Modified Bessel functions and their integrals

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1 Zero energy

The Bessel function, for computational purposes at $E = 0$ are evaluated removing the $k = \sqrt{2mE}/\hbar$ dependence.

$$\boxed{\begin{aligned} \tilde{j}_L(r) &\equiv \frac{(2L+1)!!}{k^L}\, j_L(kr)\,, \\ \tilde{y}_L(r) &\equiv \frac{k^{L+1}}{(2L+1)!!}\, f_\epsilon(r)\, y_L(kr)\,, \end{aligned}}$$

where $f_\epsilon(r)$ is a function to regolarise $y_L(kr)$ for $r \to 0$, defined as

$$f_\epsilon(r) \equiv \left(1 - e^{-\epsilon r}\right)^{2L+1} .$$

Choosing in the code $\epsilon = 0.25$ fm^{-1} one gets that $(1 - f_\epsilon(20)) \sim 0.01$ for $L \sim 1$. For $r \to 0$

$$\lim_{r \to 0} f_\epsilon(r) \sim (\epsilon r)^{2L+1} .$$

Since

$$\boxed{\begin{aligned} j_L(x) &\simeq \frac{x^L}{(2L+1)!!}\,, \\ y_L(x) &\simeq -\frac{(2L-1)!!}{x^{L+1}}\,, \end{aligned}}$$

we have for very small $x = kr$

$$\begin{aligned} \tilde{j}_L(r) &= r^L\,, \\ \tilde{y}_L(r) &= -\frac{f_\epsilon(r)}{(2L+1)}\,\frac{1}{r^{L+1}}\,. \end{aligned}$$

Specifically $x = 0$ since we chose $E = 0$ and this holds perfectly.

2 Integrals for the variational method

2.1 Asymptotic region integrals

The integrals needed for the asymptotic region are

$$
\begin{aligned}
I_{R',R} &\equiv \langle \tilde{j}_{L'}, \alpha' |\, H - E \,| j_L, \alpha \rangle \,, \\
I_{I',R} &\equiv \langle \tilde{y}_{L'}, \alpha' |\, H - E \,| j_L, \alpha \rangle \,, \\
I_{R',I} &\equiv \langle \tilde{j}_{L'}, \alpha' |\, H - E \,| j_L, \alpha \rangle \,, \\
I_{I',I} &\equiv \langle \tilde{y}_{L'}, \alpha' |\, H - E \,| y_L, \alpha \rangle \,.
\end{aligned}
$$

Since

$$
I_{X,R} = A \langle X_{L'} |\, K - E + V \,| j_L \rangle \qquad \rightarrow \qquad V_{X,R} \equiv I_{X,R} = \langle X_{L'} |\, V \,| \tilde{j}_L \rangle \,.
$$

Here we used the fact that y_L are eigenfunction of the kinetic energy K with eigenvalue E. Therefore we need to evaluate

$$
\begin{aligned}
I_{R',R} &= V_{R',R} \,, \\
I_{I',R} &= V_{I',R} \,, \\
I_{R',I} &= K_{R',I} - E \, \langle R' | I \rangle + V_{R',I} \,, \\
I_{I',I} &= K_{I',I} - E \, \langle I' | I \rangle + V_{I',I} \,.
\end{aligned}
$$

(**question** why are not we using $\langle y_L | (K - E) = 0$ to write $I_{R',I} = V_{R',I}$??? Is it numerically different?)
Since $E = 0$

$$
\begin{aligned}
I_{R',R} &= V_{R',R} \,, \\
I_{I',R} &= V_{I',R} \,, \\
I_{R',I} &= K_{R',I} + V_{R',I} \,, \\
I_{I',I} &= K_{I',I} + V_{I',I} \,.
\end{aligned}
$$

2.2 Convergence of $I_{R',R}$ and $I_{I',R}$

This is ensured by the fact that $V = V_N \rightarrow e^{-r^\alpha}$ for $r \rightarrow \inf$, in our case specifically

$$
V \simeq p(r, R_{ST}) \, e^{-(r/R_{ST})^2} \,,
$$

where p is a polynomial in r and R_{ST}.

2.3 Convergence for $I_{R',I}$

The potential part converges for the reasons already stated above.
Finally let us focus on the kinetic part

$$
K_{R',I} = \left\langle R' \middle| -\frac{\mathrm{d}^2}{\mathrm{d}r^{\,2}} - \frac{2}{r} \frac{\mathrm{d}}{\mathrm{d}r} \middle| I \right\rangle
$$

// CONTINUE