2 RAS-CI Contraction scheme $(N_\alpha \neq N_\beta)$

Scheme for the em RAS_Contrac_Odd(V,ItrRAS,M,Na,Nb) routine $(N_{alpha} \neq N_{beta})$:

```
1   use  Reduced_Lists
2   use  Addressing
3   read  Fock, integrals
4   set parameters & dimensions
5   ! Na/Nb = # alpha/beta electrons in RAS2
6   allocate amplitude vectors (jB) & responses (jR)
7   do Roots
8     read jB
9     do i1 = 1,M
10
11       if [Hole_a] then
12         do ll = 1,MNAH_a = M1N_a: LM1N_a
13           F_is =< Act_a|F|Hole_a >< Act_b|Act_b >
14           build: LAH_1a(MNAH_1a), SgnAH_1a, doLAH_1a=true
15       enddo;endif
16       if [Hole_b] then
17         do ll = 1,MNAH_b = M1N_b: LM1N_b
18           F_{\bar{i}\bar{s}} =< Act_b|F|Hole_b >< Act_a|Act_a >
19           build: LAH_1b(MNAH_1b), SgnAH_1b, doLAH_1b=true
20       enddo;endif
21       if [Part_a] then
22         do ll = 1,MNAP_a = M1N1_a: LM1N1_a
23           F_as :< Act_a|F|Part_a >< Act_b|Act_b >
24           build: LAP_1a(MNAP_1a), SgnAP_1a, doLAP_1a=true
25       enddo; endif
26       if [Part_b] then
27         do ll = 1,MNAP_b = M1N1_b: LM1N1_b
28           F_{\bar{a}\bar{s}} =< Act_b|F|Part_b >< Act_a|Act_a >
29           build: LAP_1b(MNAP_1b), SgnAP_1b, doLAP_1b=true
30       enddo; endif
31
32       do i2 = 1,i1
33         define: IFock, iXvv, iXoo1, iXoo2
34
35         if [Hole_a .and. (Hole_b .OR. Part_b)] then
36           call RAS_FormXah: LAH_2a(MNAH_a), SgnAH_2a, doLAH_2a=true
37           call RAS_FormXah: LAH_2b(MNAH_b), SgnAH_2b, doLAH_2b=true
38           do iA = 1,MNAH_a
39             define jAa_1, jAa_2, jHa_1, jHa_2
40             if [Hole_b] then
41               do iB = 1,MNAH_b = M1N_b
42                 define jAb_1, jAb_2, jHb_1, jHb_2
43                 define K_a,K_b,L_a,L_b (amplitude pointers)
44                 (is_1|\bar{j}\bar{s}_2) =< Hole_a|V|Act_a >< Act_b|V|Hole_b >  (iXoo1)
45                 if [i1 .NE. i2] (is_2|\bar{j}\bar{s}_1) =< Hole_a|V|Act_a >< Act_b|V|Hole_b >  (iXoo2)
46               enddo
47             endif
48             if [Part_b] then ! b-Part/a-Hole
49               RAS_FormXap: LAP_2b(MNAP_b), SgnAP_2b, doLAP_2b=true
50               define jAa_1, jAa_2 (from LAH_1a,LAH_2a)
51               do iB = 1,MNAP_b = M1N1_b
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```fortran
52            define jAb_1,jAb_2,jPb_1,jPb_2 (from LAP_1b,LAP_2b)
53            (a̅s̅_1|is_2) =< Part_b|V|Act_b >< Act_a|V|Hole_a > (iXvo1)
54            if [i1.NE.i2] (a̅s̅_2|is_1) =< Part_b|V|Act_b >< Act_a|V|Hole_a > (iXvo2)
55       enddo;endif;enddo;endif
56
57       if [Part_a .and. (Part_b.or.Hole_b)] then
58         RAS_FormXap: LAP_2a(MNAP_a), SgnAP_2a, doLAP_2a=true
59         do iA = 1,MNAP_a = M1N1_a
60           define jAa_1,jAa_2,jPa_1,jPa_2 (from LAP_1a,LAP_2a)
61           if [Part_b] then ! a-Part/b-Part
