_H$ no neutrons will have had time to reach the detector. For $t_m > -t_H$, there are three time regions to consider when calculating the neutron speeds that will be counted into channel m . They are $-t_H < t_m \leq 0$, $0 < t_m \leq t_H$ and $t_m > t_H$.

The easiest way to do the calculations is to consider the travel time t of the neutrons from the chopper to the detector. When integrating over the range of speeds for neutrons that will be counted into channel m , it will be necessary to include a factor that represents the triangular transmission function of the chopper. It will also be useful to introduce a new variable $y = v/v_0 = \ell/(v_0 t)$ which means $t = \ell/(v_0 y)$ and $dt = -(\ell/v_0)(1/y^2) dy$.

What we want to integrate over these three time regions is the number of neutrons whose travel time lies between t and $t + dt$. As the number whose speed is between v and $v + dv$ is proportional to $y^2 e^{-y^2} dv$ and $t = \ell/v$, the number whose travel time is between t and $t + dt$ will be proportional to $y^4 e^{-y^2} dt$.

Some useful integrals will be:

$$\begin{aligned} \int_{y_1}^{y_2} e^{-y^2} dy &= \frac{\sqrt{\pi}}{2} [\Phi(y_2) - \Phi(y_1)] \quad \text{where} \quad \Phi(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt, \\ \int_{y_1}^{y_2} y e^{-y^2} dy &= -\frac{1}{2} \int_{y_1^2}^{y_2^2} e^{-z} dz = \frac{1}{2} (e^{-y_1^2} - e^{-y_2^2}), \\ \int y^2 e^{-y^2} dy &= -\frac{1}{2} y e^{-y^2} + \frac{1}{2} \int e^{-y^2} dy. \end{aligned}$$

The calculations are given below. The neutron count rate will be proportional to $\mathcal{R}(m)$ and the factor $1/t_H$ is included to make the result dimensionless.

$$\underline{-t_H < t_m \leq 0}$$

$$\begin{aligned} \mathcal{R}(m) &= \frac{1}{t_H} \int_0^{t_H+t_m} \left(\frac{t_H + t_m - t}{t_H} \right) y(t)^4 e^{-y(t)^2} dt \\ &= \frac{\ell}{v_0 t_H} \int_{y_1}^{\infty} \left[\left(1 + \frac{t_m}{t_H} \right) y^2 - \frac{\ell}{v_0 t_H} y \right] e^{-y^2} dy \quad \text{where} \quad y_1 = \frac{\ell}{v_0(t_m + t_H)} \\ &= \frac{1}{2} \frac{\ell}{v_0 t_H} \left(1 + \frac{t_m}{t_H} \right) \left(\frac{\sqrt{\pi}}{2} [1 - \Phi(y_1)] + y_1 e^{-y_1^2} \right) - \frac{1}{2} \left(\frac{\ell}{v_0 t_H} \right)^2 e^{-y_1^2} \end{aligned}$$

$$\underline{0 < t_m \leq t_H}$$

$$\begin{aligned} \mathcal{R}(m) &= \frac{1}{t_H} \int_0^{t_m} \left(\frac{t_H - t_m + t}{t_H} \right) y(t)^4 e^{-y(t)^2} dt + \frac{1}{t_H} \int_{t_m}^{t_H+t_m} \left(\frac{t_H + t_m - t}{t_H} \right) y(t)^4 e^{-y(t)^2} dt \\ &= \frac{\ell}{v_0 t_H} \int_{y_1}^{y_m} \left[\left(1 + \frac{t_m}{t_H} \right) y^2 - \frac{\ell}{v_0 t_H} y \right] e^{-y^2} dy + \frac{\ell}{v_0 t_H} \int_{y_m}^{\infty} \left[\left(1 - \frac{t_m}{t_H} \right) y^2 + \frac{\ell}{v_0 t_H} y \right] e^{-y^2} dy \\ &= \frac{1}{2} \frac{\ell}{v_0 t_H} \left\{ \frac{\sqrt{\pi}}{2} [1 - \Phi(y_1)] + y_1 e^{-y_1^2} \right. \\ &\quad \left. - \frac{t_m}{t_H} \left(\frac{\sqrt{\pi}}{2} [1 + \Phi(y_1) - 2\Phi(y_m)] + 2y_m e^{-y_m^2} - y_1 e^{-y_1^2} \right) \right\} \\ &\quad + \frac{1}{2} \left(\frac{\ell}{v_0 t_H} \right)^2 [e^{-y_1^2} - 2e^{-y_m^2}] \quad \text{where} \quad y_m = \frac{\ell}{v_0 t_m}. \end{aligned}$$

