1 Partial wave expansion of the regularized Coulomb interaction

Using the more friendly modified Spherical Bessel functions,

$$\begin{aligned}
\frac{\mathrm{erf}(\beta|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|} &= \frac{2}{\sqrt{\pi}}\int_0^\beta \mathrm{d}u\mathrm{e}^{-u^2(r^2+r'^2)}\left[\sum_{l=0}^{\infty}(2l+1)i_l(2u^2rr')P_l\left(\cos(\theta)\right)\right] \\
&= \frac{2}{\sqrt{\pi}}\sum_{l=0}^{\infty}(2l+1)P_l\left(\cos(\theta)\right)\int_0^\beta \mathrm{d}u\mathrm{e}^{-u^2(r^2+r'^2)}i_l(2u^2rr') \\
&= 8\sqrt{\pi}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}\left(\cos(\theta),\phi\right)Y^*_{lm}\left(\cos(\theta'),\phi'\right)\int_0^\beta \mathrm{d}u\ \mathrm{e}^{-u^2(r^2+r'^2)}i_l(2u^2rr') \\
&= \sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}\left(\cos(\theta),\phi\right)Y^*_{lm}\left(\cos(\theta'),\phi'\right)\left[8\sqrt{\frac{\pi}{2rr'}}\int_0^{\beta\sqrt{2rr'}}\mathrm{d}x\ \mathrm{e}^{-x^2\left(\frac{r^2+r'^2}{2rr'}\right)}i_l(x^2)\right] \\
&= \sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}\left(\cos(\theta),\phi\right)Y^*_{lm}\left(\cos(\theta'),\phi'\right)\left(\frac{4\pi}{2l+1}\right)\mathrm{W}_l^{(\mathrm{erf})}(r,r';\beta)
\end{aligned} \tag{1.1}$$

where

$$\mathrm{W}_l^{(\mathrm{erf})}(r,r';\beta) = \left(\frac{2(2l+1)}{\sqrt{\pi}}\right)\left(\frac{1}{\sqrt{2rr'}}\right)\int_0^{\beta\sqrt{2rr'}}\mathrm{d}x\ \mathrm{e}^{-x^2\left(\frac{r^2+r'^2}{2rr'}\right)}i_l(x^2) \tag{1.2}$$

and

$$\begin{aligned}
i_0(x) &= \frac{\sinh(x)}{x} = \mathrm{sinhc}(x) \\
i_1(x) &= \frac{x\cosh(x)-\sinh(x)}{x^2} = \frac{\cosh(x)-\mathrm{sinhc}(x)}{x} = \\
i_2(x) &= \frac{(x^2+3)\sinh(x)-3x\cosh(x)}{x^3} = \frac{(x^2+3)\mathrm{sinhc}(x)-3\cosh(x)}{x^2} = \\
i_3(x) &= \frac{(x^3+15x)\cosh(x)-(6x^2+15)\sinh(x)}{x^4} = \frac{(x^2+15)\cosh(x)-(6x^2+15)\mathrm{sinhc}(x)}{x^3}
\end{aligned} \tag{1.3}$$

The symbol W is employed for the interaction as opposed to ϕ due neglect of the prefactor $e^2/4\pi\epsilon_0$ (or just e^2 in a.u.) required for the unit of the interaction to be energy. The factor $4\pi/(2l+1)$ is introduced such that $\lim_{\beta\to\infty}\mathrm{W}_l^{(\mathrm{erf})}(r,r';\beta) = r_<^l/r_>^{l+1}$, the familar partial wave expansion of the $1/|\mathbf{r}-\mathbf{r}'|$, where $r_> = \max(r,r')$ and $r_< = \min(r,r')$.

The key limits for W are

$$\begin{aligned}
\lim_{\beta\to\infty}\mathrm{W}_l^{(\mathrm{erf})}(r,r') &= \frac{r_<^l}{r_>^{l+1}} \\
\lim_{r_<\to 0}\mathrm{W}_l^{(\mathrm{erf})}(r,r') &= \frac{\mathrm{erf}(\beta r_>)}{r_>}\delta_{l,0}
\end{aligned} \tag{1.4}$$

where $r_> = \max(r,r')$, $r_< = \min(r,r')$. The first limit is the partial wave expansion of $1/|\mathbf{r}-\mathbf{r}'|$, the second limit is derived as follows:

$$
\begin{aligned}
\mathrm{W}_l^{(\mathrm{erf})}(r,r') &= \left(\frac{2(2l+1)}{\sqrt{\pi}}\right)\left(\frac{1}{\sqrt{2rr'}}\right)\int_0^{\beta\sqrt{2rr'}} \mathrm{d}x\ \mathrm{e}^{-x^2\left(\frac{r^2+r'^2}{2rr'}\right)} i_l(x^2) \\
&= \left(\frac{2(2l+1)}{\sqrt{\pi}}\right)\int_0^{\beta} \mathrm{d}x\ \mathrm{e}^{-x^2\left(r^2+r'^2\right)} i_l(2rr'x^2) \\
\mathrm{W}_l^{(\mathrm{erf})}(r,0) &= \left(\frac{2(2l+1)}{\sqrt{\pi}}\right)\int_0^{\beta} \mathrm{d}x\ \mathrm{e}^{-x^2r^2} i_l(0) \\
&= \left(\frac{2(2l+1)}{\sqrt{\pi}}\right)\int_0^{\beta} \mathrm{d}x\ \mathrm{e}^{-x^2r^2} \delta_{l,0} \\
&= (2l+1)\frac{\mathrm{erf}(\beta r_>)}{r_>}\delta_{l,0} \\
&= \frac{\mathrm{erf}(\beta r_>)}{r_>}\delta_{l,0}
\end{aligned} \tag{1.5}
$$

where the $\lim_{x\to 0} i_l(x) = \delta_{l,0}$ which can be proved from Eq.1.3, or more generally, from the small argument expansion given by Abramowitz and Stegun's book with leading order term ($i_l(x) \sim x^l$) as x goes to 0.

The required indefinite integrals are

$$
\int \mathrm{d}x\ \mathrm{e}^{-a^2x^2} i_0(x^2) = \frac{\sqrt{\pi}\mathrm{sgn}(x)}{2}\left[a_m \mathrm{erfc}(a_m|x|) - a_p \mathrm{erfc}(a_p|x|)\right] - xe^{-a^2x^2}\left[\mathrm{sinhc}(x^2)\right] \tag{1.6}
$$

$$
\begin{aligned}
\int \mathrm{d}x\ \mathrm{e}^{-a^2x^2} i_1(x^2) &= \frac{1}{6x^3}\Big[\sqrt{\pi}(2a^2+1)a_m x^3 \mathrm{erfc}(a_m|x|) - \sqrt{\pi}(2a^2-1)a_p x^3 \mathrm{erfc}(a_p|x|) \\
&\quad -e^{-(a^2+1)x^2}(2a^2(e^{2x^2}-1)x^2 + (e^{2x^2}+1)x^2 - e^{2x^2}+1)\Big] \\
&= \frac{1}{6x^3}\Big[\sqrt{\pi}(2a^2+1)a_m x^3 \mathrm{erfc}(a_m|x|) - \sqrt{\pi}(2a^2-1)a_p x^3 \mathrm{erfc}(a_p|x|) \\
&\quad -2e^{-a^2x^2}\big[(2a^2x^2-1)\sinh(x^2) + x^2\cosh(x^2)\big]\Big] \\
&= \frac{\sqrt{\pi}}{6}\big[(2a^2+1)a_m \mathrm{erfc}(a_m|x|) - (2a^2-1)a_p \mathrm{erfc}(a_p|x|)\big] \\
&\quad -\frac{e^{-a^2x^2}}{3x^3}\big[(2a^2x^2-1)\sinh(x^2) + x^2\cosh(x^2)\big] \\
&= \frac{\sqrt{\pi}}{6}\big[(2a^2+1)a_m \mathrm{erfc}(a_m|x|) - (2a^2-1)a_p \mathrm{erfc}(a_p|x|)\big] \\
&\quad -\frac{e^{-a^2x^2}}{3x}\big[(2a^2x^2-1)\mathrm{sinhc}(x^2) + \cosh(x^2)\big]
\end{aligned} \tag{1.7}
$$

