1 Partial wave expansion of the regularized Coulomb interaction

Using the more friendly modified Spherical Bessel functions,

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

where

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

and

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

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 $4\pi/(2l+1)$ is introduced such that the familiar form is produced when $\beta\to\infty$.

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:

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

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

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

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

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

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

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

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

where $r_> = \max(r, r')$ and $r_< = \min(r, r')$. Furtheremore, since the upper and lower limits of the integral are positive semi-definite, 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 and is strictly $x \geq 0$ and hence all $\mathrm{sgn}(x) \equiv 1$. However, it is nontheless convenient to introduce $r_>$ and $r_<$ everywhere rather have mixed notation of $r, r' r_>, rlt$

Using the simplified form of the integrals 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 are written in a form in which the limits $r_< = 0$, $\beta \to \infty$ and $r_> = r_<$ can be evaluated by inspection,

$$\begin{aligned} \mathrm{W}_0^{(\mathrm{erf})}(r, r') &= \frac{\mathrm{erf}(\beta(r_> + r_<)) - \mathrm{erf}(\beta(r_> - r_<))}{2 r_<} + \frac{\mathrm{erf}(\beta(r_> + r_<)) + \mathrm{erf}(\beta(r_> - r_<))}{2 r_>} \\ &- \frac{2\beta}{\sqrt{\pi}} e^{-\beta^2 (r_>^2 + r_<^2)} \left[\frac{\sinh\left(2\beta^2 r_> r_<\right)}{2\beta^2 r_> r_<} \right] \end{aligned} \tag{1.12}$$

$$\mathrm{W}_1^{(\mathrm{erf})}(r, r') = \frac{1}{3} \left[\frac{1}{r_<} + \frac{2 r_<}{r_>^2} \right]$$

$$\mathrm{W}_2^{(\mathrm{erf})}(r, r') = \tag{1.13}$$

$$\mathrm{W}_3^{(\mathrm{erf})}(r, r') = \tag{1.14}$$

The alternative form of the integral is

$$\begin{aligned} \int \mathrm{d}x \; \mathrm{e}^{-a^2 x^2} i_1(b^2 x^2) &= \frac{1}{6 b^4} \left[\sqrt{\pi} \left(-(a^2 + a_m^2) a_p \mathrm{erfc}(x a_p) + (a^2 + a_p^2) a_m \mathrm{erfc}(x a_m) \right) \right. \\ &\left. - \frac{2 b^2 e^{-x^2 a^2}}{x} \left((2 a^2 x^2 - 1) \frac{\sinh\left(b^2 x^2\right)}{b^2 x^2} + \cosh\left(b^2 x^2\right) \right) \right] \end{aligned} \tag{1.15}$$

where

$$\begin{aligned} a &= \sqrt{r_>^2 + r_<^2} \\ b &= \sqrt{2 r_> r_<} \\ a_m &= r_> - r_< \\ a_p &= r_> + r_< \end{aligned} \tag{1.16}$$

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