Explicit knowledge of the temperature and energy derivatives of the Doppler Broadening Functions not only provides analytical insight of how the cross section slope varies with energy and temperature but also specifies extreme points, exact locations of which are important for cross section interpolation (Hwang, 1992). This is required for the studies where fuel temperatures are not uniform. In reactors, nuclides exist in conditions where the temperatures are different or changing due to feedbacks. Modeling of the feedbacks requires cross section information for many nuclides over a wide range of temperatures. Cross section sensitivity and activation analysis studies not only require accurate DBFs but also their temperature derivatives. Calculation of Doppler broadened cross sections at all the required temperatures for all the nuclides are time consuming. On the other hand, interpolation schemes which involve computation of temperature derivatives of DBFs involve memory storage problems (Trumbull 2006) as numerical evaluation of temperature derivatives are prone to larger errors. Because of the huge number of calculations of the cross sections in the energy–temperature grid, there is a continuing effort to reduce calculation time and memory storage by efficient algorithms and schemes. Accurate and efficient interpolation schemes are still a topic of interest (Otuka et al 2008).

Accurate values of derivatives of line shape functions are necessary for creation of energy and temperature grids for interpolation (Hwang 1992). There
have been no standard tabulations for the energy and temperature derivatives of Doppler Broadened functions available in the literature so far. Even static neutronic calculations in power reactors require DBFs at different temperatures since the temperature distributions are non uniform (Olefht, 1970; Goltsev et al., 2000; Matsumoto et al., 2006). Monte Carlo methods are well suited to study such effects. Continuous energy Monte Carlo calculations make use of the Doppler broadened cross sections directly. For such calculations, creating resonance data at run time is prohibitive and point-wise cross sections as a function of energy and temperature are pre-computed and interpolated (Hwang, 1992; Trumbull, 2006). In section 4.1 we have obtained analytical expressions for the temperature and energy derivatives of both $\psi(x,\theta)$ and $\chi(x,\theta)$. Computations carried out for the derivatives of the DBF’s are presented in section 4.2.

### 4.1 Derivatives of $\psi(x,\theta)$ and $\chi(x,\theta)$

The fact that Steffensen’s inequality can be used to obtain DBFs to any desired accuracies suggests that the derivatives of these functions can be computed from analytic expressions obtained from direct differentiation of their integral forms.

#### 4.1.1 Temperature Derivatives

Starting from the integral forms, the first derivatives of $\psi$ and $\chi$ are easily derived and are linear functions of $\psi$ and $\chi$ with coefficients $a_i$ being functions of $\theta$ and $x$.

#### 4.1.1.1 Temperature Derivative of $\psi(x,\theta)$
\[ \frac{\partial \psi}{\partial \theta} = \frac{1}{2\sqrt{\pi}} \left( \exp\left(\frac{-\theta^2}{4} (x - t)^2\right) - \theta^2 \int_{-\infty}^{\infty} \frac{\exp\left(\frac{-\theta^2}{4} (x - t)^2\right)}{1 + t^2} dt \right) \]

\[ = \frac{1}{\theta} \psi - \frac{\theta^2}{4\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp\left(\frac{-\theta^2}{4} (x - t)^2\right)}{1 + t^2} (x^2 + t^2 - 2xt) dt \]

\[ = \frac{1}{\theta} \psi - \frac{\theta^2}{4\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp\left(\frac{-\theta^2}{4} (x - t)^2\right)}{1 + t^2} (x^2 + t^2 + 1 - 2xt) dt \]

\[ = \frac{1}{\theta} \psi - \frac{\theta^2}{4\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp\left(\frac{-\theta^2}{4} (x - t)^2\right)}{1 + t^2} (x^2 + t^2 + 1 - 2xt) dt \]

Identifying the \( \chi \) integral in the fourth term we can write this as

\[ \frac{\partial \psi}{\partial \theta} = \left[ \frac{1}{\theta} - \frac{\theta}{2} (x^2 - 1) \right] \psi + \frac{x\theta}{2} \chi - \frac{\theta}{2} = \alpha_1 \psi + \alpha_2 \chi - \alpha_3 \]  \hspace{1cm} (4.2)

