

# THE RELATION OF THE SPIN OPERATOR METHOD WITH OTHER AUTHORS' SIMILAR METHODS

By

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A spin operator method described by Pratt for constructing singlets is demonstrated to be a considerably more complicated procedure than that of Löwdin or of the present author.

The reason for elaborating the spin operator method was given by PRATT'S paper [1] entitled "Eigenfunctions of  $S^2$  by a Spin Operator Method". Studying the works of CONDON, SHORTLY [2] and RACAH [3], Pratt discovered the mathematical difficulty arising from the method of configuration interaction, and wanted it to be solved. Therefore a spin operator was constructed with the so-called  $S^+$  step-up and  $S^-$  stepdown spin operator which, when operating on determinants built up from spin-orbitals, creates each eigenfunction of the total  $S^2$ . Above all, Pratt applied his operator to find all the orthogonal singlets for a  $2N$ -electron system: the 5 singlets of the six-electron system, the 14 singlets of the eight-electron system and the 42 singlets of the ten-electron system. The formula of the operator is as follows:

$$O = \frac{1}{(N+1)^{1/2} \{n[1+(n-1)/(N+1)]\}^{3/2}} \times$$

$$\times \sum_i \left\{ 1 + \sum_{m=1}^N \frac{(-1)^m (N-M)!}{N! M!} [(S_A^- S_B^+)^M + (S_A^+ S_B^-)^M] \times \right. \quad (1)$$

$$\left. \prod_{j_{A_i}, k_{B_i}} (S_{j_{A_i}}^+ S_{j_{A_i}}^- S_{k_{B_i}}^- S_{k_{B_i}}^+ + S_{j_{A_i}}^- S_{j_{A_i}}^+ S_{k_{B_i}}^+ S_{k_{B_i}}^-) \right\}.$$

On applying operator (1) two cases have to be taken into consideration:

- 1) the operator is operating on spin-orbitals having the projection of spin  $M_s = 0$ ;
- 2) the operator is operating on spin-orbitals having the projection of spin  $M_s \neq 0$ .

In the first case, one must know when using the operator that PRATT divided the electrons of the  $2N$ -electron system into two sets: the collection of  $N$  electrons and orbitals will be termed set  $A$ , and the remaining  $N$  electrons and  $N$  orbitals denoted as set  $B$ . The determinant which on application of (1) gives the singlet

states was constructed by Pratt by composing the product of the two determinants built up from spin-orbitals of the electrons of set  $A$  and set  $B$ .  $S_A^-$  and  $S_A^+$  mean the so-called step-down and step-up operators which operate on part  $A$  and  $B$ , respectively, of the above mentioned determinant.

The summation of  $i$  means the summation of all the different sets constructed from the  $2N$  spin-orbitals by choosing the  $N$  spin-orbitals in all possible ways.  $M$  denotes the number of spin reversing in set  $A$  and  $B$ , respectively. In case of  $M_s=0$ , the value of  $n$  is one.

In the second case the projection of spin  $M_s$  differs from zero. This means that (1) operates on spin-product functions in which the number of electrons having spin  $\alpha$  don't agree with the number of electrons having spin  $\beta$ . If  $x$  denotes the number of electrons having spin  $\alpha$ , but  $y$  the number of electrons having spin  $\beta$  and  $x > 0$ ,  $n$  is given in (1) by the formula as follows:

$$n = \frac{x!}{(x-y)! y!}, \quad (2)$$

where  $y$  means the value of  $N$  in (1).

To estimate Pratt's and the present author's [4] operators together, one must investigate the deriving procedure of both operators. Pratt derived his operator in more steps. First, he constructs

the singlet of the six-electron system given with the branching diagram in Fig. 1 based on the spin-vector model.

Having experienced, the above results giving the general definition of the number of spin-reversing in  $A$  and  $B$ , he writes the operator constructing the singlets of the  $2N$ -electron systems in the following formula:

$$O^1 = \sum_{M=0}^N (-1)^M \frac{(N-M)!}{N! M! \sqrt{N+1}} (S_A^- S_B^+)^M. \quad (3)$$

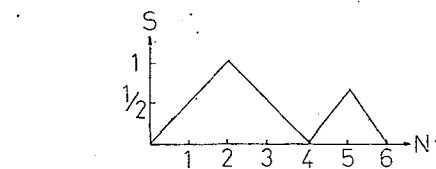


Fig. 1.

