n-ELECTRON ($n=2, 4, 6, 8$) TRIPLETS AS S^2 EIGENFUNCTIONS

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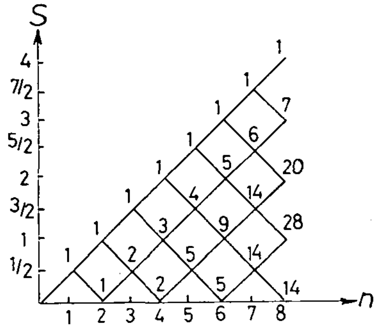
n-electron ($n=2, 4, 6, 8$) triplets as S^2 eigenfunctions were constructed by the method of spin operators.

Introduction

In previous papers [1—3] using the abstract formulation of the method of branching diagrams, a spin operator was constructed with the so-called S^+ step up and S^- step down spin operator which, when operating on the eigenfunctions of the total S_z spin operator related to maximal projections of total spin, creates each eigen-function of the total S^2 corresponding to its different eigenvalues. The branching diagram has the form:



and the formula of the operator is as follows:

$$O_{x_1 x_2 x_3 \dots x_{2n-1} x_{2n}} = \left(\frac{x_1 - x_2 + x_3 - \dots + x_{2n-1} + x_{2n} + 1}{x_1 - x_2 x_3 - \dots + x_{2n-1} + 1} \right)^{1/2} \times$$

$$\times \left(\frac{x_1 - x_2 + x_3 - \dots + x_{2n-3} - x_{2n-2} + 1}{x_1 - x_2 + x_3 - \dots + x_{2n-3} + 1} \right)^{1/2} \times \dots \times \left(\frac{x_1 - x_2 + 1}{x_1 + 1} \right)^{1/2} \times$$

$$\times \sum_{k=0}^{x_{2n}} (-1)^k \frac{(x_1 - x_2 + x_3 - \dots + x_{2n-1} - k)!}{(x_1 - x_2 + x_3 - \dots + x_{2n-1})!\, k!} \left(S^-_{x_1 x_2 x_3 \dots x_{2n-1}} S^+_{x_{2n}} \right)^k \times$$

$$\times \sum_{j=0}^{x_{2n-2}} (-1)^j \frac{(x_1-x_2+x_3-\ldots+x_{2n-3}-j)!}{(x_1-x_2+x_3-\ldots+x_{2n-3})!\,j!} (S^-_{X_1X_2X_3\ldots X_{2n-3}} S^+_{X_{2n-2}})^j \times \ldots \times$$

$$\times \sum_{i=0}^{x_2} \frac{(x_1-i)!}{x_i!\,i!} (S^-_{X_1} S^+_{X_2})^i.$$

In a next paper [4] with the proposed operator technique the n-electron ($n=2, 4, 6, 8$) singlets as S^2 eigenfunctions were constructed.

Since in the investigation of molecules by configuration interaction, by one of the most important method of quantum chemistry, all the states of definite multiplicity for the various configurations are required, in the present paper the n-electron ($n=2, 4, 6, 8$) triplets as S^2 eigenfunctions were constructed.

The n-electron triplets

Let us denote the Slater determinants describing the states of n-electron systems as follows

$n = 2$

$A = |\alpha\alpha|.$

$n = 4$

$B_1 = |\alpha\alpha\alpha\beta|, \quad B_2 = |\alpha\alpha\beta\alpha|, \quad B_3 = |\alpha\beta\alpha\alpha|, \quad B_4 = |\beta\alpha\alpha\alpha|.$

$n = 6$

$C_1 = |\alpha\alpha\alpha\alpha\beta\beta|, \quad C_2 = |\alpha\alpha\alpha\beta\beta\alpha|, \quad C_3 = |\alpha\alpha\alpha\beta\alpha\beta|,$

$C_4 = |\alpha\alpha\beta\beta\alpha\alpha|, \quad C_5 = |\alpha\alpha\beta\alpha\alpha\beta|, \quad C_6 = |\alpha\alpha\beta\alpha\beta\alpha|,$