4.1.1.2 Temperature Derivative of \( \chi(x, \theta) \)

Similarly starting from the integral form of \( \chi \)

\[ \frac{\partial \chi}{\partial \theta} = \frac{1}{\sqrt{\pi}} \left( \int_{-\infty}^{\infty} \frac{\exp\left(\frac{-\theta^2}{4} (x - t)^2\right)}{1 + t^2} dt - \theta^2 \int_{-\infty}^{\infty} \frac{\exp\left(\frac{-\theta^2}{4} (x - t)^2\right)}{2\sqrt{\pi}} (x - t)^2 dt \right) \]

\[ = \frac{1}{\theta} \chi - \frac{\theta^2}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp\left(\frac{-\theta^2}{4} (x - t)^2\right)}{1 + t^2} (x^2 + t^2 - 2xt) dt \]

\[ = \frac{1}{\theta} \chi - \frac{\theta^2}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp\left(\frac{-\theta^2}{4} (x - t)^2\right)}{1 + t^2} (x^2 + t^2 - 2xt) dt \]

\[ + \int_{-\infty}^{\infty} t e^\left(\frac{-\theta^2}{4} (x - t)^2 \right) dt - \int_{-\infty}^{\infty} \frac{\exp\left(\frac{-\theta^2}{4} (x - t)^2\right)}{1 + t^2} (2xt) dt \]
Noting that
\[ t \exp\left(-\frac{\theta^2}{4}(x-t)^2\right) = x \exp\left[-\frac{\theta^2}{4}(x-t)^2\right] - \frac{2}{\theta^2} \exp\left[-\frac{\theta^2}{4}(x-t)^2\right], \]

...(4.5)

(4.3) simplifies to
\[
\frac{\partial \psi}{\partial \theta} = \left[\frac{1}{\theta} - \frac{\theta}{2}(x^2-1)\right] \psi - 2x \theta \psi + x \theta \equiv \alpha_1 \psi - 4 \alpha_2 \psi + 2 \alpha_3 x
\]
\[
\text{(4.6)}
\]

where
\[
\left[\frac{1}{\theta} - \frac{\theta}{2}(x^2-1)\right] = \alpha_1
\]
\[
x \theta \psi = \alpha_2
\]
\[
\frac{\theta}{2} = \alpha_3
\]

Upper and lower bounds of the derivatives of \( \psi \) are given by

Case 1: \( \alpha_i \) positive
\[
\left(\frac{\partial \psi}{\partial \theta}\right)_U = \alpha_1 \psi_U + \alpha_2 \chi_U - \alpha_3
\]
\[
\text{(4.7a)}
\]
\[
\left(\frac{\partial \psi}{\partial \theta}\right)_L = \alpha_1 \psi_L + \alpha_2 \chi_L - \alpha_3
\]
\[
\text{(4.7b)}
\]

Case 2: \( \alpha_i \) negative
\[
\left(\frac{\partial \psi}{\partial \theta}\right)_U = \alpha_1 \psi_U + \alpha_2 \chi_U - \alpha_3
\]
\[
\text{(4.7c)}
\]
Upper and lower bounds of the derivatives of $\chi$ are given by

Case 1: $\alpha_i$ positive

$$\left( \frac{\partial \chi}{\partial \theta} \right)_{U} = \alpha_i \chi_U - 4 \alpha_i \psi_L + 2 \alpha_i x$$  \hspace{1cm} (4.8a)

$$\left( \frac{\partial \chi}{\partial \theta} \right)_{L} = \alpha_i \chi_L - 4 \alpha_i \psi_U + 2 \alpha_i x$$  \hspace{1cm} (4.8b)

Case 2: $\alpha_i$ negative

$$\left( \frac{\partial \chi}{\partial \theta} \right)_{U} = \alpha_i \chi_U - 4 \alpha_i \psi_L + 2 \alpha_i x$$  \hspace{1cm} (4.8c)

$$\left( \frac{\partial \chi}{\partial \theta} \right)_{L} = \alpha_i \chi_L - 4 \alpha_i \psi_U + 2 \alpha_i x$$  \hspace{1cm} (4.8d)

Once these are computed, higher order derivatives can also be obtained from recursion relations.

4.1.2 Energy derivatives

Analytical expressions for the first order energy derivatives are also obtained from differentiating their integral forms.

4.1.2.1 Energy derivative of $\psi(x, \theta)$

Energy derivative of the $\psi$ function is given by

$$\frac{\partial \psi}{\partial x} = \theta \left[ \int_{-\infty}^{\infty} \frac{\exp\left[-\frac{\theta^2(x-t)^2}{4}\right]}{1 + t^2} \left[-\frac{\theta^2}{2}(x-t)\right] dt \right]$$

$$= \theta \left[ \int_{-\infty}^{\infty} \frac{\exp\left[-\frac{\theta^2(x-t)^2}{4}\right]}{1 + t^2} \left(-\frac{\theta^2}{2}x\right) + \frac{\theta^2}{2} \int_{-\infty}^{\infty} \frac{\exp\left[-\frac{\theta^2(x-t)^2}{4}\right]}{1 + t^2} dt \right]$$