62             if [.not.doLAP_2b] RAS_FormXap: LAP_2b(MNAP_b), SgnAP_2b, doLAP_2b=true
63             do iB = 1,MNAP_b = M1N1_b
64               define jAb_1,jAb_2,jPb_1,jPb_2 (from LAP_1b,LAP_2b)
65               define iKa,iKb,iLa,iLb (amplitude pointers)
66               (as_1|b̅s̅_2) =< Part_a|V|Act_a >< Act_b|V|Part_b > (iXvv)
67               if [i1.NE.i2] (as_2|b̅s̅_1) =< Part_a|V|Act_a >< Act_b|V|Part_b > (iXvv)
68           enddo;endif
69           if [Hole_b] then ! a-Part/b-Hole
70             if [.not.doLAH_2b] call RAS_FormXah: LAH_2b(MNAH_b), SgnAH_2b, doLAH_2b=true
71             define jAa_1,jAa_2,jPa_1,jPa_2 (from LAP_1a,LAP_2a)
72             do iB = 1,MNAH_b = M1N_b
73               define jAb_1,jAb_2,jHb_1,jHb_2 (from LAH_1b,LAH_2b)
74               (as_1|ī̅s̅_2) =< Part_a|V|Act_a >< Act_b|V|Hole_b > (iXvo1)
75               if [i1.NE.i2] (as_2|ī̅s̅_1) =< Part_a|V|Act_a >< Act_b|V|Hole_b > (iXvo2)
76       enddo;endif;enddo;endif
77
78 !c*****************c
79 !c* i1 != i2 case *c
80 !c*****************c
81       if [i1.NE.i2] then
82
83         if [(M-2).ge.(Na-1) .and. Na.gt.0] then
84           do ll = 1,MNAA_12a ! MNAA_12a = M2N1_a: LM2N1_a
85             build LAA_12a
86             F_ss' =< Act_a|F|Act_a >< Act_b|Act_b >
87             if [Hole_b]
88               F_ss' =< Act_a|F|Act_a >< Hole_b|Hole_b >
89               (ss'|ī̅j̅) =< Hole_b|V|Hole_b >< Act_a|V|Act_a >
90             endif
91             if [Part_b] then
92               (ss'|a̅b̅) =< Part_b|V|Part_b >< Act_a|V|Act_a >
93               F_ss' =< Act_a|F|Act_a >< Part_b|Part_b >
94             endif
95             if [Hole_a .and. Part_a] then
96                 (as|is') =< Hole_a|V|Part_a >< Act_b|Act_b >
97         endif;enddo;endif
98         if [(M-2).ge.(Nb-1) .and. Nb.gt.0] then
99           do ll = 1,MNAA_12b ! MNAA_12b = M2N1_b: LM2N1_b
100            build LAA_12b
101            F_s̅s̅' =< Act_b|F|Act_b >< Act_a|Act_a >
102            if [Hole_a] then
103              F_s̅s̅' =< Act_b|F|Act_b >< Hole_a|Hole_a >
104              (s̅s̅'|ij) =< Hole_a|V|Hole_a >< Act_b|V|Act_b >
105            endif
106            if [Part_a] then
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107            (s̄s̄′|ab) =< Part_a|V|Part_a >< Act_b|V|Act_b >
108            F_{s̄s̄′} =< Act_b|F|Act_b >< Part_a|Part_a >
109          endif
110          if [Hole_b .and. Part_b] then
111             (ās̄|īs̄′) =< Hole_b|V|Part_b >< Act_a|Act_a >
112      endif;enddo;endif
113
114      if [Hole_a .and. (M−2).ge.Na] then
115        do ll = 1,MNHH_12a ! MNHH_12a = M2N_a: LM2N_a
116           F_{ss′} =< Hole_a|F|Hole_a >< Act_b|Act_b >
117           (ss′|ij) =< Hole_a|V|Hole_a >< Act_b|Act_b >
118           (si|s′j) =< Hole_a|V|Hole_a >< Act_b|Act_b >
119        enddo;endif
120      if [Hole_b .and. (M−2).ge.Nb] then
121        do ll = 1,MNHH_12b ! MNHH_12b = M2N_b: LM2N_b
