E1-20: Computer generation of many electron spin eigen functions

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Quite often we have to deal with many electron Hamiltonian operators which are spin independent. The corresponding stationary states are eigen functions of the usual spin operators S^2 and S_x Some of these applications (eg. photoionization calculations using Schwinger variational principle) require the

knowledge of the explicit form of the wave function. A configuration interaction (CI) expansion of such an N-electron wave function takes the form $\Phi = \Sigma_i \phi_i$, where

$$\phi_i = \hat{A}4[(core)(open)\alpha(1)ß(2)....\alpha(2n\text{-}1)ß(2n)\Theta_i(2n+1,...,N)]$$

Here $\hat{A}$ is the antisymmetrizer.

(core) = $\phi_1(1)\ \phi_1(2)\ ....\ \phi_n(2n\text{-}1)\ \phi_n(2n)$;
it is a product of doubly occupied orbitals.

(open) = $\phi_a(2n+1)\phi_b(2n+2)\ ....\ \phi_x(N)$;
is a product of (N-2n) singly occupied orbitals.

α and ß are the usual single electron spin states.

$\Theta_i(2n+1, ..., N)$ is a spin eigen function corresponding to (N-2n) electrons.

The construction of ϕ requires the construction of Θ. As the number of electrons increases, the number of Θ functions (for given S and S_z values) increase very rapidly and manual construction becomes impractical.

For example there are only 5 such functions with $S = S_z = 0$ when the number of electrons is 6. However, there are 16,796 such functions when the electron number is 20. A computer program, using the character handling facilities in FORTRAN was developed to do the necessary algebra, to explicitly generate all the spin eigen fnctions, with given S and S_z, corresponding to a given number of electrons. A typical output from the program is displayed below. This is a function with $S = S_z = 0$ for 6 electrons.

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 0.353553D+00 ABABAB  -  0.353553D+00 ABABBA
 - 0.353553D+00 ABBAAB + 0.353553D+00 ABBABA
 - 0.353553D+00 BAABAB + 0.353553D+00 BAABBA
 + 0.353553D+00 BABAAB  -  0.353553D+00 BABABA
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Here A and B represent the α and ß spin states of an electron.