Integrals
$F^k(i,j), i \neq j; F^k(i,i); G^k(i,j)$

- $F^k(i,j), i \neq j$

$$\begin{aligned}
F^k(1,2) &= \int_0^\infty \int_0^\infty P_1^2(r_1) \frac{r_<^k}{r_>^{k+1}} P_2^2(r_2) dr_1 dr_2 \\
P_1 &= \sum_i C_{i1} B_i^{k_s} \\
P_2 &= \sum_i C_{i2} B_i^{k_s} \\
F^k(1,2) &= \sum_i C_{i1}^2 f(i,i) \\
&+ \sum_i \sum_{i'}^{i<i'} 2C_{i1} C_{i'1} f(i,i') \\
f(i,i') &= \sum_j C_{j2}^2 r^k(i,j;i'j) \\
&+ \sum_j \sum_{j'}^{j<j'} 2C_{j2} C_{j'2} r^k(i,j;i'j') \\
F^k(1,2) &= \sum_i C_{i1}^2 \sum_j C_{j2}^2 r^k(i,j;i,j) \\
&+ 2\sum_i \sum_{i'}^{i<i'} C_{i1} C_{i'1} \sum_j C_{j2}^2 r^k(i,j;i',j) \\
&+ 2\sum_i \sum_{i'}^{i<i'} C_{i2} C_{i'2} \sum_j C_{j1}^2 r^k(i,j,;i',j)
\end{aligned}$$

$$
\begin{aligned}
&+ \quad 4\sum_i \sum_{i'}^{i<i'} C_{i1}C_{i'1} \sum_j \sum_{j'}^{j<j'} C_{j2}C_{j'2} r^k(i,j;i'j') \\
&= \quad \sum_i C_{i1}^2 \left[C_{i2}^2 r^k(i,i;i,i) + \sum_j^{i<j} C_{j2}^2 r^k(j,i;j,i) \right] \\
&+ \quad \sum_i C_{i2}^2 \sum_j^{i<j} C_{j1}^2 r^k(j,i;j,i) \\
&+ \quad 2\sum_i C_{i2}^2 \sum_j \sum_{j'}^{j<j'} C_{j1}C_{j'1} r^k(j,i;j',i) \\
&+ \quad 2\sum_i C_{i1}^2 \sum_j \sum_{j'}^{j<j'} C_{j2}C_{j'2} r^k(j,i;j',i) \\
&+ \quad 4\sum_i \sum_{i'}^{i<i'} C_{i1}C_{i'1} \sum_{j'} \left[C_{i2}C_{j'2} r^k(i,i;i',j') + \sum_j^{j<j',i<j} C_{j2}C_{j'2} r^k(j,i;j',i') \right] \\
&+ \quad 4\sum_i \sum_{i'}^{i<i'} C_{i2}C_{i'2} \sum_{j'} \sum_j^{j<j',i<j} C_{j1}C_{j'1} r^k(j,i;j',i')
\end{aligned}
$$

- $F^k(i,i)$

$$
\begin{aligned}
F^k(1,1) &= 2\sum_i C_{i1}^2 \left[0.5 C_{i1}^2 r^k(i,i;i,i) + \sum_j^{i<j} C_{j1}^2 r^k(j,i;j,i) \right] \\
&+ 4\sum_i C_{i1}^2 \sum_j \sum_{j'}^{j<j'} C_{j1}C_{j'1} r^k(j,i;j',i) \\
&+ 8\sum_i \sum_{i'}^{i<i'} C_{i1}C_{i'1} \sum_{j'}^{i<j'} \left[0.5 C_{i1}C_{j'1} r^k(i,i;j',i') + \sum_j^{j<j',i<j} C_{j1}C_{j'1} r^k(j,i;j',i') \right]
\end{aligned}
$$

