

Gauss-Laguerre Hyperradial Basis

The hyperradial functions are of the form

$$R_n(\rho) = (RR)^{-3} [n!/(n+5)!]^{1/2} L_n^5(z) \exp(-z/2)$$

where $z = \rho/RR$. (The initial problem, without singling out the $\rho^{-5/2}$ factor is considered.) They are orthonormalized:

$$\int_0^\infty d\rho \rho^5 R_n R_{n'} = \delta_{nn'}.$$

RR is a free (or variational) parameter.

$L_n^{\alpha=5.d0}$ are calculated with polag.f.

The normalizing factor $[n!/(n+5)!]^{1/2}$ is calculated with lagnorm.f

Kinetic energy matrix elements are calculated analytically with ekin.f.

Matrix elements of potential energy have the form

$$[n!/(n+5)!]^{1/2} \times [n'!/(n'+5)!]^{1/2} \int_0^\infty dz z^5 \exp(-z) L_n^5(z) L_{n'}^5(z) W(z \times RR).$$

The integrals are calculated using the Gauss-Laguerre quadrature formula

$$\int_0^\infty dz z^5 \exp(-z) f(z) = \sum_{i=1}^I W_i f(z_i).$$

The weights W_i and the quadrature points z_i are generated by qualag.f