122           F_{s̄s̄′} =< Hole_b|F|Hole_b >< Act_a|Act_a >
123           (s̄s̄′|īj̄) =< Hole_b|V|Hole_b >< Act_a|Act_a >
124           (s̄ī|s̄′j̄) =< Hole_b|V|Hole_b >< Act_a|Act_a >
125        enddo;endif
126
127      if [Part_a .and. Na.ge.2] then
128        do ll = 1,MNPP_12a ! MNPP_12a = M2N2_a: LM2N2_a
129           (ss′|ab) =< Part_a|V|Part_a >< Act_b|Act_b >
130           (sa|s′b) =< Part_a|V|Part_a >< Act_b|Act_b >
131           F_{ss′} =< Part_a|F|Part_a >< Act_b|Act_b >
132        enddo;endif
133      if [Part_b .and. Nb.ge.2] then
134        do ll = 1,MNPP_12b ! MNPP_12b = M2N2_b: LM2N2_b
135           (s̄s̄′|āb̄) =< Part_b|V|Part_b >< Act_a|Act_a >
136           (s̄ā|s̄′b̄) =< Part_b|V|Part_b >< Act_a|Act_a >
137           F_{s̄s̄′} =< Part_b|F|Part_b >< Act_a|Act_a >
138        enddo;endif
139
140 !c*****************c
141 !c* i1 = i2 case *c
142 !c*****************c
143      else ! [i1.EQ.i2]
144
145      if [(M−1).ge.(Na−1) .and. Na.gt.0] then
146        do ll = 1,MNAA_12a ! MNAA_12a = M1N1_a: LM1N1_a
147           build LAA_12a
148           F_{ss} =< Act_a|F|Act_a >< Act_b|Act_b >
149           if [Hole_b] then
150              F_{ss} =< Act_a|F|Act_a >< Hole_b|Hole_b >
151              (ss|īj̄) =< Hole_b|V|Hole_b >< Act_a|V|Act_a >
152           endif
153           if [Part_b] then
154              (ss|āb̄) =< Part_b|V|Part_b >< Act_a|V|Act_a >
155              F_{ss} =< Act_a|F|Act_a >< Part_b|Part_b >
156      endif;enddo;endif
157
158      if [(M−1).ge.(Nb−1) .and. Nb.gt.0] then
159        do ll = 1,MNAA_12b ! MNAA_12b = M1N1_b: LM1N1_b
160           build LAA_12b
161           F_{s̄s̄} =< Act_b|F|Act_b >< Act_a|Act_a >
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```fortran
162              if [Hole_a]  then
163                  F_ss̄ = < Act_b|F|Act_b > < Hole_a|Hole_a >
164                  (s̄s̄|ij) = < Hole_a|V|Hole_a > < Act_b|V|Act_b >
165              endif
166              if [Part_a]  then
167                  (s̄s̄|ab) = < Part_a|V|Part_a > < Act_b|V|Act_b >
168                  F_s̄s̄ = < Act_b|F|Act_b > < Part_a|Part_a >
169          endif ; enddo ; endif

171          if [Hole_a]  then
172            do ll = 1,MNHH_12a  ! MNHH_12a = M1N_a: LM1N_a
173                F_ss = < Hole_a|F|Hole_a > < Act_b|Act_b >
174                (ss|ij) = < Hole_a|V|Hole_a > < Act_b|Act_b >
175                (si|sj) = < Hole_a|V|Hole_a > < Act_b|Act_b >
176          enddo ; endif
177          if [Hole_b]  then
178            do ll = 1,MNHH_12b  ! MNHH_12b = M1N_b: LM1N_b
179                F_s̄s̄ = < Hole_b|F|Hole_b > < Act_a|Act_a >
180                (s̄s̄|īj̄) = < Hole_b|V|Hole_b > < Act_a|Act_a >
181                (s̄i|s̄j̄) = < Hole_b|V|Hole_b > < Act_a|Act_a >
182          enddo ; endif

184          if [Part_a .and. Na.ge.2]  then
185            do ll = 1,MNPP_12a  ! MNPP_12a = M1N2_a: LM1N2_a