$t_m > t_H$

$$\begin{aligned}
\mathcal{R}(m) &= \frac{1}{t_H} \int_{t_m - t_H}^{t_m} \left(\frac{t_H - t_m + t}{t_H} \right) y(t)^4 e^{-y(t)^2} dt + \frac{1}{t_H} \int_{t_m}^{t_H + t_m} \left(\frac{t_H + t_m - t}{t_H} \right) y(t)^4 e^{-y(t)^2} dt \\
&= \frac{\ell}{v_0 t_H} \int_{y_1}^{y_m} \left[\left(1 + \frac{t_m}{t_H} \right) y^2 - \frac{\ell}{v_0 t_H} y \right] e^{-y^2} dy + \frac{\ell}{v_0 t_H} \int_{y_m}^{y_2} \left[\left(1 - \frac{t_m}{t_H} \right) y^2 + \frac{\ell}{v_0 t_H} y \right] e^{-y^2} dy \\
&= \frac{1}{2} \frac{\ell}{v_0 t_H} \left\{ \frac{\sqrt{\pi}}{2} [\Phi(y_2) - \Phi(y_1)] + y_1 e^{-y_1^2} - y_2 e^{-y_2^2} \right. \\
&\quad \left. - \frac{t_m}{t_H} \left(\frac{\sqrt{\pi}}{2} [\Phi(y_2) + \Phi(y_1) - 2\Phi(y_m)] + 2y_m e^{-y_m^2} - y_1 e^{-y_1^2} - y_2 e^{-y_2^2} \right) \right\} \\
&\quad + \frac{1}{2} \left(\frac{\ell}{v_0 t_H} \right)^2 \left[e^{-y_1^2} + e^{-y_2^2} - 2e^{-y_m^2} \right] \quad \text{where } y_2 = \frac{\ell}{v_0(t_m - t_H)}.
\end{aligned}$$

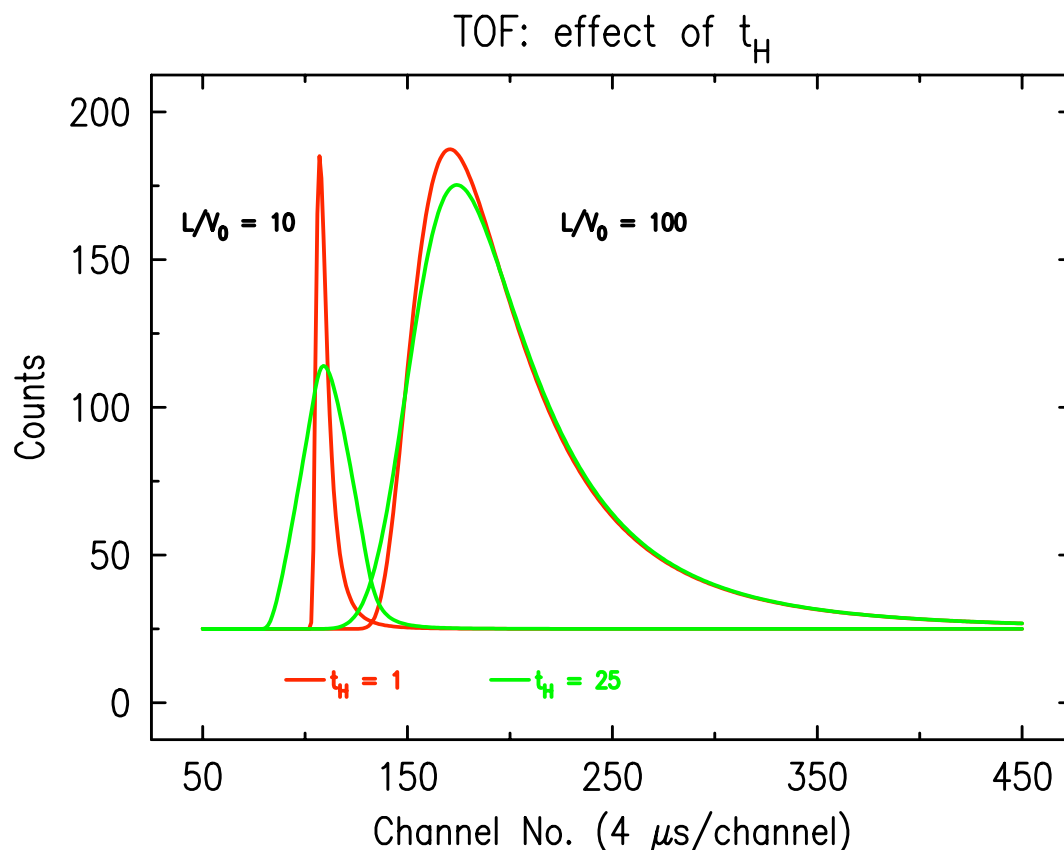
Thus $\mathcal{R}(m)$ has exponentials along with error functions. These should not be too hard to evaluate numerically for fitting purposes. Most compiler libraries provide them. The Gnu Scientific Library (<http://www.gnu.org/software/gsl/>) has routines for both of these functions. The exponential function goes rapidly to zero for large x and can lead to floating point underflows. I used code provided in the GSL library to deal with that.