- $G^k(i,j)$

$$
\begin{aligned}
G^k(1,2) &= \int_0^\infty \int_0^\infty P_1(r_1)P_2(r_2) \frac{r_<^k}{r_>^{k+1}} P_2(r_1)P_1(r_2)\,dr_1 dr_2 \\
P_1 &= \sum_i C_{i1} B_i^{k_s}
\end{aligned}
$$

$$
\begin{aligned}
P_2 &= \sum_i C_{i2} B_i^{k_s} \\
G^k(1,2) &= 2\sum_i C_{i1}^2 \left[0.5 C_{i1}^2 r^k(i,i;i,i) + \sum_j^{i<j} C_{j1}^2 r^k(j,i;j,i) \right] \\
&+ 2\sum_i C_{i1} C_{i2} \sum_j \sum_{j'}^{j<j'} \left[C_{j1} C_{j'2} + C_{j'1} C_{j2} \right] r^k(j,i;j',i) \\
&+ 2\sum_i \sum_{i'}^{i<i'} \left[C_{i1} C_{i'2} + C_{i'1} C_{i2} \right] \sum_{j'}^{i<j'} \Big[0.5 \left(C_{i1} C_{j'2} + C_{j'1} C_{i2} \right) r^k(i,i;j',i') \\
&\qquad + \sum_j^{j<j',i<j} \left(C_{j1} C_{j'2} + C_{j'1} C_{j2} \right) r^k(j,i;j',i') \Big]
\end{aligned}
$$

Integral N^k

$$
\begin{aligned}
N^k(i,j;i',j') &= \int_0^\infty \int_0^\infty B_i(r_1)B_j(r_2)\frac{r_2^k}{r_1^{k+3}}\epsilon(r_1-r_2)B_{i'}(r_1)B_{j'}(r_2)dr_1dr_2 \\
&= \int_0^\infty dr_1 B_i(r_1)B_{i'}(r_1)\frac{1}{r_1^{k+3}}\int_0^{r_1} dr_2 B_j(r_2)B_{j'}(r_2)r_2^k
\end{aligned}
$$

- Scaling law in the logarithmic step region

$$
\int_{r_{iv+1}}^{r_{iv+2}} B_{i+1}^{k_s}(r)B_{j+1}^{k_s}(r)r^k dr = (1+h)^{1+k}\int_{r_{iv}}^{r_{iv+1}} B_i^{k_s}(r)B_j^{k_s}(r)r^k dr
$$

Proof:

$$
\begin{aligned}
& \int_{r_{iv+1}}^{r_{iv+2}} B_{i+1}^{k_s}(r)B_{j+1}^{k_s}(r)r^k dr \\
& \text{Let } r - r_{iv+1} = t \\
= \; & \int_0^{(r_{iv+2}-r_{iv+1})} B_{i+1}^{k_s}(t+r_{iv+1})B_{j+1}^{k_s}(t+r_{iv+1})(t+r_{iv+1})^k dt \\
& \text{Let } t/(1+h) = x \\
= \; & (1+h)\int_0^{(r_{iv+2}-r_{iv+1})/(1+h)} B_{i+1}^{k_s}[(1+h)(x+r_{iv})]B_{j+1}^{k_s}[(1+h)(x+r_{iv})](1+h)^k(x+r_{iv})^k d \\
= \; & (1+h)^{1+k}\int_0^{r_{(iv+1}-r_{iv})} B_i^{k_s}(x+r_{iv})B_j^{k_s}(x+r_{iv})(x+r_{iv})^k dx \\
& \text{Let } x + r_{iv} = r \\
= \; & (1+h)^{1+k}\int_{r_{iv}}^{r_{iv+1}} B_i^{k_s}(r)B_j^{k_s}(r)r^k dr.
\end{aligned}
$$

For cell integrals of N^k, there are two possibilities: $iv = jv$ and $iv < jv$.

1) $iv < jv$.

$$\int_{r_{iv+1}}^{r_{iv+2}} \int_{r_{jv+1}}^{r_{jv+2}} \frac{r_2^k}{r_1^{k+3}} B_{i+1}^{k_s}(r_1) B_{j+1}^{k_s}(r_2) B_{i'+1}^{k_s}(r_1) B_{j'+1}^{k_s}(r_2) dr_1 dr_2$$
$$= (1+h)^{-1} \int_{r_{iv}}^{r_{iv+1}} \int_{r_{jv}}^{r_{jv+1}} \frac{r_2^k}{r_1^{k+1}} B_i^{k_s}(r_1) B_j^{k_s}(r_2) B_{i'}^{k_s}(r_1) B_{j'}^{k_s}(r_2) dr_1 dr_2$$