186                (ss|ab) = < Part_a|V|Part_a > < Act_b|Act_b >
187                (sa|sb) = < Part_a|V|Part_a > < Act_b|Act_b >
188                F_ss = < Part_a|F|Part_a > < Act_b|Act_b >
189          enddo ; endif
190          if [Part_b .and. Nb.ge.2]  then
191            do ll = 1,MNPP_12b  ! MNPP_12b = M1N2_b: LM1N2_b
192                (s̄s̄|āb̄) = < Part_b|V|Part_b > < Act_a|Act_a >
193                (s̄a|s̄b̄) = < Part_b|V|Part_b > < Act_a|Act_a >
194                F_s̄s̄ = < Part_b|F|Part_b > < Act_a|Act_a >
195          enddo ; endif

197      endif  ! [i1.EQ.i2]

199      do i3 = 1,i1
200        do i4 = 1,i4max
201          define: iXssss , I_ijkl
202          CALL FormXij: LAA_34a,LHH_34a,LPP_34a ! excitation lists and signs
203          CALL FormXij: LAA_34b,LHH_34b,LPP_34b ! excitation lists and signs

205  !***********************
206  !*  2 elec alpha/beta  *
207  !***********************
208          do iA = 1,MNAA_12a
209            do iB = 1,MNAA_34b  ! [Act−Act]
210                (s_1 s_2|s̄_3 s̄_4) = < Act_a|V|Act_a > < Act_b|V|Act_b > ! (1)
211                if [I_ijkl.ge.7]  (s_1 s_2|s̄_4 s̄_3) = < Act_a|V|Act_a > < Act_b|V|Act_b > ! (1')
212            enddo
213            do iB = 1,MNHH_34b  ! [Hole_b−Hole_b]
214                (s_1 s_2|s̄_3 s̄_4) = < Act_a|V|Act_a > < Hole_b|V|Hole_b > ! (1)
215                if [I_ijkl.ge.7]  (s_1 s_2|s̄_4 s̄_3) = < Act_a|V|Act_a > < Hole_b|V|Hole_b >   ! (1')
216            enddo
```

```fortran
            do  iB = 1,MNPP_34b  !  [Part_b−Part_b]
                (s_1s_2|s̄_3s̄_4) =< Act_a|V|Act_a >< Part_b|V|Part_b >  !  (1)
                if [I_ijkl.ge.7]  (s_1s_2|s̄_4s̄_3) =< Act_a|V|Act_a >< Part_b|V|Part_b >  !  (1')
            enddo
        enddo

        if [MNHH_12a.gt.0 .or. MNPP_12a.gt.0]  then
            do  iB = 1,MNAA_34b
                do  iA = 1,MNHH_12a  !  [Hole_a−Hole_a]
                    (s_1s_2|s̄_3s̄_4) =< Hole_a|V|Hole_a >< Act_b|V|Act_b >  !  (3)
                    if [I_ijkl.ge.7]  (s_1s_2|s̄_4s̄_3) =< Hole_a|V|Hole_a >< Act_b|V|Act_b >  !  (3')
                enddo
                do  iA = 1,MNPP_12a  !  [Part_a−Part_a]
                    (s_1s_2|s̄_3s̄_4) =< Part_a|V|Part_a >< Act_b|V|Act_b >  !  (3)
                    if [I_ijkl.ge.7]  (s_1s_2|s̄_4s̄_3) =< Part_a|V|Part_a >< Act_b|V|Act_b >  !  (3')
                enddo
            enddo
        endif

        if [I_ijkl.ne.1,7]  then
            do  iB = 1,MNAA_12b
                do  iA = 1,MNAA_34a  !  [Act−Act]
                    (s̄_1s̄_2|s_3s_4) =< Act_a|V|Act_a >< Act_b|V|Act_b >  !  (2)
                    if [I_ijkl.gt.7]  (s̄_1s̄_2|s_4s_3) =< Act_a|V|Act_a >< Act_b|V|Act_b >  !  (2')
                enddo
                if [MNHH_34a.gt.0]  then  !  [Hole_a−Hole_a]
                    do  iA = 1,MNHH_34a
                        (s̄_1s̄_2|s_3s_4) =< Hole_a|V|Hole_a >< Act_b|V|Act_b >  !  (2)