Second term can be identified as the $\chi$ integral. After simplification we get...
\[ \frac{\partial \psi}{\partial x} = \frac{\theta^2}{2} [\chi - x\psi] \quad (4.10) \]

### 4.1.2 Energy derivative of \( \chi(x, \theta) \)

Likewise energy derivative of \( \chi \) integral is written as

\[
\frac{\partial \chi}{\partial x} = \frac{\theta}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp\left[-\frac{\theta^2}{4}(x-t)^2\right] \frac{-\theta^2}{2} (x-t) dt (4.11)
\]

\[
\frac{\partial \chi}{\partial x} = \frac{\theta}{\sqrt{\pi}} \left[ \int_{-\infty}^{\infty} \left( -\theta^2 x \right) dt + \theta^2 \int_{-\infty}^{\infty} \frac{-(x-t)^2}{1+t^2} t^2 dt \right] 
\]

Second integral on RHS of equation (12) can be written as

\[
\frac{\theta^2}{2} \int_{-\infty}^{\infty} \exp\left[-\frac{\theta^2}{4}(x-t)^2\right] t^2 dt = \frac{\theta^2}{2} \int_{-\infty}^{\infty} \frac{\exp\left[-\frac{\theta^2}{4}(x-t)^2\right]}{1+t^2} (t^2 + 1 - 1) dt 
\]

\[
= \frac{\theta^2}{2} \left\{ \int_{-\infty}^{\infty} \exp\left[-\frac{\theta^2}{4}(x-t)^2\right] dt - \int_{-\infty}^{\infty} \frac{\exp\left[-\frac{\theta^2}{4}(x-t)^2\right]}{1+t^2} dt \right\} 
\]

Derivative given by (4.12) now simplifies to

\[ \frac{\partial \chi}{\partial x} = -\theta^2 [\frac{x\chi}{2} + \psi - 1] \quad (4.13) \]

The upper and lower bounds of the derivatives are given by

\[ \frac{\partial \psi}{\partial x} = (\chi_U - 2x\psi_U) \frac{\theta^2}{4} \quad (4.14a) \]

\[ \frac{\partial \psi}{\partial x} = (\chi_L - 2x\psi_U) \frac{\theta^2}{4} \quad (4.14b) \]

\[ \frac{\partial \chi}{\partial x} = -\theta^2 [\frac{x\chi_L}{2} + \psi_L - 1] \quad (4.14c) \]
\[
\frac{\partial \chi}{\partial x} = -\theta^2 \left[ \frac{x \psi}{2} + \psi_x - 1 \right]
\] (4.14d)

Again, higher order derivatives can be computed recursively, once the first order derivatives are computed using the above expressions.

4.2. Relative accuracies and illustrative computations

As discussed in Chapter 2, the important region of \( \theta \) and \( x \) for Doppler effect is between 0 and 12 for \( u(=x\theta) \). Beyond this value of \( u \), the temperature effects are negligible. We have carried out computations of upper and lower bound approximations of the derivatives for values of \( u \) up to 12.

4.2.1 Computations for the temperature derivatives

The parameter \( \theta \) for a resonance depends on temperature. The 6.673 eV resonance of U-238, for example, has approximate \( \theta \) values of 0.5 and 0.3 corresponding to temperatures around 250 and 700 K. High energy resonances of fertile and structural materials have much lower values of \( \theta \). Bounds of temperature derivatives of both \( \psi \) and \( \chi \) functions are computed using (4.7a) to (4.7d) and (4.8a) to (4.8d). If \( \theta_0 \) corresponds to temperature 300 K, it follows from the definition of Doppler width that \( \theta \) corresponding to a temperature \( T \) is \( \theta_0 \sqrt{\frac{300}{T}} \). For purposes of illustration, we consider a temperature range 300 to 900 K and \( \theta_0 \) values of 0.1 and 0.5. In the computations, \( \psi \) and \( \chi \) functions with relative accuracies \( 10^{-4} \) and \( 10^{-6} \) are used. Relative errors of the temperature derivatives, calculated as described in section (2.4), are plotted as a function of \( \theta \) in Figs 4.1-4.4 for typical values of \( x \). The relative errors of derivatives depend on relative accuracies of \( \psi \) and
\( \chi \) functions used. For example, even when DBFs with relative accuracies as good as \( 10^{-4} \) are used, the relative errors of the derivatives can be as high as \( 10^{-2} \). To achieve relative accuracies better than \( 10^{-3} \) in the derivatives, DBFs with accuracies \( 10^{-6} \) have to be used. It is clear from the figures that relative errors show an increasing trend as \( \theta \) increases. Derivatives of \( \chi \) function, relative to those of \( \psi \), require higher number of terms to achieve desired accuracies.