Proof: In this case, the two dimensional integration is completely separable.

$$\begin{aligned}
& \int_{r_{iv+1}}^{r_{iv+2}} \int_{r_{jv+1}}^{r_{jv+2}} \frac{r_2^k}{r_1^{k+3}} B_{i+1}^{k_s}(r_1) B_{j+1}^{k_s}(r_2) B_{i'+1}^{k_s}(r_1) B_{j'+1}^{k_s}(r_2) dr_1 dr_2 \\
= & \int_{r_{iv+1}}^{r_{iv+2}} \frac{1}{r_1^{k+3}} B_{i+1}^{k_s}(r_1) B_{i'+1}^{k_s}(r_1) dr_1 \int_{r_{jv+1}}^{r_{jv+2}} r_2^k B_{j+1}^{k_s}(r_2) B_{j'+1}^{k_s}(r_2) dr_2 \\
= & (1+h)^{-k-2} \int_{r_{iv}}^{r_{iv+1}} \frac{1}{r_1^{k+3}} B_i^{k_s}(r_1) B_{i'}^{k_s}(r_1) dr_1 \cdot (1+h)^{1+k} \int_{r_{jv}}^{r_{jv+1}} r_2^k B_j^{k_s}(r_2) B_{j'}^{k_s}(r_2) dr_2 \\
= & (1+h)^{-1} \int_{r_{iv}}^{r_{iv+1}} \int_{r_{jv}}^{r_{jv+1}} \frac{r_2^k}{r_1^{k+3}} B_i^{k_s}(r_1) B_j^{k_s}(r_2) B_{i'}^{k_s}(r_1) B_{j'}^{k_s}(r_2) dr_1 dr_2
\end{aligned}$$

2) $iv = jv$.

$$\begin{aligned}
& \int_{r_{iv+1}}^{r_{iv+2}} \int_{r_{iv+1}}^{r_1} \frac{r_2^k}{r_1^{k+3}} B_{i+1}^{k_s}(r_1) B_{j+1}^{k_s}(r_2) B_{i'+1}^{k_s}(r_1) B_{j'+1}^{k_s}(r_2) dr_1 dr_2 \\
= & (1+h)^{-1} \int_{r_{iv}}^{r_{iv+1}} \int_{r_{iv}}^{r_1} \frac{r_2^k}{r_1^{k+3}} B_i^{k_s}(r_1) B_j^{k_s}(r_2) B_{i'}^{k_s}(r_1) B_{j'}^{k_s}(r_2) dr_1 dr_2
\end{aligned}$$

Proof:

$$\begin{aligned}
& \int_{r_{iv+1}}^{r_{iv+2}} \int_{r_{iv+1}}^{r_1} \frac{r_2^k}{r_1^{k+3}} B_{i+1}^{k_s}(r_1) B_{j+1}^{k_s}(r_2) B_{i'+1}^{k_s}(r_1) B_{j'+1}^{k_s}(r_2) dr_1 dr_2 \\
= & \int_{r_{iv+1}}^{r_{iv+2}} B_{i+1}^{k_s}(r_1) B_{i'+1}^{k_s}(r_1) dr_1 \left\{ \frac{1}{r_1^{k+3}} \int_{r_{iv+1}}^{r_1} r_2^k B_{j+1}^{k_s}(r_2) B_{j'+1}^{k_s}(r_2) dr_2 \right\} \\
& \text{Let } t_1 = r_1 - r_{iv+1},\ t_2 = r_2 - r_{iv+1} \\
= & \int_0^{(r_{iv+2}-r_{iv+1})} B_{i+1}^{k_s}(t_1 + r_{iv+1}) B_{i'+1}^{k_s}(t_1 + r_{iv+1}) dt_1
\end{aligned}$$