                        if [I_ijkl.gt.7]  (s̄_1s̄_2|s_4s_3) =< Hole_a|V|Hole_a >< Act_b|V|Act_b >  !  (2')
                    enddo
                endif
                if [MNPP_34a.gt.0]  then  !  [Part_a−Part_a]
                    do  iA = 1,MNPP_34a
                        (s̄_1s̄_2|s_3s_4) =< Part_a|V|Part_a >< Act_b|V|Act_b >  !  (2)
                        if [I_ijkl.gt.7]  (s̄_1s̄_2|s_4s_3) =< Part_a|V|Part_a >< Act_b|V|Act_b >  !  (2')
                    enddo
                endif
            enddo

            if [MNHH_12b.gt.0 .or. MNPP_12b.gt.0]  then
                do  iA = 1,MNAA_34a
                    do  iB = 1,MNHH_12b  !  [Hole_b−Hole_b]
                        (s̄_1s̄_2|s_3s_4) =< Hole_b|V|Hole_b >< Act_a|V|Act_a >  !  (4)
                        if [I_ijkl.gt.7]  (s̄_1s̄_2|s_4s_3) =< Hole_b|V|Hole_b >< Act_a|V|Act_a >  !  (4')
                    enddo
                    do  iB = 1,MNPP_12b  !  [Part_b−Part_b]
                        (s̄_1s̄_2|s_3s_4) =< Part_b|V|Part_b >< Act_a|V|Act_a >  !  (4)
                        if [I_ijkl.gt.7]  (s̄_1s̄_2|s_4s_3) =< Part_b|V|Part_b >< Act_a|V|Act_a >  !  (4')
                    enddo
                enddo
            endif
        endif
```

```fortran
! ************************
! *   2-elec alpha/alpha   *
! ************************
               if [I_{ijkl}=1,3,5]  then !************************
                  deallocate  LAA_34σ,LHH_34σ,LPP_34σ  (σ = a,b)
                  cycle i4

               elseif [I_{ijkl} = 2,7 .and. M.ge.2]  then !************************

                  if [Na.ge.2]  then
                    do  ll = 1,LM2N2_a
                      (ss|ss) =< Act_a|V|Act_a >< Act_b|Act_b >
                      if [Hole_b]  then
                        (ss|ss) =< Act_a|V|Act_a >< Hole_b|Hole_b >
                      endif
                      if [Part_b]  then
                        (ss|ss) =< Act_a|V|Act_a >< Part_b|Part_b >
                    endif;enddo;endif
                    if [Nb.ge.2]
                      do  ll = 1,LM2N2_b
                        (s̄s̄|s̄s̄) =< Act_b|V|Act_b >< Act_a|Act_a >
                        if [Hole_a]  then
                          (s̄s̄|s̄s̄) =< Act_b|V|Act_b >< Hole_a|Hole_a >
                        endif
                        if [Part_a]  then
                          (s̄s̄|s̄s̄) =< Act_b|V|Act_b >< Part_a|Part_a >
                    endif;enddo;endif

                    if [Hole_a .and. (M-2).ge.(Na-1) .and. Na.gt.0]  then
                      do   ll = 1,LM2N1_a
                        (ss|ss) =< Hole_a|V|Hole_a >< Act_b|Act_b >
                    enddo;endif
                    if [Hole_b .and. (M-2).ge.(Nb-1) .and. Nb.gt.0]  then
                      do  ll = 1,LM2N1_b
                        (s̄s̄|s̄s̄) =< Hole_b|V|Hole_b >< Act_a|Act_a >
                    enddo;endif

