Problems - VB

- Write the structures of O_2 at R_e and ∞
- Find out in **all** formula's what changes with orbital orthogonality
- In a direct CI the program is simplified by "group theory" (*I can explain*); Would a direct VB be possible/feasable/attractive ??
- Consider singular value decomposition; Show how it can be used to evaluate determinants and directed hybrids
- Determine the # Kekule and total number of covalent structures of a cyclopentafused pyrene; how many determinants has one structure ?? (in which spincoupling scheme)
- Show how one can derive 2nd order cofactor from the first-order ones and the 1st-order from the 2nd order ones. Which algorithm is most favourable; When ??
- Show the relation between a Fock-matrix element and the Brilliouin theorem and the corresponding matrix element.
- Give an estimate of the amount of work in a VB or VBSCF