$$
\begin{aligned}
\int \mathrm{d}x\ \mathrm{e}^{-a^2x^2} i_2(x^2) \quad &= \quad \frac{1}{10x^5}\left[-\sqrt{\pi}(4a^4+2a^2-1)x^4a_m|x|\mathrm{erf}(a_m|x|)+\sqrt{\pi}(4a^4-2a^2-1)x^4a_p|x|\mathrm{erf}(a_p|x|)\right.\\
&\quad +\sqrt{\pi}x^4(2a^2(a_m|x|+a_p|x|)-a_m|x|+a_p|x|+4a^4(a_m|x|-a_p|x|))\\
&\quad +e^{-(a^2-1)x^2}((2a^2+3)x^2+(-4a^4-2a^2+1)x^4-3)\\
&\quad \left.+e^{-(a^2+1)x^2}((3-2a^2)x^2+(4a^4-2a^2-1)x^4+3)\right]\\
&= \quad \frac{\mathrm{sgn}(x)}{10}\left[-\sqrt{\pi}(4a^4+2a^2-1)a_m\mathrm{erf}(a_m|x|)+\sqrt{\pi}(4a^4-2a^2-1)a_p\mathrm{erf}(a_p|x|)\right.\\
&\quad \left.+\sqrt{\pi}(2a^2(a_m+a_p)-a_m+a_p+4a^4(a_m-a_p))\right]\\
&+ \quad \frac{1}{5x^5}\left[+e^{-a^2x^2}(2a^2x^2\sinh(x^2)+(-4a^4+1)x^4\sinh(x^2)+(3x^2-2a^2x^4)\cosh(x^2)-3\sinh(x^2))\right]\\
&= \quad \frac{\sqrt{\pi}\mathrm{sgn}(x)}{10}\left[(4a^4+2a^2-1)a_m\mathrm{erfc}(a_m|x|)-(4a^4-2a^2-1)a_p\mathrm{erfc}(a_p|x|)\right]\\
&+ \quad \frac{e^{-a^2x^2}}{5x^3}\left[((1-4a^4)x^4+2a^2x^2-3)\mathrm{sinhc}(x^2)+(3-2a^2x^2)\cosh(x^2)+4a^4x^4\right]\\
&- \quad \frac{4xa^4e^{-a^2x^2}}{5}
\end{aligned} \tag{1.8}
$$

Here, the integrals are presented in a form in which is easier to check by differentiating wrt to x and ensuring that the limit $x \to 0$ is well defined.

$$
\int \mathrm{d}x\ \mathrm{e}^{-a^2x^2} i_3(x^2) \quad = \tag{1.9}
$$

where

$$
\begin{aligned}
a_m &= \sqrt{a^2-1}\\
a_p &= \sqrt{a^2+1}
\end{aligned} \tag{1.10}
$$

In order to evalute the partial waves, we insert the definition of the a's

$$
\begin{aligned}
a &= \frac{\sqrt{r_>^2+r_<^2}}{\sqrt{2r_>r_<}}\\
a_m &= \frac{r_>-r_<}{\sqrt{2r_>r_<}}\\
a_p &= \frac{r_>+r_<}{\sqrt{2r_>r_<}}
\end{aligned} \tag{1.11}
$$

where as aboave $r_> = \max(r, r')$ and $r_< = \min(r, r')$. Furtheremore, since the upper and lower limits of the integral are positive semi-definite ($x \geq 0$), we only need to be careful about the absolute value in the evalution of a_p and a_m and not in x which is evaluted at the limits. Hence $\mathrm{sgn}(x) \equiv 1$ and $|x| \equiv x$. It is nontheless convenient to introduce $r_>$ and $r_<$ everywhere rather have mixed notation of $r, r'r_>, r_<$

Using the simplified form of the integrals above and the definition of the a's in terms of $r_>$ and $r_<$, the coefficients of the partial wave expansion of the regularized / cutoff Coulomb interaction can be written in a form in which the limits $r_< \to 0$, $\beta \to \infty$ and $r_> \to r_<$ can be evaluated by easily. For convenience functions,

$$
\begin{aligned}
\mathrm{D}_p^{(\mathrm{erf})}(r_<, r_>;\beta) &= \frac{1}{2}\left[\mathrm{erf}(\beta(r_>+r_<))+\mathrm{erf}(\beta(r_>-r_<))\right]\\
\mathrm{D}_m^{(\mathrm{erf})}(r_<, r_>;\beta) &= \frac{1}{2}\left[\mathrm{erf}(\beta(r_>+r_<))-\mathrm{erf}(\beta(r_>-r_<))\right]\\
G_H(r_<, r_>, \beta) &= \left(\frac{2\beta}{\sqrt{\pi}}\right)e^{-\beta^2(r_>^2+r_<^2)}
\end{aligned} \tag{1.12}
$$

