Notes EESL

Jaco ter Hoeve

October 20, 2020

Goal: we want to find the single scattering distribution $S(E)$ from a Gaussian signal $J(E)$ that got smeared out by a Gaussian zero loss peak (ZLP).

1 All orders calculation

As our definitions of the Fourier Transform we take

$$f(E) = \int_{-\infty}^{\infty} d\nu \hat{f}(\nu) e^{-2\pi i \nu E} \tag{1}$$

$$\hat{f}(\nu) = \int_{-\infty}^{\infty} dE f(E) e^{2\pi i \nu E}. \tag{2}$$

According to eq. (4.8) in Egerton, the Fourier transforms of the zero-loss peak $Z(E)$, the single scattering distribution $S(E)$ and the recorded spectrum $J(E)$ are related as

$$s(\nu) = I_0 \log \left[\frac{j(\nu)}{z(\nu)} \right], \tag{3}$$

where the Fourier transforms have been written in lower case.

Next, we want to find $z(\nu)$ and $j(\nu)$. Since $Z(E)$ is a Gaussian centered around zero, we have

$$Z(E) = \frac{I_0}{\sqrt{2\pi\sigma_B^2}} e^{-E^2/2\sigma_B^2}. \tag{4}$$

The recorded spectrum is also Gaussian, but centered around $E_s \neq 0$:

$$J(E) = \frac{I_s}{\sqrt{2\pi\sigma_s^2}} e^{-(E-E_s)^2/2\sigma_s^2}. \tag{5}$$

Let us Fourier transform $Z(E)$ in order to find $z(\nu)$:

$$\begin{aligned}
z(\nu) &= \frac{I_0}{\sqrt{2\pi\sigma_B^2}} \int dE \exp\left[-E^2/2\sigma_B^2\right] \exp[2\pi i\nu E] \\
&= \frac{I_0}{\sqrt{2\pi\sigma_B^2}} \int dE \exp\left[-\frac{1}{2\sigma_B^2}(E^2 - 4\pi i\sigma_B^2\nu E)\right] \\
&= \frac{I_0}{\sqrt{2\pi\sigma_B^2}} \int dE \exp\left[-\frac{1}{2\sigma_B^2}\left((E - 2\pi i\sigma_B^2\nu)^2 + 4\pi^2\sigma_B^4\nu^2\right)\right] \\
&= \frac{I_0}{\sqrt{2\pi\sigma_B^2}} \sqrt{2\pi\sigma_B^2} \exp[-2\pi^2\sigma_B^2\nu^2] \\
&= I_0 \exp[-2\pi^2\sigma_B^2\nu^2], \qquad (6)
\end{aligned}$$

which is another Gaussian. The Fourier Transform of $J(E)$ can readily be found by noting that the Fourier transform of a translated function f is related to the Fourier transform of the original function by a complex phase multiplication:

$$\mathcal{F}[f(E - E_s)] = e^{2\pi i\nu E_s}\mathcal{F}[f(E)] \qquad (7)$$

We will quickly show this.

$$\begin{aligned}
f(E - E_s) &= \int d\nu \hat{f}(\nu) e^{-2\pi i\nu(E-E_s)} \qquad (8) \\
&= \int d\nu \hat{f}(\nu) e^{2\pi i\nu E_s} e^{-2\pi i\nu E} \qquad (9) \\
&= \int d\nu \mathcal{F}[f(E - E_s)] e^{-2\pi i\nu E}, \qquad (10)
\end{aligned}$$

which proves (7). Therefore, using identity (7) together with equations (5) and (6) gives

$$j(\nu) = I_s e^{2\pi i\nu E_s} e^{-2\pi^2\sigma_s^2\nu^2}. \qquad (11)$$

Note that the Fourier transform of a shifted Gaussian is no longer real. We now substitute (6) and (11) into (3) to find

$$\begin{aligned}
\frac{s(\nu)}{I_0} &= \log j(\nu) - \log z(\nu) \\
&= -2\pi^2\sigma_s^2\nu^2 + 2\pi i\nu E_s + 2\pi^2\sigma_B^2\nu^2 + \log\frac{I_s}{I_0} \\
&= 2\pi^2\nu^2(\sigma_B^2 - \sigma_s^2) + 2\pi i\nu E_s + \log\frac{I_s}{I_0}. \qquad (12)
\end{aligned}$$

Neglecting noise effects, we can recover $S(E)$ by inverting $s(\nu)$ using the inverse Fourier transform. This requires us to first find $\mathcal{F}^{-1}[\nu]$ and $\mathcal{F}^{-1}[\nu^2]$.