$C_7 = |\alpha\beta\alpha\alpha\alpha\beta|, \quad C_8 = |\alpha\beta\alpha\alpha\beta\alpha|, \quad C_9 = |\alpha\beta\alpha\beta\alpha\alpha|,$

$C_{10} = |\alpha\beta\beta\alpha\alpha\alpha|, \quad C_{11} = |\beta\beta\alpha\alpha\alpha\alpha|, \quad C_{12} = |\beta\alpha\beta\alpha\alpha\alpha|,$

$C_{13} = |\beta\alpha\alpha\beta\alpha\alpha|, \quad C_{14} = |\beta\alpha\alpha\alpha\beta\alpha|, \quad C_{15} = |\beta\alpha\alpha\alpha\alpha\beta|.$

$n = 8$

$D_1 = |\alpha\alpha\alpha\alpha\alpha\beta\beta\beta|, \quad D_2 = |\alpha\alpha\alpha\alpha\beta\beta\beta\alpha|, \quad D_3 = |\alpha\alpha\alpha\alpha\beta\beta\alpha\beta|,$

$D_4 = |\alpha\alpha\alpha\alpha\beta\alpha\beta\beta|, \quad D_5 = |\alpha\alpha\alpha\beta\beta\beta\alpha\alpha|, \quad D_6 = |\alpha\alpha\alpha\beta\beta\alpha\alpha\beta|,$

$D_7 = |\alpha\alpha\alpha\beta\beta\alpha\beta\alpha|, \quad D_8 = |\alpha\alpha\alpha\beta\alpha\alpha\beta\beta|, \quad D_9 = |\alpha\alpha\alpha\beta\alpha\beta\beta\alpha|,$

$D_{10} = |\alpha\alpha\alpha\beta\alpha\beta\alpha\beta|, \quad D_{11} = |\alpha\alpha\beta\beta\alpha\alpha\alpha\beta|, \quad D_{12} = |\alpha\alpha\beta\beta\alpha\alpha\beta\alpha|,$

$D_{13} = |\alpha\alpha\beta\beta\alpha\beta\alpha\alpha|, \quad D_{14} = |\alpha\alpha\beta\alpha\alpha\alpha\beta\beta|, \quad D_{15} = |\alpha\alpha\beta\alpha\alpha\beta\beta\alpha|,$

$D_{16} = |\alpha\alpha\beta\alpha\beta\beta\alpha\alpha|, \quad D_{17} = |\alpha\alpha\beta\alpha\alpha\beta\alpha\alpha|, \quad D_{18} = |\alpha\alpha\beta\alpha\beta\alpha\alpha\beta|,$

$D_{19} = |\alpha\alpha\beta\alpha\beta\alpha\beta\alpha|, \quad D_{20} = |\alpha\beta\alpha\alpha\alpha\alpha\beta\beta|, \quad D_{21} = |\alpha\beta\alpha\alpha\alpha\beta\beta\alpha|,$

$D_{22} = |\alpha\beta\alpha\alpha\alpha\beta\alpha\beta|$, $D_{23} = |\alpha\beta\alpha\alpha\beta\beta\alpha\alpha|$, $D_{24} = |\alpha\beta\alpha\alpha\beta\alpha\alpha\beta|$,

$D_{25} = |\alpha\beta\alpha\alpha\beta\alpha\beta\alpha|$, $D_{26} = |\alpha\beta\alpha\beta\alpha\alpha\alpha\beta|$, $D_{27} = |\alpha\beta\alpha\beta\alpha\alpha\beta\alpha|$,

$D_{28} = |\alpha\beta\alpha\beta\alpha\beta\alpha\alpha|$, $D_{29} = |\alpha\beta\beta\beta\alpha\alpha\alpha\alpha|$, $D_{30} = |\alpha\beta\beta\alpha\alpha\alpha\alpha\beta|$,