$$
\begin{aligned}
& \cdot\left\{\frac{1}{(t_1+r_{iv+1})^{k+3}}\int_0^{t_1}(t_2+r_{iv+1})^k B_{j+1}^{k_s}(t_2+r_{iv+1})B_{j'+1}^{k_s}(t_2+r_{iv+1})dt_2\right\} \\
& \text{Let } r_{iv+1}=(1+h)r_{iv},\ (1+h)x_1=t_1,\ (1+h)x_2=t_2 \\
= & (1+h)^{-1}\int_0^{(r_{iv+1}-r_{iv})} B_{i+1}^{k_s}[(1+h)(x_1+r_{iv})]B_{i'+1}^{k_s}[(1+h)(x_1+r_{iv})]dx_1 \\
& \cdot\left\{\frac{1}{(x_1+r_{iv})^{k+3}}\int_0^{x_1}(x_2+r_{iv})^k B_{j+1}^{k_s}[(1+h)(x_2+r_{iv})]B_{j'+1}^{k_s}[(1+h)(x_2+r_{iv})]dx_2\right\} \\
= & (1+h)^{-1}\int_0^{(r_{iv+1}-r_{iv})} B_i^{k_s}(x_1+r_{iv})B_{i'}^{k_s}(x_1+r_{iv})dx_1 \\
& \cdot\left\{\frac{1}{(x_1+r_{iv})^{k+3}}\int_0^{x_1}(x_2+r_{iv})^k B_j^{k_s}(x_2+r_{iv})B_{j'}^{k_s}(x_2+r_{iv})dx_2\right\} \\
& \text{Let } x_1+r_{iv}=r_1, \text{ and } x_2+r_{iv}=r_2 \\
= & (1+h)^{-1}\int_{r_{iv}}^{r_{iv+1}} B_i^{k_s}(r_1)B_{i'}^{k_s}(r_1)dr_1\cdot\left\{\frac{1}{{r_1}^{k+3}}\int_{r_{iv}}^{r_1} r_2^k B_j^{k_s}(r_2)B_{j'}^{k_s}(r_2)dr_2\right\} \\
= & (1+h)^{-1}\int_{r_{iv}}^{r_{iv+1}}\int_{r_{iv}}^{r_1}\frac{r_2^k}{r_1^{k+3}}B_i^{k_s}(r_1)B_j^{k_s}(r_2)B_{i'}^{k_s}(r_1)B_{j'}^{k_s}(r_2)dr_1dr_2
\end{aligned}
$$

- Symmetry

$$
\begin{aligned}
N^k(i,j;i',j') &= N^k(i',j;i,j') \\
&= N^k(i,j';i',j) \\
&= N^k(i',j';i,j)
\end{aligned}
$$

- N^k storage mode:

$$N^k(ns,ns,ks,ks)$$

- subroutines

  q_n

  q_n_pmoments

  q_n_pdiag

  moment in the SPLINE library

  gauss

  qbsplvb in the SPLINE lirary

Integral T^k

$$T^k(i,j;i',j') = \int_0^\infty \int_0^\infty B_i(r_1)B_j(r_2)\frac{r_<^k}{r_>^{k+1}}\bar{B}_{i'}(r_1)\bar{B}_{j'}(r_2)dr_1dr_2$$

- Scaling law in the logarithmic step region

$$\int_{r_{iv+1}}^{r_{iv+2}} B_{i+1}^{k_s}(r)\bar{B}_{j+1}^{k_s}(r)r^k dr = (1+h)^k \int_{r_{iv}}^{r_{iv+1}} B_i^{k_s}(r)\bar{B}_j^{k_s}(r)r^k dr$$

$$\int_{r_{iv+1}}^{r_{iv+2}} \int_{r_{jv+1}}^{r_{jv+2}} \frac{r_<^k}{r_>^{k+1}} B_{i+1}^{k_s}(r_1)B_{j+1}^{k_s}(r_2)\bar{B}_{i'+1}^{k_s}(r_1)\bar{B}_{j'+1}^{k_s}(r_2)dr_1dr_2$$
$$= (1+h)^{-1} \int_{r_{iv}}^{r_{v+1}} \int_{r_{jv}}^{r_{jv+1}} \frac{r_<^k}{r_>^{k+1}} B_i^{k_s}(r_1)B_j^{k_s}(r_2)\bar{B}_{i'}^{k_s}(r_1)\bar{B}_{j'}^{k_s}(r_2)dr_1dr_2$$

- Symmetry

$$T^k(i,j;i',j') \quad = \quad T^k(j,i;j',i')$$

- T^k storage mode:

$$T^k(ns, ns, 2*ks-1, 2*ks-1)$$

- subroutines

q_t

q_t_pmoments

q_t_moment

q_t_pdiag

gauss

bsplvd: Use de Boor's original code.

