

Table 1: Convergence of two-electron Coloumb potential $1/r_{12}$ with respect to ℓ_{\max} in the Neumann expansion in prolate spheroidal coordinates. Internuclear separation R is 1.4. All the quanties are given in atomic units.

Electron 1	(0.2, -0.3, 0.0)	(1.0, -2.0, -1.0)	(10, -2, -50)
Electron 2	(0.5, 0.1, -1.0)	(-1.0, 3.0, 1.0)	(5, 1, -3)
$\ell_{\max} = 10$	0.8944912425297	0.1759041023385	0.02111472177686
$\ell_{\max} = 20$	0.8944272224030	0.1739625665290	0.02111472177657
$\ell_{\max} = 30$	0.8944271910024	0.1740764143734	0.02111472177657
$\ell_{\max} = 40$	0.8944271909999	0.1740778613865	0.02111472177657
$\ell_{\max} = 50$	0.8944271909999	0.1740776557020	0.02111472177657
Exact $1/r_{12}$	0.8944271909999	0.1740776559557	0.02111472177657

The von Neumann expansion of $1/r_{12}$ in prolate spheroidal coordinates is given by

$$\frac{1}{r_{12}} = \frac{2}{R} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (-1)^{|m|} (2\ell+1) \left(\frac{(\ell-|m|)!}{(\ell+|m|)!} \right)^2 P_{\ell}^{|m|}(\xi_{<}) Q_{\ell}^{|m|}(\xi_{>}) P_{\ell}^{|m|}(\eta_1) P_{\ell}^{|m|}(\eta_2) e^{im(\varphi_1-\varphi_2)}, \quad (1)$$

where $\xi_{<} = \min(\xi_1, \xi_2)$ and $\xi_{>} = \max(\xi_1, \xi_2)$.