$D_{31} = |\alpha\beta\beta\alpha\alpha\alpha\beta\alpha|$, $D_{32} = |\alpha\beta\beta\alpha\beta\alpha\alpha\alpha|$, $D_{33} = |\alpha\beta\beta\alpha\alpha\beta\alpha\alpha|$,

$D_{34} = |\alpha\beta\alpha\beta\beta\alpha\alpha\alpha|$, $D_{35} = |\alpha\alpha\beta\beta\beta\alpha\alpha\alpha|$, $D_{36} = |\beta\beta\beta\alpha\alpha\alpha\alpha\alpha|$,

$D_{37} = |\beta\beta\alpha\alpha\alpha\alpha\alpha\beta|$, $D_{38} = |\beta\beta\alpha\alpha\alpha\alpha\beta\alpha|$, $D_{39} = |\beta\beta\alpha\alpha\alpha\beta\alpha\alpha|$,

$D_{40} = |\beta\beta\alpha\alpha\beta\alpha\alpha\alpha|$, $D_{41} = |\beta\beta\alpha\beta\alpha\alpha\alpha\alpha|$, $D_{42} = |\beta\alpha\alpha\alpha\alpha\alpha\beta\beta|$,

$D_{43} = |\beta\alpha\alpha\alpha\alpha\beta\beta\alpha|$, $D_{44} = |\beta\alpha\alpha\alpha\alpha\beta\alpha\beta|$, $D_{45} = |\beta\alpha\alpha\alpha\beta\beta\alpha\alpha|$,

$D_{46} = |\beta\alpha\alpha\alpha\beta\alpha\beta\alpha|$, $D_{47} = |\beta\alpha\alpha\alpha\beta\alpha\alpha\beta|$, $D_{48} = |\beta\alpha\alpha\beta\alpha\alpha\alpha\beta|$,

$D_{49} = |\beta\alpha\alpha\beta\alpha\alpha\beta\alpha|$, $D_{50} = |\beta\alpha\alpha\beta\alpha\beta\alpha\alpha|$, $D_{51} = |\beta\alpha\alpha\beta\beta\alpha\alpha\alpha|$,

$D_{52} = |\beta\alpha\beta\beta\alpha\alpha\alpha\alpha|$, $D_{53} = |\beta\alpha\beta\alpha\alpha\alpha\alpha\beta|$, $D_{54} = |\beta\alpha\beta\alpha\alpha\alpha\beta\alpha|$,

$D_{55} = |\beta\alpha\beta\alpha\alpha\beta\alpha\alpha|$, $D_{56} = |\beta\alpha\beta\alpha\beta\alpha\alpha\alpha|$.

The relating eigenfunctions are as follows

$n = 2$

$\Phi_1^2 = A.$

$n = 4$

$$\Phi_1^4 = O_{X_1X_2}B_1 = \frac{1}{\sqrt{12}}[3B_1-(B_2+B_3+B_4)];$$

$$\Phi_2^4 = O_{X_1X_2}B_2 = \frac{1}{\sqrt{6}}[2B_2-(B_3+B_4)];$$

$$\Phi_3^4 = O_{X_1X_2}B_3 = \frac{1}{\sqrt{2}}(B_3-B_4).$$

$n = 6$

$$\Phi_1^6 = O_{X_1X_2}C_1 = \frac{1}{2\sqrt{60}}[12C_1-3(C_2+C_3+C_5+C_6+C_7+C_8+C_{14}+C_{15})+$$
$$+2(C_4+C_9+C_{10}+C_{11}+C_{12}+C_{13})];$$

$$\Phi_2^6 = O_{X_1X_2}C_2 = \frac{1}{12\sqrt{2}}[12C_2-4(C_4+C_6+C_8+C_9+C_{13}+C_{14})+4(C_{10}+C_{11}+C_{12})];$$