When writing the fitting code, it is easy to measure time in MCS channel number units and use the dwell time to convert to μs after the fit. Pages 7 and 8 list the model function code that I used. It is written in C and there are some global variables: **NO** is n_0 , **X** is the channel number so that **m** = **X** - **NO** is t_m , **HW** is t_H , **PK** - **NO** is ℓ/v_0 , all expressed in channel number units. The quantities **NO**, **PK**, **HW**, **BG** and **SF** are the parameters that may be varied in the fit. Once **HW** and **NO** have been found from fitting data taken with the detector close to the chopper, they are then held fixed. (The value of **HW** found from the fit should, of course, agree with the calculated value from the chopper and slit dimensions and chopper rotation speed.)

My code was written for a nice fitting/plotting package called *C-Plot*, available from Certified Scientific Software (<http://www.certif.com/>). You could use it as pseudocode to guide code you write for *Matlab* or some other package.

Necessity:

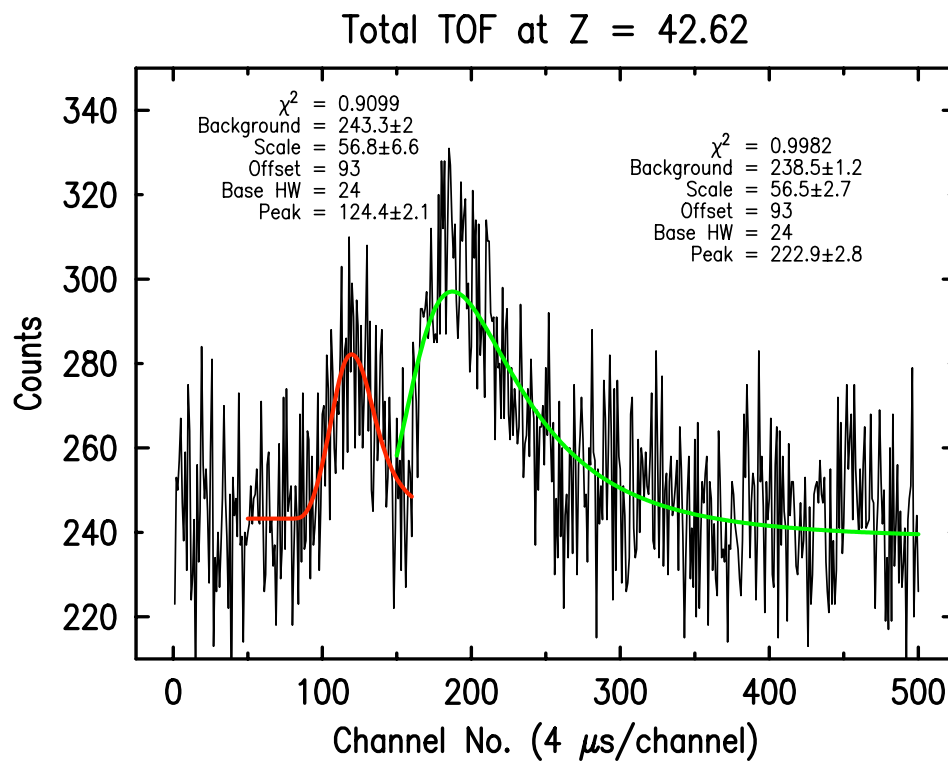
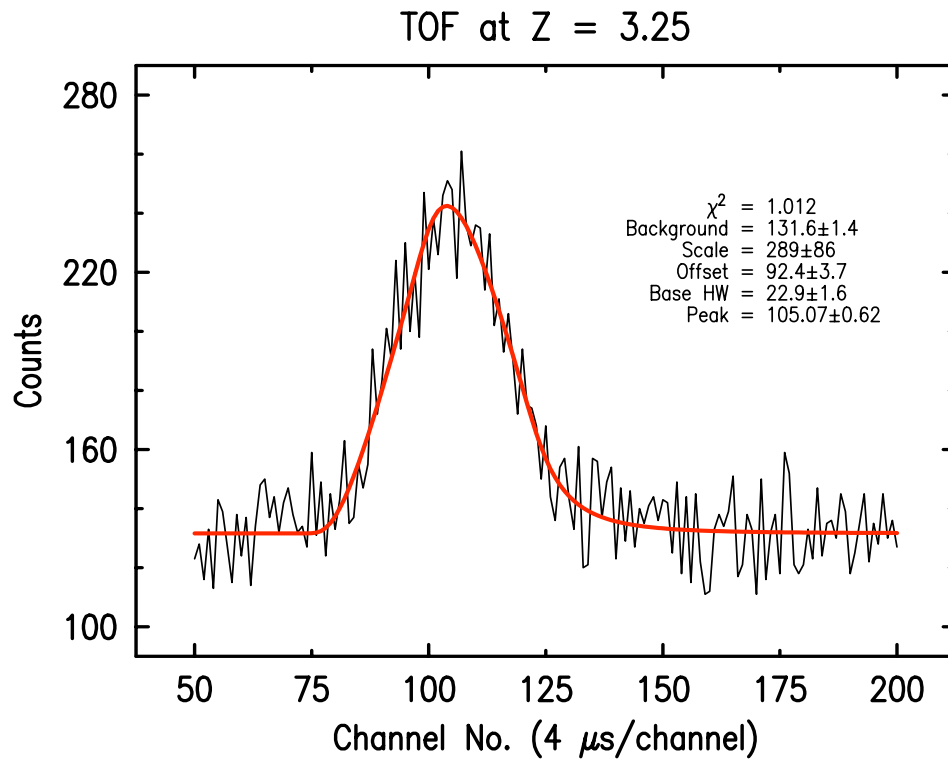
How necessary is this correction for the finite opening time of the chopper? As you might expect, it depends on how t_H compares to the time for the neutrons to travel to the detector. The graph below shows some calculated fits with $t_H = 25$ channels (close to the $95 \mu s$ calculated value for the chopper) and $t_H = 1$ channel, essentially no correction for chopper open time. I used $n_0 = 100$ channels, which is close to correct for the apparatus. The plots are for thermal spectra with $\ell/v_0 = 10$ channels and $\ell/v_0 = 100$ channels; the latter is about what one expects for $t_D = 4 \mu s$ and thermal neutrons when $\ell = 1$ m.



The correction is not important for thermal neutrons at $\ell = 1$ m, but it matters close to the chopper and for the epithermal peak seen in the spectrum at $\ell = 1$ m.