                    if [Part_a .and. Na.ge.3]  then
                      do   ll = 1,LM2N3_a
                        (ss|ss) =< Part_a|V|Part_a >< Act_b|Act_b >
                    enddo;endif
                    if [Part_b .and. Nb.ge.3]  then
                      do   ll = 1,LM2N3_b
                        (s̄s̄|s̄s̄) =< Part_b|V|Part_b >< Act_a|Act_a >
                    enddo;endif

               elseif  [I_{ijkl} = 4,6,8,9,10 .and. M.ge.3]  then !************************

                  if [Na.ge.2 .and. (M-3).ge.(Na-2)]  then ! <Act_a|V|Act_a> <X_b|X_b>
                    do   ll = 1,LM3N2_a
                      (ss|ss) =< Act_a|V|Act_a >< Act_b|Act_b >
                      if [Hole_b]  then
                        (ss|ss) =< Act_a|V|Act_a >< Hole_b|Hole_b >
                      endif
                      if [Part_b]  then
```

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```fortran
327                        (ss|ss) =< Act_a|V|Act_a >< Part_b|Part_b >
328                     endif; enddo; endif
329                     if [Nb.ge.2 .and. (M-3).ge.(Nb-2)] then ! <Act_b|V|Act_b> <X_a|X_a>
330                        do  ll = 1,LM3N2_b
331                          (s̄s̄|s̄s̄) =< Act_b|V|Act_b >< Act_a|Act_a >
332                          if [Hole_a] then
333                            (s̄s̄|s̄s̄) =< Act_b|V|Act_b >< Hole_a|Hole_a >
334                          endif
335                          if [Part_a] then
336                            (s̄s̄|s̄s̄) =< Act_b|V|Act_b >< Part_a|Part_a >
337                     endif; enddo; endif
338
339                     if [Hole_a .and. (M-3).ge.(Na-1) .and. Na.gt.0] then
340                        do ll = 1,LM3N1_a
341                          (ss|ss) =< Hole_a|V|Hole_a >< Act_b|Act_b >
342                     enddo; endif
343                     if [Hole_b .and. (M-3).ge.(Nb-1) .and. Nb.gt.0] then
344                        do ll = 1,LM3N1_b
345                          (s̄s̄|s̄s̄) =< Hole_b|V|Hole_b >< Act_a|Act_a >
346                     enddo; endif
347
348                     if [Part_a .and. Na.ge.3] then
349                        do ll = 1,LM3N3_a
350                          (ss|ss) =< Part_a|V|Part_a >< Act_b|Act_b >
351                     enddo; endif
352                     if [Part_b .and. Nb.ge.3] then
353                        do ll = 1,LM3N3_b
354                          (s̄s̄|s̄s̄) =< Part_b|V|Part_b >< Act_a|Act_a >
355                     enddo; endif
356
357               elseif [I_{ijkl} = 11 .and. M.ge.4] the !********************************
358
359                     if [Na.ge.2 .and. (M-4).ge.(Na-2)] then ! <Act_a|V|Act_a> <X_b|X_b>
360                        do ll = 1,LM4N2_a
361                          (ss|ss) =< Act_a|V|Act_a >< Act_b|Act_b >  (2 times)
362                          if [Hole_b] then