Our starting point here is the integral representation of the dirac delta function:

$$\delta(E) = \int d\nu e^{-2\pi i\nu E}. \tag{13}$$

Differentiating once and twice with respect to E, gives respectively

$$\delta'(E) = -2\pi i \int d\nu \nu e^{-2\pi i\nu E} \tag{14}$$

$$\delta''(E) = -4\pi^2 \int d\nu \nu^2 e^{-2\pi i\nu E}. \tag{15}$$

Hence,

$$\mathcal{F}^{-1}[\nu] = \frac{i\delta'(E)}{2\pi} \qquad \text{and} \qquad \mathcal{F}^{-1}[\nu^2] = \frac{i\delta''(E)}{4\pi^2}. \tag{16}$$

Taking the inverse Fourier transform of (12), then leads to

$$\frac{S(E)}{I_0} = \log\left(\frac{I_s}{I_0}\right)\delta(E) - E_s\delta'(E) + \frac{(\sigma_B^2 - \sigma_s^2)}{2}\delta''(E). \tag{17}$$

2 Finite order calculation

Let us calculate $S(E)$ neglecting contributions $J^n(E)$ with $n > 1$. In other words,

$$\begin{aligned} J(E) &= Z(E) + J^1(E) + \dots \\ &= I_0 R(E) * \delta(E) + R(E) * S(E) + \dots \end{aligned} \tag{18}$$

Taking the Fourier transform results in

$$\begin{aligned} j(\nu) &= z(\nu) + \frac{z(\nu)}{I_0} s(\nu) + \dots \\ &= z(\nu)\left[1 + \frac{s(\nu)}{I_0}\right] + \dots, \end{aligned} \tag{19}$$

where the dots represent higher order scatterings. Eliminating $s(\nu)$ gives

$$s(\nu) = I_0\left(\frac{j(\nu)}{z(\nu)} - 1\right) + \dots, \tag{20}$$

which can also be found by expanding eq. (3) up to first order in $j(\nu)/z(\nu)$. From now on we will no longer write the dots. Upon substituting eq. (11) and (6) into (20), we obtain

$$\begin{aligned} s(\nu) &= I_s \exp[-2\pi^2\nu^2(\sigma_s^2 - \sigma_B^2) + 2\pi i\nu E_s] - I_0 \\ &= I_s \exp\left[-2\pi^2(\sigma_s^2 - \sigma_B^2)\left(\nu^2 - \frac{2\pi i\nu E_s}{2\pi^2(\sigma_s^2 - \sigma_B^2)}\right)\right] - I_0 \\ &= I_s \exp\left[-2\pi^2(\sigma_s^2 - \sigma_B^2)\left(\left[\nu - \frac{iE_s}{2\pi(\sigma_s^2 - \sigma_B^2)}\right]^2 + \left[\frac{E_S}{2\pi(\sigma_s^2 - \sigma_B^2)}\right]^2\right)\right] - I_0 \end{aligned}$$

Extracting the ν dependence gives

$$s(\nu) = I_s \exp\left[-\frac{E_s^2}{2(\sigma_s^2 - \sigma_B^2)}\right] \cdot \exp\left[-2\pi(\sigma_s^2 - \sigma_B^2)\left(\nu - \frac{iE_s}{2\pi(\sigma_s^2 - \sigma_B^2)}\right)^2\right] - I_0.$$

Hence,

$$S(E) = I_s \exp\left[-\frac{E_s^2}{2(\sigma_s^2 - \sigma_B^2)}\right] \mathcal{F}^{-1}\left\{\exp\left[-2\pi(\sigma_s^2 - \sigma_B^2)\left(\nu - \frac{iE_s}{2\pi(\sigma_s^2 - \sigma_B^2)}\right)^2\right]\right\} - I_0\delta(E).$$

By shifting $\nu \to \nu + iE_s/2\pi(\sigma_s^2 - \sigma_B^2)$, we find

$$\begin{aligned}
S(E) &= I_s \exp\left[-\frac{E_s^2}{2(\sigma_s^2 - \sigma_B^2)}\right] \exp\left[\frac{E_s E}{\sigma_s^2 - \sigma_B^2}\right] \mathcal{F}^{-1}\left\{\exp[-2\pi^2(\sigma_s^2 - \sigma_B^2)\nu^2]\right\} - I_0\delta(E) \\
&= I_s \exp\left[\cdot\right] \exp\left[\cdot\right] \frac{1}{\sqrt{2\pi(\sigma_s^2 - \sigma_B^2)}} \exp\left[-\frac{E^2}{2(\sigma_s^2 - \sigma_B^2)}\right] - I_0\delta(E) \\
&= \frac{I_s}{\sqrt{2\pi(\sigma_s^2 - \sigma_B^2)}} \exp\left[-\frac{E_s^2}{2(\sigma_s^2 - \sigma_B^2)}\right] \exp\left[-\frac{E^2 - 2EE_s}{2(\sigma_s^2 - \sigma_B^2)}\right] - I_0\delta(E).
\end{aligned}$$

After completing the square in the last exponential, we obtain

$$S(E) = \frac{I_s}{\sqrt{2\pi(\sigma_s^2 - \sigma_B^2)}} \exp\left[-\frac{(E - E_s)^2}{2(\sigma_s^2 - \sigma_B^2)}\right] - I_0\delta(E). \tag{21}$$

Note that the recovered single scattering distribution is still centered around E_s. It also has a smaller width than the experimental signal $J(E)$. The spread transforms as $\sigma_s^2 \to \sigma_s^2 - \sigma_B^2$ upon deconvolution up to first order. Furthermore, for $\sigma_s \gg \sigma_B$ and $I_s \gg I_0$, the SSD $S(E)$ reduces to $J(E)$.