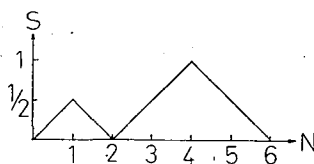


Fig. 2

Fig. 3

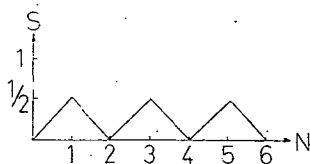


Fig. 4

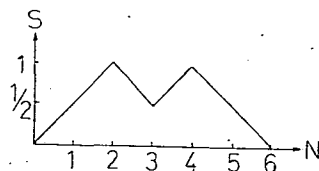


Fig. 5

Then he investigates the remaining singlets of the six-electron systems, given in Figs. 2 and 5. It was established that operator (3) must be generalized to the following formula:

$$O = 1 \frac{1}{(N+M)^{1/2}} \sum_i \left\{ 1 + \sum_{M=1}^N (-1)^M \frac{(N-M)!}{N! M!} \times \right. \\ \times [(S_{A_i}^- S_{B_i}^+)^M + (S_{A_i}^+ S_{B_i}^-)^M] \times \\ \left. \times \prod_{j_{A_i}, j_{B_i}} (S_{j_{A_i}}^+ S_{j_{A_i}}^- S_{k_{B_i}}^- S_{k_{B_i}}^+ + S_{j_{A_i}}^- S_{j_{A_i}}^+ S_{k_{B_i}}^+ S_{k_{B_i}}^-) \right\}. \quad (4)$$

But this operator isn't general enough because it's applicable only to the spin product functions having the projection of spin  $M_s=0$ . Operator (4) is to be generalized for the case  $M_s \neq 0$ . Formula (1) of the operator originates from this generalization.

After constructing the operator on the basis of the formula

$$S^2 = -\frac{1}{4} N(N+4) + \sum_{i < j} P_{ij}^{\sigma}, \quad (5)$$

it was proved, that 0 can be transposed with  $S^2$ .  $P_{ij}$  denotes the permutation operator.

As against the former way of derivation, it was shown by the present author that in uniting the systems, having spins  $\alpha$  and  $\beta$ , respectively, into a system having the resulting spin  $s+s'-l$ , the spin summation formula of van der Waerden results in the linear combination of the original configurations, which is an eigenfunction of operator  $S^2$  corresponding to eigenvalues  $(s+s'-\lambda)(s+s'-\lambda+1)$ . Then the formula of the spin summation will be put in its operator form, which will be transformed by the branching diagram into the case of eigenfunctions given by Slater-determinants. So the present author's operator takes the following form:

$$O_{X_1 X_2 X_3 \dots X_{2n-1} X_{2n}} = \left( \frac{x_1 - x_2 + x_3 - \dots + x_{2n-1} + x_{2n} + 1}{x_1 - x_2 x_3 - \dots + x_{2n-1} + 1} \right)^{1/2} \times \\ \times \left( \frac{x_1 - x_2 + x_3 - \dots + x_{2n-3} + x_{2n-2} + 1}{x_1 - x_2 + x_3 - \dots + x_{2n-3} + 1} \right)^{1/2} \times \dots \times \left( \frac{x_1 - x_2 + 1}{x_1 + 1} \right)^{1/2} \times \\ \times \sum_{k=0}^{x_{2n}} (-1)^k \frac{(x_1 - x_2 + x_3 - \dots + x_{2n-1} - k)!}{(x_1 - x_2 + x_3 - \dots + x_{2n-1})! k!} (S_{X_1 X_2 X_3 \dots X_{2n-1}}^- S_{X_{2n}}^+)^k \times \\ \times \sum_{j=0}^{x_{2n-2}} (-1)^j \frac{(x_1 - x_2 + x_3 - \dots + x_{2n-3} - j)!}{(x_1 - x_2 + x_3 - \dots + x_{2n-3})! j!} (S_{X_1 X_2 X_3 \dots X_{2n-3}}^- S_{X_{2n-2}}^+)^j \times \dots \times \\ \times \sum_{i=0}^{x_2} \frac{(x_1 - i)!}{x_i! i!} (S_{X_1}^- S_{X_2}^+)^i. \quad (6)$$

This way of derivation seems to be easier then that of Pratt.

