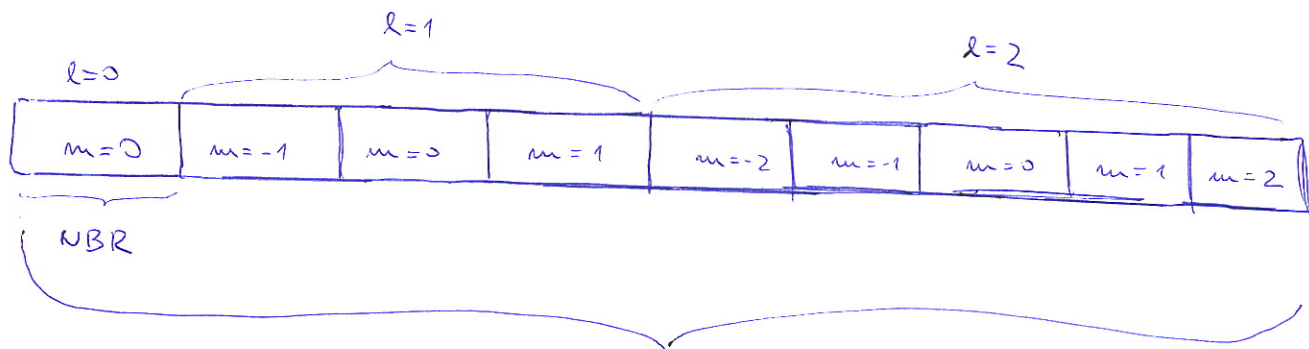## HF and higher angular momenta

- Increase $LMAX = 1, 2$, must be done before the generation of

  the radial repulsion integrals table by:

  | call rkb_alloc (2* LMAX)
  | call rkb_cell

- Do not incorporate new basis set indeces "l" and "m". Create

  one linear basis set index "ib" which organizes the basis

  as follows (motivation by Q.chemistry programs, no radial symmetry):

$$NB = NBR * NPW \text{ (number of partial waves)}$$

$$NPW = (LMAX + 1)^2$$

- Basis set loop is formed by a "triple-loop" (i, l, m), C-syntax:

```
for (l1=0 | ib1=0; l1 ≤ LMAX ; l1++)
  for( m1 = -l1 ; m1 ≤ l1 ; m1++ )
    for ( i1 =0 ; i1 ≤ NBR ; i1++ , ib1++ )  {
      array[ib1][.] = ...
    }
```

– The calculations slow down because formation of

J and k matrices scale as $\underline{NB^4 \times \bar{N}}$. ($\bar{N} = 1$ for singlet

and $\bar{N} = 2$ for triplet)