$$\Phi_3^6 = O_{X_1\dots X_4}C_3 = \frac{1}{12}[9C_3-3(C_2+C_5+C_7+C_{15})-2(C_4+C_9+C_{13})+$$
$$+2(C_6+C_8+C_{10}+C_{11}+C_{12}+C_{14})];$$

$$\Phi_4^6 = O_{X_1X_2}C_4 = \frac{1}{2\sqrt{3}}[2C_4-(C_9+C_{10}+C_{12}+C_{13})+2C_{11}];$$

$$\Phi_5^6 = O_{X_1\ldots X_4}C_5 = \frac{1}{6\sqrt{2}}[6C_5-3(C_7+C_{15})-2(C_4+C_6)-(C_{10}+C_{12})+C_8+C_9+ \\ +2C_{11}+C_{13}+C_{14}];$$

$$\Phi_6^6 = O_{X_1\ldots X_4}C_6 = \frac{1}{6}[4C_6-2(C_4+C_8+C_{14})-(C_{10}+C_{12})+C_9+2C_{11}+C_{13}];$$

$$\Phi_7^6 = O_{X_1\ldots X_4}C_7 = \frac{1}{2\sqrt{6}}[3(C_7-C_{15})-(C_8+C_9+C_{10})+C_{12}+C_{13}+C_{14}];$$

$$\Phi_8^6 = O_{X_1\ldots X_4}C_8 = \frac{1}{2\sqrt{3}}[2(C_8-C_{14})-(C_9+C_{10})+C_{12}+C_{13}];$$

$$\Phi_9^6 = O_{X_1\ldots X_4}C_9 = \frac{1}{2}[C_9+C_{12}-(C_{10}+C_{13})].$$

$n = 8$

$$\Phi_1^8 = O_{X_1\ldots X_2}D_1 = \frac{1}{10\sqrt{2}}[10D_1+D_5+D_6+D_7+D_{11}+D_{12}+D_{13}+D_{16}+D_{18}+D_{19}+ \\ +D_{23}+D_{24}+D_{25}+D_{26}+D_{27}+D_{28}+D_{30}+D_{31}+D_{33}+D_{37}+D_{38}+D_{39}+D_{45}+ \\ +D_{46}+D_{47}+D_{48}+D_{49}+D_{50}+D_{53}+D_{54}+D_{55}-2(D_2+D_3+D_4+D_8+D_9+D_{10}+ \\ +D_{14}+D_{15}+D_{17}+D_{20}+D_{21}+D_{22}+D_{42}+D_{43}+D_{44})-(D_{29}+D_{32}+D_{34}+D_{35}+ \\ +D_{36}+D_{40}+D_{41}+D_{51}+D_{52}+D_{56})];$$

$$\Phi_2^8 = O_{X_1X_2}D_2 = \frac{1}{6\sqrt{10}}[12D_2-3(D_5+D_7+D_9+D_{15}+D_{16}+D_{19}+D_{21}+D_{23}+D_{25}+ \\ +D_{43}+D_{45}+D_{46})+2(D_{12}+D_{13}+D_{27}+D_{28}+D_{31}+D_{32}+D_{33}+D_{34}+D_{35}+D_{38}+ \\ +D_{39}+D_{40}+D_{49}+D_{50}+D_{51}+D_{54}+D_{55}+D_{56})+3(D_{29}+D_{36}+D_{41}+D_{52})];$$

$$\Phi_3^8 = O_{X_4\ldots X_4}D_3 = \frac{1}{48\sqrt{5}}[72D_3+66(D_{13}+D_{28}+D_{32}+D_{33}+D_{34}+D_{35}+D_{39}+D_{40}+ \\ +D_{50}+D_{51}+D_{55}+D_{56})+12(D_{11}+D_{26}+D_{30}+D_{37}+D_{48}+D_{53})+6(D_7+D_9+ \\ +D_{15}+D_{19}+D_{21}+D_{25}+D_{44}+D_{46})-24D_2-18(D_6+D_{10}+D_{17}+D_{18}+D_{22}+ \\ +D_{24}+D_{44}+D_{47})-12(D_5+D_{16}+D_{23}+D_{45})-3(D_{29}+D_{36}+D_{41}+D_{52})-(D_{12}+ \\ +D_{27}+D_{31}+D_{38}+D_{49}+D_{54})];$$