Previously we saw that on applying Pratt's operator, because of its structure, we had to distinguish between spin orbitals having the projection of spins  $M_s=0$  and  $M_s \neq 0$ . In this fact the application of the operator is complicated to some extent. Such difficulties are not occurring to the present author's operator, because it genera-

tes the eigenfunctions of  $S^2$  with a projection of the maximum spin uniformly. From these eigenfunctions the eigenfunctions having the projection of the other spins can be obtained by applying the following formula:

$$\psi(s, s-i) = \frac{1}{i!} \frac{1}{\sqrt{\binom{2s}{i}}} (S^-)^i \psi(s, s). \quad (7)$$

In connection with the structure of Pratt's operator one must also speak about the fact, that it operates on sets  $A$  and  $B$  constructed in all possible ways from electron orbitals  $\varphi_i$ . This fact raises an additional difficulty in applying Pratt's operator because increasing the number of electrons results in a sum of many members making calculation more difficult. For instance, in case of the three-electron system  $[(\alpha\alpha\beta)]$ , the operator has the form as follows:

$$\begin{aligned} O = \frac{1}{\sqrt{2}} \{ & [1 - (S_1^- S_2^+ + S_1^+ S_2^-)] \times [S_1^+ S_1^- S_2^- S_3^+ + S_1^- S_1^+ S_2^+ S_2^-] + \\ & + [1 - (S_1^- S_3^+ + S_1^+ S_3^-)] \times [S_1^+ S_1^- S_3^- S_3^+ + S_1^- S_1^+ S_3^+ S_3^-] + \\ & + [1 - (S_2^- S_3^+ + S_2^+ S_3^-)] \times [S_2^+ S_2^- S_3^- S_3^+ + S_2^- S_2^+ S_3^+ S_3^-] \}. \end{aligned} \quad (8)$$

The above-mentioned circumstance was eliminated from the present author's operator by uniting the state of the  $N$ -electron system, having the total spin  $S$ , with the branching diagram from part systems on the basis of the spin summation formula of van der Waerden, and the operators constructing the eigenfunctions of  $S^2$  were built up in succession from the operators acting on the part systems. In the above mentioned case of three-electron systems, the present author's operator has the form as follows:

$$O = \sqrt{\frac{2}{3}} (1 - S_{\alpha}^- S_{\beta}^+), \quad (9)$$

where  $S_{\alpha}^-$  denotes the step-down operator acting on the  $(\alpha\alpha)$  spinproduct function,  $S_{\beta}^+$  the step-up operator acting on the  $\beta$  spinfunction.

It follows from the above mentioned comparison, that the present author's spin operator method is mathematically easier to treat than Pratt's method being simpler and more homogeneous.

Finally, the projection operator method [5] is to be mentioned as well. The essence of this is to give the eigenfunction of an operator when the eigenvalues are known. Par-Olov Löwdin has given a spin projection operator which, when operating on a determinant built up from spin orbitals of  $N$  antisymmetric particles with a half spin, such as electrons or nucleons, selects a state of multiplicity  $(2l+1)$ . This operator has the following form:

$${}^{(2l+1)}O = \prod_k^{k \neq l} \frac{S^2 - k(k+1)}{l(l+1) - k(k+1)}, \quad (10)$$

where  $S$  denotes the spin operator. Measuring the spin in units of  $\hbar$ :

$$l = \frac{N}{2}, \frac{N}{2} - 1, \frac{N}{2} - 2, \dots, 0 \quad \text{or} \quad \frac{1}{2}$$

depending on whether  $N$  is even or odd; the smallest and the largest values of  $k$  are the minimum and maximum values of the resulting spins, respectively.

On giving the Slater-determinants built up from  $2N$  spin orbitals with eigenvalue  $S_z=0$ , Löwdin introduced the following quantities:

$$\begin{aligned} T_0 &= \{\alpha\alpha \dots \alpha | \beta\beta \dots \beta\}, \\ T_1 &= \{(\beta\alpha\alpha \dots) + (\alpha\beta\alpha \dots) + \dots | (\alpha\beta\beta \dots) + (\beta\alpha\beta \dots) + \dots\} \\ T_2 &= \{(\beta\beta\alpha \dots) + (\beta\alpha\beta \dots) + \dots | (\alpha\alpha\beta \dots) + (\alpha\beta\alpha \dots) + \dots\} \\ &\vdots \\ T_N &= \{\beta\beta \dots \beta | \alpha\alpha \dots \alpha\}. \end{aligned} \quad (11)$$

$T_0$  is evidently the original Slater determinant, having  $N$  columns with spin  $\alpha$  and spin  $\beta$  respectively, and  $T_k$  is the sum of all the different determinants obtained from the  $k$  interchanges of the spin functions between the two originally given orbital  $A$  and  $B$ , in all possible order. Hence,  $T_k$  is a product of two factors, each of which is containing  $\binom{n}{k}$  terms and  $T_k$  consists, therefore, of a sum of  $\binom{n}{k}^2$  determinants.