363                            (ss|ss) =< Act_a|V|Act_a >< Hole_b|Hole_b >  (2 times)
364                          endif
365                          if [Part_b] then
366                            (ss|ss) =< Act_a|V|Act_a >< Part_b|Part_b >  (2 times)
367                     endif; enddo; endif
368                     if [Nb.ge.2 .and. (M-4).ge.(Nb-2)] then ! <Act_b|V|Act_b> <X_a|X_a>
369                        do ll = 1,LM4N2_b
370                          (s̄s̄|s̄s̄) =< Act_b|V|Act_b >< Act_a|Act_a >  (2 times)
371                          if [Hole_a] then
372                            (s̄s̄|s̄s̄) =< Act_b|V|Act_b >< Hole_a|Hole_a >  (2 times)
373                          endif
374                          if [Part_a] then
375                            (s̄s̄|s̄s̄) =< Act_b|V|Act_b >< Part_a|Part_a >  (2 times)
376                     endif; enddo; endif
377
378                     if [Hole_a .and. (M-4).ge.(Na-1) .and. Na.gt.0] then
379                        do ll = 1,LM4N1_a
380                          (ss|ss) =< Hole_a|V|Hole_a >< Act_b|Act_b >  (2 times)
381                     enddo; endif
```

13

```fortran
382              if [Hole_b .and. (M-4).ge.(Nb-1) .and. Nb.gt.0] then
383                do ll = 1,LM4N1_b
384                  (s̄s̄|s̄s̄) =< Hole_b|V|Hole_b >< Act_a|Act_a >  (2 times)
385              enddo; endif
386
387              if [Part_a .and. Na.ge.3 .and. (M-4).ge.(Na-3)]
388                do ll = 1,LM4N3_a
389                  (ss|ss) =< Part_a|V|Part_a >< Act_b|Act_b >  (2 times)
390              enddo; endif
391              if [Part_b .and. Nb.ge.3 .and. (M-4).ge.(Nb-3)]
392                do ll = 1,LM4N3_b
393                  (s̄s̄|s̄s̄) =< Part_b|V|Part_b >< Act_a|Act_a >  (2 times)
394              enddo; endif
395
396          deallocate LAA_34σ, LHH_34σ, LPP_34σ
397        enddo ! i4, i3
398
399      if [Hole .or. Part] then
400        do i3 = 1,M
401          if [Na.lt.1 .and. Nb.lt.1] cycle i3
402
403 !*********************
404 !*  2-elec alpha/beta  *
405 !*********************
406          do iA = 1,MNAA_12a ! LAA_12a(MNAA_12a)
407            if [Hole_b .and. (M-1).ge.Nb] then  ! <Act_b|V|Hole_b> <Act_a|V|Act_a>
408              do ll = 1,LM1N_b
409                (ss|s̄ī) =< Act_b|V|Hole_b >< Act_a|V|Act_a >
410                if [I_{ijkl}.ge.9] (ss|s̄ī) =< Act_b|V|Hole_b >< Act_a|V|Act_a >
411            enddo; endif
412            if [Part_b] then  ! <Act_b|V|Part_b> <Act_a|V|Act_a>
413              do ll = 1,LM1N1_b
414                (ss|s̄ā) =< Act_b|V|Part_b >< Act_a|V|Act_a >
415                if [I_{ijkl}.ge.9] (ss|s̄ā) =< Act_b|V|Part_b >< Act_a|V|Act_a >
416          enddo; endif; enddo
417
418          do iB = 1,MNAA_12b ! LAA_12b(MNAA_12b)
419            if [Hole_a .and. (M-1).ge.Na] then  ! <Act_a|V|Hole_a> <Act_b|V|Act_b>
420              do ll = 1,LM1N_a
421                (s̄s̄|si) =< Act_a|V|Hole_a >< Act_b|V|Act_b >