$$\Phi_4^8 = O_{X_1\ldots X_4}D_4 = \frac{1}{40\sqrt{3}}[48D_4+6(D_5+D_{16}+D_{23}+D_{45})+4(D_{32}+D_{34}+D_{35}+$$

$$+D_{40}+D_{51}+D_{56})+6(D_{11}+D_{12}+D_{26}+D_{27}+D_{30}+D_{31}+D_{37}+D_{38}+D_{48}+D_{49}+$$
$$+D_{53}+D_{54})-9(D_7+D_8+D_{18}+D_{19}+D_{24}+D_{25}+D_{46}+D_{47})+3(D_9+D_{10}+D_{15}+$$
$$+D_{17}+D_{21}+D_{22}+D_{43}+D_{44})-12(D_2+D_3+D_6+D_{14}+D_{20}+D_{42})-6(D_{29}+$$
$$+D_{36}+D_{41}+D_{52})-4(D_{13}+D_{28}+D_{33}+D_{39}+D_{50}+D_{55})];$$

$$\Phi_5^8=O_{X_1X_2}D_5=\frac{1}{6}[3(D_5-D_{36})+D_{29}+D_{32}+D_{33}+D_{39}+D_{40}+D_{41}+D_{52}+D_{55}+$$
$$+D_{56}-(D_{13}+D_{16}+D_{23}+D_{28}+D_{34}+D_{35}+D_{45}+D_{50}+D_{51})];$$

$$\Phi_6^8\quad O_{X_1\ldots X_4}D_6=\frac{1}{6\sqrt{6}}[9D_6+2(D_{34}+D_{35}+D_{51})+D_{12}+D_{13}+D_{16}+D_{19}+D_{23}+$$
$$+D_{25}+D_{27}+D_{28}+D_{29}+D_{32}+D_{40}+D_{41}+D_{45}+D_{46}+D_{49}+D_{50}+D_{52}+D_{56}-$$
$$-(D_{31}+D_{33}+D_{38}+D_{39}+D_{54}+D_{55})-3(D_5+D_7+D_{18}+D_{24}+D_{34}+D_{35}+D_{36}+$$
$$+D_{47}+D_{51})];$$

$$\Phi_7^8=O_{X_1\ldots X_4}D_7=\frac{1}{6\sqrt{3}}[6D_7+2(D_{31}+D_{38}+D_{54})+D_{13}+D_{16}+D_{23}+D_{28}+D_{29}+$$
$$+D_{32}+D_{40}+D_{41}+D_{45}+D_{50}+D_{52}+D_{56}-3(D_5+D_{36})-2(D_{12}+D_{19}+D_{25}+$$
$$+D_{27}+D_{46}+D_{49})-(D_{33}+D_{34}+D_{35}+D_{39}+D_{51}+D_{55})];$$

$$\Phi_8^8=O_{X_1\ldots X_4}D_8=\frac{1}{48\sqrt{5}}[72D_8+2(D_{30}+D_{31}+D_{37}+D_{38}+D_{53}+D_{54})+8(D_{13}+$$
$$+D_{28}+D_{34}+D_{35}+D_{50}+D_{51})+6(D_{15}+D_{17}+D_{18}+D_{19}+D_{21}+D_{22}+D_{24}+D_{25}+$$
$$+D_{43}+D_{44}+D_{46}+D_{47})+4(D_{29}+D_{41}+D_{52})-3D_5-24(D_{14}+D_{20}+D_{42})-$$
$$-28(D_6+D_7+D_9+D_{10})-12(D_{11}+D_{12}+D_{26}+D_{27}+D_{36}+D_{48}+D_{49})-8(D_{32}+$$
$$+D_{33}+D_{39}+D_{40}+D_{55}+D_{56})-4(D_{16}+D_{23}+D_{45})];$$