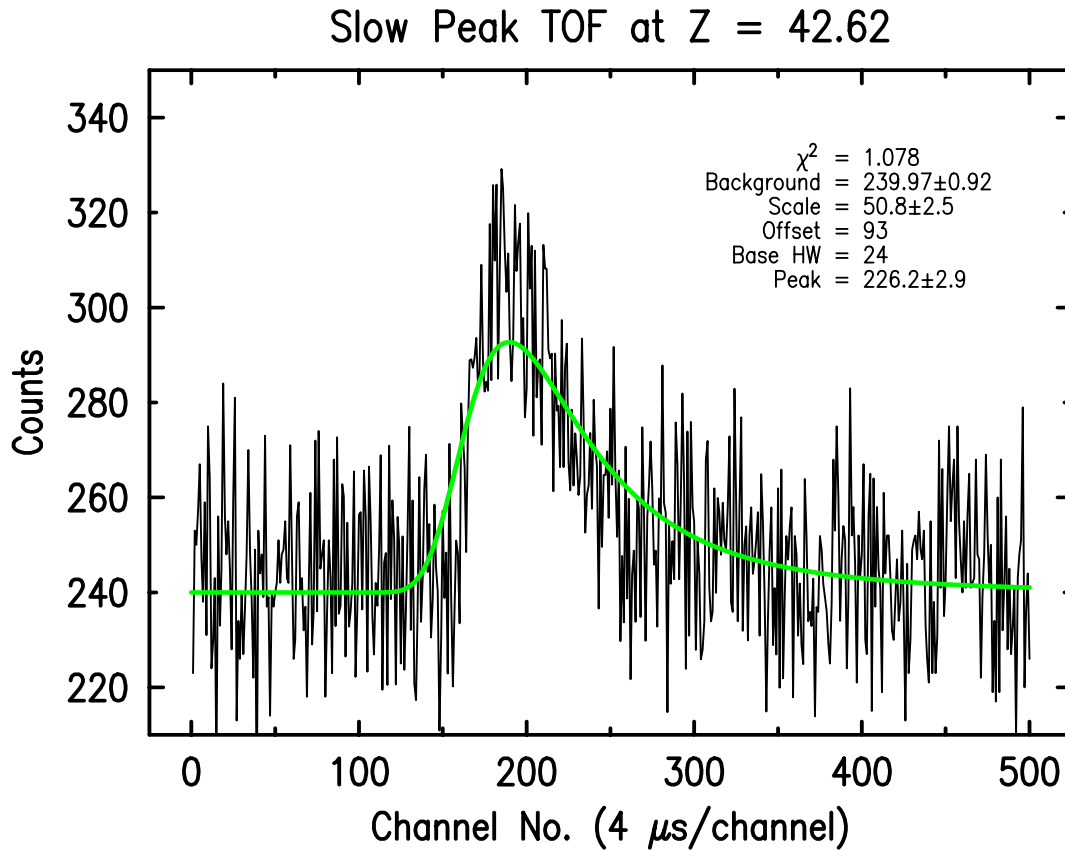
The fast peak above has a speed about $2.5 \times 10^4 \text{ m s}^{-1}$, obtained from the peak position shift of about $45 \mu s$ as the detector was moved 1.0 m. As the plot shows, a Maxwell-Boltzmann distribution with this v_0 would rise and fall so rapidly that the fit function is essentially the triangular transmission of the chopper. (The same must be true for whatever is the actual speed distribution of the fast neutrons.) This v_0 would correspond to a thermal distribution for $T \approx 3 \times 10^4$ K. The epithermal neutrons are moving so fast and their speed distribution is sufficiently narrow that even after they have travelled 1 m we cannot determine it with a chopper whose time resolution is given by $t_H \simeq 100 \mu s$. However it is very unlikely to be thermal.

Fits of the thermal functions to my data are shown on the next page; the fits and plots were made with *C-Plot*.



After 1 m, the scan appears to separate into two peaks. Each was fit individually to a thermal spectrum. One seems to have v_0 about 12 times the other.

Finally, the fit obtained to the fast peak portion of the scan was subtracted (with zero background) from the total data. This should, in principle, leave only the background and the neutron counts from the slow (thermal) neutrons. The data that resulted are shown in the plot below along with the fit to all of the data.



The result agrees with that obtained only by fitting data in channels above number 150. The value of v_0 obtained from the fit is about 2000 m/s. The value obtained using the peak shift from $Z = 3.25$ to $Z = 42.62$ ($\Delta\ell = 1.00$ m) would be 2100 m/s. The fast peak shift suggests a speed about 13000 m/s, while the average speed obtained from the fit of the $Z = 3.25$ data to a thermal spectrum (unreliable, in my view) would be $v_0 \simeq 20000$ m/s.