Then Löwdin has proved among others that in case of singlets the following relation is valid:

$${}^1O T_0 = C_0^{(0)} \sum_{k=0}^n (-1)^k \binom{n}{k}^{-1} T_k. \quad (12)$$

On the basis of operator (12) it can be verified that for singlets Löwdin's operator and Pratt's operator, given under (3), are identical up to a constant factor. Therefore, the effect of the step-up and step-down operators ( $S_A^- S_B^+$ ) on the  $T_k$  introduced above should be investigated.  $q$  operator reverses in the Slater determinant all the  $\alpha$  spins into  $\beta$  spins; and  $S_B^+$  operator reverses in the Slater determinant all the  $\beta$  spins into  $\alpha$  spins, and so  $(S_A^- S_B^+) T_0$  gives the sum of all the different determinants obtained by an interchange of the spin functions between the two originally given groups  $A$  and  $B$  of the orbitals, in all possible order. But this is just the way  $T_1$  was introduced, therefore,

$$(S_A^- S_B^+) T_0 = T_1 = 1^2 T_1. \quad (13)$$

When  $(S_A^- S_B^+)$  operates on  $T_1$ , we obtain, before the line as well as after terms which contain two  $\beta$  and two  $\alpha$  spins respectively, in all possible order. Of these terms, however, due to the structure of  $T_1$  two are equivalent before the line as well as after, therefore,

$$(S_A^- S_B^+) T_1 = 2^2 T_2. \quad (14)$$

Quite similarly

$$(S_A^- S_B^+) T_{k-1} = k^2 T_k. \quad (15)$$

From (13), (14), and (15)

$$T_1 = \frac{1}{1^2} (S_A^- S_B^+) T_0 \quad (16)$$

$$T_2 = \frac{1}{2^2} (S_A^- S_B^+) T_1 = \frac{1}{(2!)^2} (S_A^- S_B^+)^2 T_0 \quad (17)$$

⋮

$$T_k = \frac{1}{(k!)^2} (S_A^- S_B^+)^k T_0 \quad (18)$$

Let us substitute (18) for (12)

$$\begin{aligned} {}^1O T_0 &= C_0^{(0)} \sum_{k=0}^N (-1)^k \binom{N}{k}^{-1} T_k = C_0^{(0)} \sum_{k=0}^N (-1)^k \frac{1}{(k!)^2} (S_A^- S_B^+)^k T_0 = \quad (19) \\ &= C_0^{(0)} \sum_{k=0}^N (-1)^k \frac{(N-k)!}{N! k!} (S_A^- S_B^+)^k T_0. \end{aligned}$$

Comparing (19) with (12) — as  $k=M$  — we can verify that for constructing singlets Löwdin's and Pratt's operators are with the exception of a constant factor identical.

Since Löwdin's spin projection operator is suitable for constructing the eigenfunctions of all the multiplet states, and for singlets, it agrees with the simplest form of Pratt's operator, it can be laid down as a fact that Pratt, by generalizing his operator, makes it rather complicated.

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#### СВЯЗЬ МЕТОДА СПИНОВЫХ ОПЕРАТОРОВ С ПОДОБНЫМИ МЕТОДАМИ ДРУГИХ АВТОРОВ

Ф. Беренц

Пратт разработал спинопаторный формализм для конструирования синглетов. Нами показано, что его метод в значительном мере сложнее метода Левдина или автора данной работы.

# ***n*-ELECTRON (*n*=4, 6, 8) QUINTETS, SEPTETS, AND NONETS AS $S^2$ EIGENFUNCTIONS**

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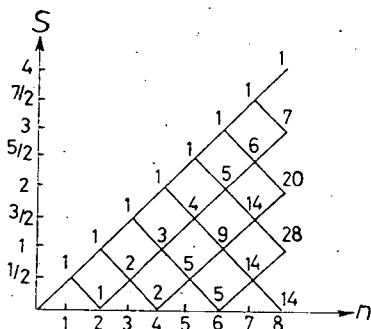
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*n*-electron (*n*=4, 6, 8) quintets, septets and nonets were constructed as  $S^2$  eigenfunctions by the method of spin operators.