$$\Phi_9^8=O_{X_1\ldots X_4}D_9=\frac{1}{6\sqrt{6}}[9D_9+2(D_{31}+D_{33}+D_{34}+D_{35}+D_{38}+D_{39}+D_{51}+D_{54}+$$
$$+D_{55})+D_{16}+D_{19}+D_{23}+D_{25}+D_{29}+D_{41}+D_{45}+D_{46}+D_{52}-3(D_5+D_7+D_{15}+$$
$$+D_{21}+D_{36}+D_{43})-2(D_{12}+D_{13}+D_{26}+D_{28}+D_{32}+D_{40}+D_{49}+D_{50}+D_{56})];$$

$$\Phi_{10}^8=O_{X_1\ldots X_6}D_{10}=\frac{1}{24\sqrt{3}}[27D_{10}+6(D_{30}+D_{37}+D_{53})+4(D_{33}+D_{34}+D_{35}+D_{39}+$$
$$+D_{51}+D_{55})+3(D_7+D_{15}+D_{18}+D_{21}+D_{24}+D_{43}+D_{47})-2(D_{12}+D_{16}+D_{23}+$$
$$+D_{27}+D_{29}+D_{41}+D_{45}+D_{49}+D_{52})-9(D_6+D_9+D_{17}+D_{22}+D_{44})-6(D_5+$$

$$+D_{11}+D_{26}+D_{36}+D_{48})-4(D_{13}+D_{28}+D_{32}+D_{40}+D_{50}+D_{56})-2(D_{31}+D_{38}+$$
$$+D_{54})-(D_{19}+D_{25}+D_{46})];$$

$$\Phi_{11}^{8}=O_{X_1\dots X_4}D_{11}=\frac{1}{24}[12(D_{11}+D_{37})+3(D_{36}+D_{41})+2(D_{27}+D_{28}+D_{31}+D_{32}+$$
$$+D_{33}+D_{34}+D_{49}+D_{50}+D_{51}+D_{54}+D_{55}+D_{56})-6(D_{26}+D_{30}+D_{48}+D_{53})-$$
$$-4(D_{12}+D_{13}+D_{35})-(D_{38}+D_{39}+D_{40})];$$

$$\Phi_{12}^{8}=O_{X_1\dots X_4}D_{12}=\frac{1}{6\sqrt{2}}[4(D_{12}+D_{38})+D_{28}+D_{32}+D_{33}+D_{34}+D_{50}+D_{51}+D_{55}+$$
$$+D_{56}-2(D_{13}+D_{27}+D_{31}+D_{35}+D_{39}+D_{40}+D_{49}+D_{54})];$$

$$\Phi_{13}^{8}=O_{X_1\dots X_4}D_{13}=\frac{1}{2\sqrt{6}}[2(D_{13}+D_{32}+D_{34}+D_{39}+D_{51}+D_{56})-2(D_{35}+D_{40})-$$
$$-(D_{28}+D_{33}+D_{50}+D_{55})];$$

$$\Phi_{14}^{8}=O_{X_1\dots X_4}D_{14}=\frac{1}{12\sqrt{10}}[24D_{14}+6(D_{37}+D_{38})+4(D_{13}+D_{16}+D_{35})+3(D_{21}+$$
$$+D_{22}+D_{24}+D_{25}+D_{26}+D_{27}+D_{43}+D_{44}+D_{46}+D_{47}+D_{48}+D_{49})+2(D_{29}+D_{32}+$$
$$+D_{33}+D_{52}+D_{55}+D_{56})-12(D_{20}+D_{42})-6(D_{11}+D_{12}+D_{15}+D_{17}+D_{18}+D_{19})-$$
$$-4(D_{39}+D_{40}+D_{41})-3(D_{30}+D_{31}+D_{53}+D_{54})-2(D_{23}+D_{28}+D_{34}+D_{45}+$$
$$+D_{50}+D_{51})];$$