This suggests to me that 93 is too low for the offset channel number and a better value would be somewhere from 95 to 100. If the angle the chopper wheel has to rotate after the light pulse until the first slit is fully open were to be measured, then the offset channel number n_0 could be calculated.

```

#define RP 0.88622693 /* \sqrt{\pi}/2 */

double model(deriv_flag)
int deriv_flag;
{
    double m, p, yfit;
    double y1, y2, ym, r;
    double ey1, ey2, eym; /* exponentials */
    double py1, py2, pym; /* error functions */

    m = X - NO;
    p = PK - NO;
    if (p < 1.0) p = 1.0;
    if (m <= (-HW)) {
        r = 0;
    }
    else if (m <= 0) {
        y1 = p/(m+HW);
        py1 = gsl_sf_erf(y1);
        status = gsl_sf_exp_e(-y1*y1, &result);
        if (status) {
            ey1 = 0.0;
            if (status != GSL_EUNDRFLW)
                printf("exp(-y1*y1) m=%g %s\n", m, gsl_strerror(status));
        }
        else ey1 = result.val;
        r = (p/HW)*( RP*(1.0 - py1) + y1*ey1
            + (m/HW)*( RP*(1.0 - py1) + y1*ey1 ) - (p/HW)*ey1 );
    }
    else if (m <= HW) {
        y1 = p/(m+HW);
        py1 = gsl_sf_erf(y1);
        status = gsl_sf_exp_e(-y1*y1, &result);
        if (status) {
            ey1 = 0.0;
            if (status != GSL_EUNDRFLW)
                printf("exp(-y1*y1) m=%g %s\n", m, gsl_strerror(status));
        }
        ym = p/m;
        pym = gsl_sf_erf(ym);
        status = gsl_sf_exp_e(-ym*ym, &result);
        if (status) {
            eym = 0.0;
            if (status != GSL_EUNDRFLW)
                printf("exp(-ym*ym) m=%g %s\n", m, gsl_strerror(status));
        }
        else eym = result.val;
        r = (p/HW)*( RP*(1.0 - py1) + y1*ey1
            + (m/HW)*( RP*(2.0*pym - py1 - 1.0) - 2.0*ym*eym + y1*ey1 )
            - (p/HW)*(2.0*eym - ey1) );
    }
}

```

```

else { /* m > HW */
    y1 = p/(m+HW);
    py1 = gsl_sf_erf(y1);
    status = gsl_sf_exp_e(-y1*y1, &result);
    if (status) {
        ey1 = 0.0;
        if (status != GSL_EUNDRFLW)
            printf("exp(-y1*y1) m=%g %s\n", m, gsl_strerror(status));
    }
    else ey1 = result.val;
    ym = p/m;
    pym = gsl_sf_erf(ym);
    status = gsl_sf_exp_e(-ym*ym, &result);
    if (status) {
        eym = 0.0;
        if (status != GSL_EUNDRFLW)
            printf("exp(-ym*ym) m=%g %s\n", m, gsl_strerror(status));
    }
    else eym = result.val;
    y2 = p/(m-HW);
    py2 = gsl_sf_erf(y2);
    status = gsl_sf_exp_e(-y2*y2, &result);
    if (status) {
        ey2 = 0.0;
        if (status != GSL_EUNDRFLW)
            printf("exp(-y2*y2) m=%g %s\n", m, gsl_strerror(status));
    }
    else ey2 = result.val;
    r = (p/HW)*( RP*((py2 - py1) + y1*ey1 - y2*ey2
        + (m/HW)*(RP*(2.0*pym - py1 - py2)) - 2.0*ym*eym + y1*ey1 + y2*ey2 )
        - (p/HW)*(2.0*eym - ey1 - ey2) );
}
yfit = BG + SF * r;
if (deriv_flag) {
    if (fBG) dBG = 1;
    if (fSF) dSF = r;
}
return(yfit);
}

```


Consider a general case, convolving $y^\mu e^{-y^2}$ with a triangular chopper function. Here, μ does not have to be an integer. This gives incomplete Γ functions:

$$\int_{y_1}^{y_2} y^\mu e^{-y^2} = \frac{1}{2} \left\{ \Gamma\left(\frac{\mu+1}{2}, y_1^2\right) - \Gamma\left(\frac{\mu+1}{2}, y_2^2\right) \right\} \quad \text{where } \Gamma(\nu, x) = \int_x^\infty t^{\nu-1} e^{-t} dt.$$