4.2.2 Computations for the energy derivatives

The bounds of energy derivatives of the \( \psi \) and \( \chi \) functions are computed using (4.14a) to (4.14d) and are given in Tables 4.1 and 4.2 for representative \((\theta,x)\) values. The relative errors of the energy derivatives of the bound approximations are also plotted as a function of \( x \) in Figs.4.5 -4.6. DBFs with relative accuracies of \( 10^{-4} \) and \( 10^{-6} \) are used in the computations. It can again be observed that the relative errors are higher when DBFs of lower accuracy are used. The peaking of relative error of derivative of the \( \chi \) function is seen to occur, as expected, at the point of inflexion for the energy derivative.

Usefulness of Steffensen’s inequality is thus demonstrated for accurate evaluation of not only the Doppler broadening functions but also their temperature and energy derivatives. This has also given rise to a method of generating tabulations for the derivatives.
Table 4.1:
Computed upper and lower bounds of $\psi$ function and its temperature derivative for typical values of $(x, \theta)$. The relative error is $10^{-6}$ for all arithmetic mean values of $\psi$

<table>
<thead>
<tr>
<th></th>
<th>$\theta$</th>
<th>$\psi_U$</th>
<th>$\psi_L$</th>
<th>$\frac{\partial \psi}{\partial \theta}_U$</th>
<th>$\frac{\partial \psi}{\partial \theta}_L$</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>0.20</td>
<td>0.11540036</td>
<td>0.11540014</td>
<td>0.17086877</td>
<td>0.17086825</td>
</tr>
<tr>
<td></td>
<td>0.25</td>
<td>0.11934436</td>
<td>0.11934414</td>
<td>-0.00544130</td>
<td>-0.00544138</td>
</tr>
<tr>
<td></td>
<td>0.30</td>
<td>0.11571036</td>
<td>0.11571014</td>
<td>-0.13096469</td>
<td>-0.13096513</td>
</tr>
<tr>
<td>10</td>
<td>0.10</td>
<td>0.06622613</td>
<td>0.06622600</td>
<td>0.32360578</td>
<td>0.32360504</td>
</tr>
<tr>
<td></td>
<td>0.15</td>
<td>0.07327782</td>
<td>0.07327768</td>
<td>-0.02484946</td>
<td>-0.02484957</td>
</tr>
<tr>
<td></td>
<td>0.20</td>
<td>0.06614275</td>
<td>0.06614262</td>
<td>-0.23318631</td>
<td>-0.23318694</td>
</tr>
</tbody>
</table>
Table 4.2:
The computed upper and lower bounds of $\chi$ function and its energy derivative for typical values of $(x,\theta)$. The relative error is $10^{-6}$ for all arithmetic mean values of $\chi$.

<table>
<thead>
<tr>
<th>$\theta$</th>
<th>$x$</th>
<th>$\chi_U$</th>
<th>$\chi_L$</th>
<th>$\frac{\partial \chi}{\partial x}_U$</th>
<th>$\frac{\partial \chi}{\partial x}_L$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>8</td>
<td>0.18537489</td>
<td>0.18537454</td>
<td>0.00672924</td>
<td>0.00672918</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>0.19091292</td>
<td>0.19091255</td>
<td>-0.00082822</td>
<td>-0.00082829</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>0.11754315</td>
<td>0.11754292</td>
<td>-0.00730219</td>
<td>-0.00730228</td>
</tr>
<tr>
<td>0.5</td>
<td>4</td>
<td>0.40075682</td>
<td>0.40075603</td>
<td>0.00845033</td>
<td>0.00844985</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>0.35997561</td>
<td>0.35997493</td>
<td>-0.03834537</td>
<td>-0.03834591</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>0.27978897</td>
<td>0.27978845</td>
<td>-0.03735056</td>
<td>-0.03735110</td>
</tr>
</tbody>
</table>
Fig 4.1. Relative error of temperature derivatives with respect to $\theta$ using equations (4.7) and (4.8) for $x = 6$
Fig 4.2. Relative error of temperature derivatives with respect to $\theta$ using equations (4.7) and (4.8) for $x = 20$
Fig 4.3. Relative error of temperature derivatives with respect to $\theta$ using equations (4.7) and (4.8) for $x = 30$
Fig 4.4. Relative error of temperature derivatives with respect to $\theta$ using equations (4.7) and (4.8) for $x = 100$
Fig 4.5. Relative error of energy derivatives with respect to $x$ using equations (4.14a), (4.14b), (4.14c) and (4.14d) for $\theta = 0.1$
Relative error of energy derivatives with respect to $x$ using equations (4.14a), (4.14b), (4.14c), and (4.14d) for $\theta = 0.5$