Integral V^k

$$V^k(i,j;i',j') = \int_0^\infty \int_0^\infty B_i(r_1)B_j(r_2)\frac{r_<^k}{r_>^{k+3}}\bar{B}_{i'}(r_1)B_{j'}(r_2)dr_1dr_2$$

- Scaling law in the logarithmic step region

$$\int_{r_{iv+1}}^{r_{iv+2}} B_{i+1}^{k_s}(r)B_{j+1}^{k_s}(r)r^k dr = (1+h)^{1+k}\int_{r_{iv}}^{r_{iv+1}} B_i^{k_s}(r)B_j^{k_s}(r)r^k dr$$

$$\int_{r_{iv+1}}^{r_{iv+2}} B_{i+1}^{k_s}(r)\bar{B}_{j+1}^{k_s}(r)r^k dr = (1+h)^{k}\int_{r_{iv}}^{r_{iv+1}} B_i^{k_s}(r)\bar{B}_j^{k_s}(r)r^k dr$$

$$\int_{r_{iv+1}}^{r_{iv+2}}\int_{r_{jv+1}}^{r_{jv+2}} \frac{r_<^k}{r_>^{k+3}} B_{i+1}^{k_s}(r_1)B_{j+1}^{k_s}(r_2)\bar{B}_{i'+1}^{k_s}(r_1)B_{j'+1}^{k_s}(r_2)dr_1dr_2$$
$$= (1+h)^{-2}\int_{r_{iv}}^{r_{iv+1}}\int_{r_{jv}}^{r_{jv+1}} \frac{r_<^k}{r_>^{k+3}} B_{i}^{k_s}(r_1)B_{j}^{k_s}(r_2)\bar{B}_{i'}^{k_s}(r_1)B_{j'}^{k_s}(r_2)dr_1dr_2$$

- Symmetry

$$\begin{aligned} V^k(i,j;i',j') &= V^k(i,j';i',j) \\ &= V^k(j,i;j',i') \end{aligned}$$

- V^k storage mode:

$$V^k(ns, ns, 2*ks-1, ks)$$

- subroutines

q_v

q_v_pmoments

moment

q_v_moment

q_v_pdiag

gauss

bsplvd: Use de Boor's original code.

Integral R^k with relativistic shift

$$R^k(i,j;i',j') + (2k+1)X^k(i,j;i'j')$$

where

$$X^k(i,j;i'j') = \frac{\alpha^2}{4}\int_0^\infty B_i^{k_s}(r)B_j^{k_s}(r)\frac{1}{r^2}B_{i'}^{k_s}(r)B_{j'}^{k_s}(r)$$

- V^k storage mode:
$$R^k(ns,ns,ks,ks)$$

- subroutines

  q_mrk1

  pmoments in the SPLINE library

  moment in the SPLINE library

  pdiag in the SPLINE library

  gauss

Integral $L_C(i,j)$ with relativistic shift

$$L_c(i,j) - C(i,j)$$

where

$$C(i,j) = \frac{\alpha^2}{4} \int_0^\infty \left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right) B_i^{k_s}(r) \left(\frac{d^2}{dr^2} - \frac{l'(l'+1)}{r^2} \right) B_j^{k_s}(r) dr$$

- L_c storage mode:
$$L_c(ns, 2*ks-1)$$

- subroutines

  q_l

  hlm in the SPLINE library

  q_bb2:
$$\int_0^\infty \frac{d^2}{dr^2} B_i^{k_s}(r) \frac{d^2}{dr^2} B_j^{k_s}(r)$$

  q_bdb2:
$$\int_0^\infty B_i^{k_s}(r) \frac{1}{r^2} \frac{d^2}{dr^2} B_j^{k_s}(r)$$