$$\underline{-t_H < t_m \leq 0}$$

$$\begin{aligned} \mathcal{R}(m) &= \frac{1}{t_H} \int_0^{t_H+t_m} \left(\frac{t_H+t_m-t}{t_H} \right) y(t)^\mu e^{-y(t)^2} dt \\ &= \frac{\ell}{v_0 t_H} \int_{y_1}^\infty \left[\left(1 + \frac{t_m}{t_H} \right) y^{\mu-2} - \frac{\ell}{v_0 t_H} y^{\mu-3} \right] e^{-y^2} dy \quad \text{where } y_1 = \frac{\ell}{v_0(t_m+t_H)} \\ &= \frac{1}{2} \frac{\ell}{v_0 t_H} \left(1 + \frac{t_m}{t_H} \right) \Gamma\left(\frac{\mu-1}{2}, y_1^2\right) - \frac{1}{2} \left(\frac{\ell}{v_0 t_H} \right)^2 \Gamma\left(\frac{\mu-2}{2}, y_1^2\right) \end{aligned}$$

$$\underline{0 < t_m \leq t_H}$$

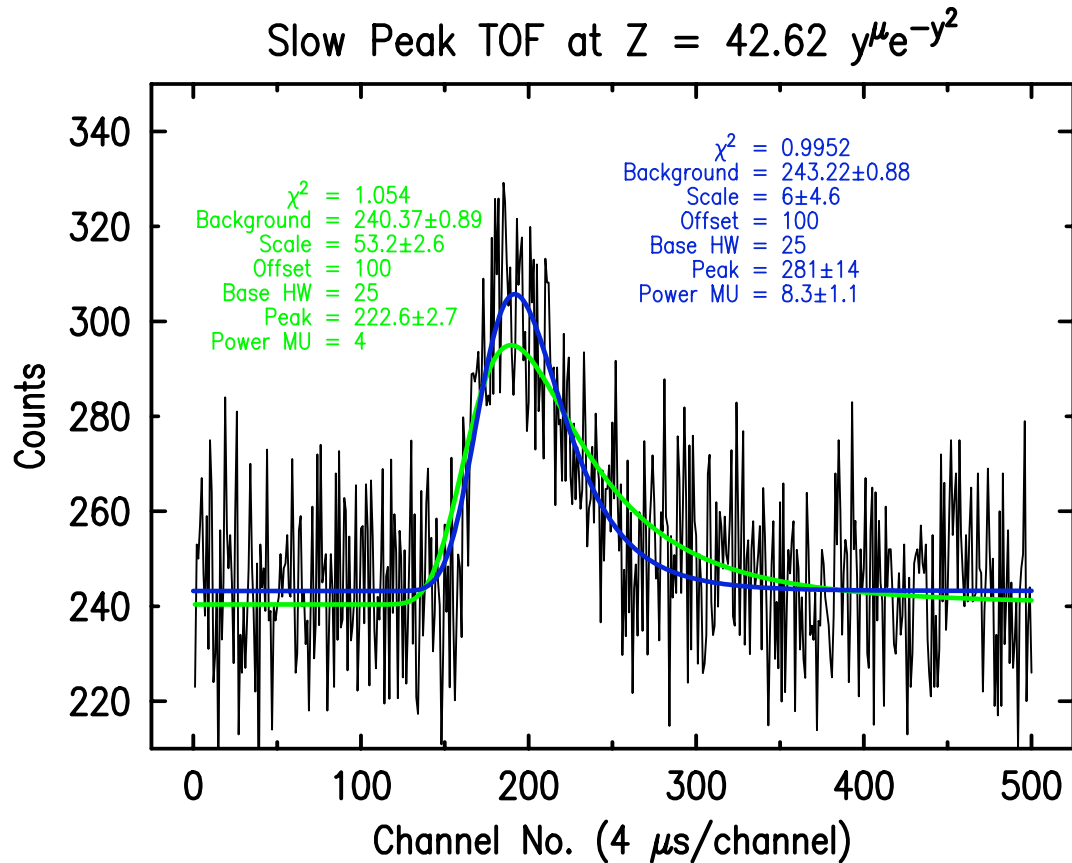
$$\begin{aligned} \mathcal{R}(m) &= \frac{1}{t_H} \int_0^{t_m} \left(\frac{t_H-t_m+t}{t_H} \right) y(t)^\mu e^{-y(t)^2} dt + \frac{1}{t_H} \int_{t_m}^{t_H+t_m} \left(\frac{t_H+t_m-t}{t_H} \right) y(t)^\mu e^{-y(t)^2} dt \\ &= \frac{\ell}{v_0 t_H} \int_{y_1}^{y_m} \left[\left(1 + \frac{t_m}{t_H} \right) y^{\mu-2} - \frac{\ell y^{\mu-3}}{v_0 t_H} \right] e^{-y^2} dy + \frac{\ell}{v_0 t_H} \int_{y_m}^\infty \left[\left(1 - \frac{t_m}{t_H} \right) y^{\mu-2} + \frac{\ell y^{\mu-3}}{v_0 t_H} \right] e^{-y^2} dy \\ &= \frac{1}{2} \frac{\ell}{v_0 t_H} \left\{ \Gamma\left(\frac{\mu-1}{2}, y_1^2\right) + \frac{t_m}{t_H} [\Gamma\left(\frac{\mu-1}{2}, y_1^2\right) - 2\Gamma\left(\frac{\mu-1}{2}, y_m^2\right)] \right\} \\ &\quad - \frac{1}{2} \left(\frac{\ell}{v_0 t_H} \right)^2 [\Gamma\left(\frac{\mu-2}{2}, y_1^2\right) - 2\Gamma\left(\frac{\mu-2}{2}, y_m^2\right)] \quad \text{where } y_m = \frac{\ell}{v_0 t_m}. \end{aligned}$$