$$\Phi_{15}^{8}=O_{X_1\dots X_4}D_{15}=\frac{1}{6\sqrt{3}}[6D_{15}+2(D_{38}+D_{39})+D_{23}+D_{25}+D_{27}+D_{28}+D_{35}+D_{45}+$$
$$+D_{46}+D_{49}+D_{50}-3(D_{21}+D_{43})-2(D_{12}+D_{13}+D_{16}+D_{19}+D_{40}+D_{41})-(D_{32}+$$
$$+D_{33}+D_{35}+D_{36}+D_{51}+D_{54}+D_{55})];$$

$$\Phi_{16}^{8}=O_{X_1\dots X_4}D_{16}=\frac{1}{6\sqrt{2}}[4(D_{16}-D_{41})+2(D_{29}+D_{39}+D_{40}+D_{52})+D_{28}+D_{34}+$$
$$+D_{50}+D_{51}-2(D_{13}+D_{23}+D_{35}+D_{45})-(D_{32}+D_{33}+D_{55}+D_{56})];$$

$$\Phi_{17}^{8}=O_{X_1\dots X_4}D_{17}=\frac{1}{6\sqrt{12}}[18D_{17}+6D_{37}+4(D_{35}+D_{39})+3(D_{21}+D_{24}+D_{26}+D_{43}+$$
$$+D_{47}+D_{48})+2(D_{12}+D_{19}+D_{23}+D_{28}+D_{29}+D_{32}+D_{45}+D_{50}+D_{52}+D_{56})+$$
$$+D_{31}+D_{54}-9(D_{22}+D_{44})-6(D_{11}+D_{15}+D_{18})-4(D_{13}+D_{16}+D_{40}+D_{41})-$$
$$3(D_{30}+D_{53})-2(D_{28}+D_{33}+D_{34}+D_{51}+D_{55})-(D_{25}+D_{27}+D_{46}+D_{49})];$$

$$\Phi_{18}^8 = O_{X_1 \dots X_5} D_{18} = \frac{1}{12\sqrt{3}} [12D_{18} + 6D_{37} + 3(D_{26} + D_{48}) + 2(D_{12} + D_{13} + D_{23} + D_{25} + D_{29} + D_{40} + D_{45} + D_{46} + D_{52}) + D_{31} + D_{33} + D_{34} + D_{51} + D_{54} + D_{55} - 6(D_{11} + D_{24} + D_{47}) - 4(D_{16} + D_{19} + D_{41}) - 3(D_{30} + D_{53}) - 2(D_{35} + D_{38} + D_{39}) - (D_{27} + D_{28} + D_{32} + D_{49} + D_{50} + D_{56})];$$

$$\Phi_{19}^8 = O_{X_1 \dots X_6} D_{19} = \frac{1}{6\sqrt{6}} [8D_{19} + 4D_{38} + 2(D_{13} + D_{23} + D_{27} + D_{29} + D_{31} + D_{40} + D_{45} + D_{52} + D_{55}) + D_{33} + D_{34} + D_{50} - 4(D_{12} + D_{16} + D_{25} + D_{41} + D_{46}) - 2(D_{35} + D_{39} + D_{49} + D_{54}) - (D_{28} + D_{32} + D_{50} + D_{55} + D_{56})];$$

$$\Phi_{20}^8 = O_{X_1 \dots X_4} D_{20} = \frac{1}{12\sqrt{5}} [12(D_{20} - D_{42}) + 3(D_{43} + D_{44} + D_{46} + D_{47} + D_{48} + D_{49} + D_{53} + D_{54}) + 2(D_{23} + D_{28} + D_{29} + D_{32} + D_{33} + D_{34}) - 3(D_{21} + D_{22} + D_{24} + D_{25} + D_{26} + D_{27} + D_{30} + D_{31}) - 2(D_{45} + D_{50} + D_{51} + D_{53} + D_{55} + D_{56})];$$