are defined. The partial wave are

$$\begin{aligned}
\mathrm{W}_0^{(\mathrm{erf})}(r,r';\beta) &= \left[\mathrm{D}_p^{(\mathrm{erf})}(r_<,r_>;\beta)\right]\left[\frac{1}{r_>}\right] + \left[\mathrm{D}_m^{(\mathrm{erf})}(r_<,r_>;\beta) - r_< G_H(r_<,r_>,\beta)\right]\left[\frac{1}{r_<}\right] \\
&- G_H(r_<,r_>,\beta)\left[\mathrm{sinhc}(2\beta^2 r_> r_<) - 1\right]
\end{aligned} \tag{1.13}$$

$$\begin{aligned}
\mathrm{W}_1^{(\mathrm{erf})}(r,r';\beta) &= \left[\mathrm{D}_p^{(\mathrm{erf})}(r_<,r_>;\beta) - r_> G_H(r_<,r_>,\beta)\right]\left[\frac{r_<}{r_>^2}\right] \\
&+ \left[\mathrm{D}_m^{(\mathrm{erf})}(r_<,r_>;\beta) - r_< G_H(r_<,r_>,\beta)\right]\left[\frac{r_>}{r_<^2}\right] \\
&- G_H(r_<,r_>,\beta)\left[\frac{(2\beta^2(r_>^2+r_<^2)-1)\mathrm{sinhc}(2\beta^2 r_> r_<) + \cosh\left(2\beta^2 r_> r_<\right) - 2\beta^2(r_>^2+r_<^2)}{2\beta^2 r_> r_<}\right]
\end{aligned} \tag{1.14}$$

$$\mathrm{W}_2^{(\mathrm{erf})}(r,r';\beta) = \tag{1.15}$$

$$\mathrm{W}_3^{(\mathrm{erf})}(r,r';\beta) = \tag{1.16}$$

The alternative form of the integral is

$$\begin{aligned}\int \mathrm{d}x\ \mathrm{e}^{-a^2x^2} i_1(b^2x^2) \quad &= \quad \frac{1}{6b^4}\Big[\sqrt{\pi}\left(-(a^2+a_m^2)a_p\mathrm{erfc}(xa_p)+(a^2+a_p^2)a_m\mathrm{erfc}(xa_m)\right) \\ &\quad -\frac{2b^2e^{-x^2a^2}}{x}\left((2a^2x^2-1)\frac{\sinh\left(b^2x^2\right)}{b^2x^2}+\cosh\left(b^2x^2\right)\right)\Big]\end{aligned} \tag{1.17}$$

where

$$\begin{aligned} a &= \sqrt{r_>^2+r_<^2} \\ b &= \sqrt{2r_>r_<} \\ a_m &= r_> - r_< \\ a_p &= r_> + r_< \end{aligned} \tag{1.18}$$

To evaluate the partial wave, the limits are simple, 0 and β.

$$
\begin{aligned}
I_2(x) &= \frac{\sqrt{\pi}}{10}\left[(4a^4+2a^2-1)a_m\mathrm{erfc}(a_m x)-(4a^4-2a^2-1)a_p\mathrm{erfc}(a_p x)\right] \\
&+ \frac{e^{-a^2x^2}}{5x^3}\left[((1-4a^4)x^4+2a^2x^2-3)\mathrm{sinhc}(x^2)+(3-2a^2x^2)\cosh\!\left(x^2\right)+4a^4x^4\right] \\
&- \frac{4xa^4e^{-a^2x^2}}{5}
\end{aligned}
$$

$$
\begin{aligned}
\frac{10}{\sqrt{\pi}}\frac{I_2(\beta\sqrt{2r_>r_<})}{\sqrt{2r_>r_<}} &= \left\{\frac{\sqrt{\pi}}{10}\left[(4a^4+2a^2-1)a_m\mathrm{erfc}(a_m x)-(4a^4-2a^2-1)a_p\mathrm{erfc}(a_p x)\right]\right. \\
&\quad \frac{1}{\sqrt{2r_>r_<}}
\end{aligned}
\tag{1.20}
$$