$$\underline{t_m > t_H}$$

$$\begin{aligned} \mathcal{R}(m) &= \frac{1}{t_H} \int_{t_m-t_H}^{t_m} \left(\frac{t_H-t_m+t}{t_H} \right) y(t)^\mu e^{-y(t)^2} dt + \frac{1}{t_H} \int_{t_m}^{t_H+t_m} \left(\frac{t_H+t_m-t}{t_H} \right) y(t)^\mu e^{-y(t)^2} dt \\ &= \frac{\ell}{v_0 t_H} \int_{y_1}^{y_m} \left[\left(1 + \frac{t_m}{t_H} \right) y^{\mu-2} - \frac{\ell y^{\mu-3}}{v_0 t_H} \right] e^{-y^2} dy + \frac{\ell}{v_0 t_H} \int_{y_m}^{y_2} \left[\left(1 - \frac{t_m}{t_H} \right) y^{\mu-2} + \frac{\ell y^{\mu-3}}{v_0 t_H} \right] e^{-y^2} dy \\ &= \frac{1}{2} \frac{\ell}{v_0 t_H} \left\{ \Gamma\left(\frac{\mu-1}{2}, y_1^2\right) - \Gamma\left(\frac{\mu-1}{2}, y_2^2\right) + \frac{t_m}{t_H} [\Gamma\left(\frac{\mu-1}{2}, y_1^2\right) + \Gamma\left(\frac{\mu-1}{2}, y_2^2\right) - 2\Gamma\left(\frac{\mu-1}{2}, y_m^2\right)] \right\} \\ &\quad - \frac{1}{2} \left(\frac{\ell}{v_0 t_H} \right)^2 [\Gamma\left(\frac{\mu-2}{2}, y_1^2\right) + \Gamma\left(\frac{\mu-2}{2}, y_2^2\right) - 2\Gamma\left(\frac{\mu-2}{2}, y_m^2\right)] \quad \text{where } y_2 = \frac{\ell}{v_0(t_m-t_H)}. \end{aligned}$$

A Puzzle?

I derived the result on the previous page so I could write a fitting program that would convolve $y^3 e^{-y^2}$ to see if the TOF approach would be able to measure the $1/v$ absorption cross section of materials placed in the beam. Once I had a program that could vary the exponent of y^μ continuously, I thought it would be interesting to try it on the slow thermal peak of page 6. Here is the result.



The data are too noisy to permit a claim that one fit is to be preferred to the other. The sharper and narrower peak of the $y^{8.3}$ model does seem to look a bit better, but my understanding of the spectrometer gives no reason to support the idea.

Certainly, this approach does not seem to be a good one to test if absorbing materials have a $1/v$ cross section. These data were taken with a 1 hour counting time; it might be interesting to see what would emerge from a run of 9 hours.