$$\Phi_{21}^8 = O_{X_1 \dots X_4} D_{21} = \frac{1}{6} [3(D_{21} - D_{43}) + D_{29} + D_{32} + D_{34} + D_{45} + D_{46} + D_{49} + D_{50} + D_{54} + D_{55} - (D_{23} + D_{25} + D_{27} + D_{28} + D_{31} + D_{33} + D_{51} + D_{52} + D_{56})];$$

$$\Phi_{22}^8 = O_{X_1 \dots X_6} D_{22} = \frac{1}{12\sqrt{2}} [9(D_{22} - D_{44}) + 3(D_{43} + D_{47} + D_{48} + D_{53}) + 2(D_{29} + D_{32} + D_{34} + D_{45} + D_{50} + D_{55}) + D_{25} + D_{27} + D_{31} - 3(D_{21} + D_{24} + D_{26} + D_{29}) - 2(D_{23} + D_{28} + D_{33} + D_{51} + D_{52} + D_{56}) - (D_{46} + D_{49} + D_{54})];$$

$$\Phi_{23}^8 = O_{X_1 \dots X_4} D_{23} = \frac{1}{2\sqrt{6}} [2(D_{23} + D_{29} - D_{45} - D_{52}) + D_{50} + D_{51} + D_{55} + D_{56} - (D_{28} + D_{32} + D_{33} + D_{34})];$$

$$\Phi_{24}^8 = O_{X_1 \dots X_6} D_{24} = \frac{1}{12} [6(D_{24} - D_{47}) + 3(D_{48} + D_{53}) + 2(D_{29} + D_{45} + D_{46}) + D_{27} + D_{28} + D_{31} + D_{33} + D_{51} + D_{56} - 3(D_{26} + D_{30}) - 2(D_{23} + D_{25} + D_{52}) - (D_{32} + D_{34} + D_{49} + D_{50} + D_{54} + D_{55})];$$

$$\Phi_{25}^8 = O_{X_1 \dots X_6} D_{25} = \frac{1}{6\sqrt{2}} [4(D_{25} - D_{46}) + 2(D_{29} + D_{45} + D_{49} + D_{54}) + D_{28} + D_{33} + D_{51} + D_{56} - 2(D_{23} + D_{27} + D_{31} + D_{52}) - (D_{32} + D_{34} + D_{50} + D_{55})];$$

$$\Phi_{26}^{8} = O_{X_1 \dots X_6} D_{26} = \frac{1}{4\sqrt{3}} [3(D_{26} - D_{30} - D_{48} + D_{53}) + D_{31} + D_{32} + D_{33} + D_{49} + D_{50} +$$

$$+ D_{51} - (D_{27} + D_{28} + D_{34} + D_{54} + D_{55} + D_{56})];$$

$$\Phi_{27}^{8} = O_{X_1 \dots X_6} D_{27} = \frac{1}{2\sqrt{6}} [2(D_{27} - D_{31} - D_{49} + D_{54}) + D_{32} + D_{33} + D_{50} + D_{51} -$$

$$- (D_{29} + D_{34} + D_{55} + D_{56})];$$

$$\Phi_{28}^{8} = O_{X_1 \dots X_6} D_{28} = \frac{1}{2\sqrt{2}} [D_{28} + D_{32} + D_{51} + D_{55} - (D_{33} + D_{34} + D_{49} + D_{56})].$$

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n-ЭЛЕКТРОН (n=2, 4, 6, 8) ТРИПЛЕТЫ КАК СОБСТВЕННЫЕ ФУНКЦИИ S^2

Ф. Беренц

n-электрон (n=2, 4, 6, 8) триплеты, как собственные функции S^2 были созданы методом спиновых операторов.