422                if [I_{ijkl}.ge.9] (s̄s̄|si) =< Act_a|V|Hole_a >< Act_b|V|Act_b >
423            enddo; endif
424            if [Part_a] then  ! <Act_a|V|Part_a> <Act_b|V|Act_b>
425              do ll = 1,LM1N1_a
426                (s̄s̄|si) =< Act_a|V|Part_a >< Act_b|V|Act_b >
427                if [I_{ijkl}.ge.9] (s̄s̄|si) =< Act_a|V|Part_a >< Act_b|V|Act_b >
428          enddo; endif; enddo
429
430 !*********************
431 !*  2-elec alpha/alpha  *
432 !*********************
433          NMin = 1; if [.not.Hole] NMin = 2
434          if [(Na.lt.NMin .and. Nb.lt.NMin) .or. I_{ijkl} = 5] then !*****************
435            cycle i3
436
```

```fortran
437          elseif [I_{ijkl} = 6,9,10] then !**************************
438            if [Hole_a .and. (M-2).ge.(Na-1) .and. Na.gt.0] then
439              do ll = 1,LM2N1_a
440                (ss|si) =< Act_a|V|Hole_a >< Act_b|Act_b >
441            enddo;endif
442            if [Hole_b .and. (M-2).ge.(Nb-1) .and. Nb.gt.0] then
443              do ll = 1,LM2N1_b
444                (s̄s̄|s̄ī) =< Act_b|V|Hole_b >< Act_a|Act_a >
445            enddo;endif
446
447            if [Part_a .and. Na.ge.2] then
448              do ll = 1,LM2N2_a
449                (ss|sa) =< Act_a|V|Part_a >< Act_b|Act_b >
450            enddo;endif
451            if [Part_b .and. Nb.ge.2] then
452              do ll = 1,LM2N2_b
453                (s̄s̄|s̄ā) =< Act_b|V|Part_b >< Act_a|Act_a >
454            enddo;endif
455
456          elseif [I_{ijkl} = 11 .and. M.ge.3] then !**************************
457            if [Hole_a .and. (M-3).ge.(Na-1) .and. Na.gt.0] then
458              do ll = 1,LM3N1_a
459                (ss|si) =< Act_a|V|Hole_a >< Act_b|Act_b > (2 times)
460            enddo;endif
461            if [Hole_b .and. (M-3).ge.(Nb-1) .and. Nb.gt.0] then
462              do ll = 1,LM3N1_b
463                (s̄s̄|s̄ī) =< Act_b|V|Hole_b >< Act_a|Act_a > (2 times)
464            enddo;endif
465
466            if [Part_a .and. Na.ge.2 .and. (M-3).ge.(Na-2)] then
467              do ll = 1,LM3N2_a
468                (ss|sa) =< Act_a|V|Part_a >< Act_b|Act_b > (2 times)
469            enddo;endif
470            if [Part_b .and. Nb.ge.2 .and. (M-3).ge.(Nb-2)] then
471              do ll = 1,LM3N2_b
472                (s̄s̄|s̄ā) =< Act_b|V|Part_b >< Act_a|Act_a > (2 times)
473            enddo;endif
474      enddo ! i3,i2,i1
475
476      if [Part_a] then
477        F_{ab} =< Part_a|F|Part_a >< Act_b|Act_b >
478      endif
479      if [Part_b] then
480        F_{āb̄} =< Part_b|F|Part_b >< Act_a|Act_a >
481      endif
482      if [Hole_a] then
483        F_{ij} =< Hole_a|F|Hole_a >< Act_b|Act_b >
484      endif
485      if [Hole_b] then
486        F_{īj̄} =< Hole_b|F|Hole_b >< Act_a|Act_a >
487      endif
488      write response vector (jR) into disk
489 end Roots
```