## *Introduction*

In previous papers [1—3] on the basis of the branching diagram a spin operator was constructed which, when operating on the eigenfunctions of the total  $S_z$  spin operator, creates the eigenfunctions of the total  $S^2$  operator.

The branching diagram has the form:



and the formula of the operator is as follows:

$$\begin{aligned}
 O_{X_1 X_2 X_3 \dots X_{2n-1} X_{2n}} &= \left( \frac{x_1 - x_2 + x_3 - \dots + x_{2n-1} - x_{2n} + 1}{x_1 - x_2 + x_3 - \dots + x_{2n-1} + 1} \right)^{1/2} \times \\
 &\times \left( \frac{x_1 - x_2 + x_3 - \dots - x_{2n-3} - x_{2n-2} + 1}{x_1 - x_2 + x_3 - \dots - x_{2n-3} + 1} \right)^{1/2} \times \dots \times \left( \frac{x_1 - x_2 + 1}{x_1 + 1} \right)^{1/2} \times \\
 &\times \sum_{k=0}^{x_{2n}} (-1)^k \frac{(x_1 - x_2 + x_3 - \dots + x_{2n-1} - k)!}{(x_1 - x_2 + x_3 - \dots + x_{2n-1})! k!} (S_{X_1 X_2 X_3 \dots X_{2n-1}}^- S_{X_{2n}}^+)^k \times
 \end{aligned}$$

$$\begin{aligned} & \times \sum_{j=0}^{x_{2n-2}} (-1)^j \frac{(x_1 - x_2 + x_3 - \dots + x_{2n-3} - j)!}{(x_1 - x_2 + x_3 - \dots + x_{2n-3})! j!} (S_{x_1}^- S_{x_2}^- \dots S_{x_{2n-3}}^- S_{x_{2n-2}}^+)^j \times \\ & \quad \times \dots \times \sum_{i=0}^{x_2} \frac{(x_1 - i)!}{x_1! i!} (S_{x_1}^- S_{x_2}^+)^i, \end{aligned}$$

where  $S^+$  and  $S^-$  mean the so-called step-up and step-down spin operators respectively and  $X_i$  the  $i$ -th part system to be united, containing  $x_i$  electrons with parallel  $\alpha$  and  $\beta$  spins.

Similarly, in previous papers [4, 5], with the aid of the proposed operator technique the  $n$ -electron ( $n=2, 4, 6, 8$ ) singlets and triplets and, in the present paper, quintets, septets and nonets were constructed as  $S^2$  eigenfunctions.

### The $n$ -electron quintets

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

$$n = 4$$

$$A = |\alpha\alpha\alpha\alpha|.$$

$$n = 6$$

$$B_1 = |\alpha\alpha\alpha\alpha\beta|, \quad B_2 = |\alpha\alpha\alpha\alpha\beta\alpha|,$$

$$B_3 = |\alpha\alpha\alpha\beta\alpha\alpha|, \quad B_4 = |\alpha\alpha\beta\alpha\alpha\alpha|,$$

$$B_5 = |\alpha\beta\alpha\alpha\alpha\alpha|, \quad B_6 = |\beta\alpha\alpha\alpha\alpha\alpha|.$$

$$n = 8$$

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

$$D_3 = |\alpha\alpha\alpha\alpha\alpha\beta\alpha\beta|, \quad D_4 = |\alpha\alpha\alpha\alpha\beta\beta\alpha\alpha|,$$

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

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

$$D_9 = |\alpha\alpha\alpha\beta\alpha\alpha\beta\alpha|, \quad D_{10} = |\alpha\alpha\alpha\beta\alpha\beta\alpha\alpha|,$$

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

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

$$D_{15} = |\alpha\alpha\beta\alpha\beta\alpha\alpha\alpha|, \quad D_{16} = |\alpha\beta\alpha\alpha\alpha\alpha\alpha\beta|,$$

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

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

$$D_{21} = |\alpha\beta\beta\alpha\alpha\alpha\alpha\alpha|, \quad D_{22} = |\beta\beta\alpha\alpha\alpha\alpha\alpha\alpha|,$$

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

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

$$D_{27} = |\beta\alpha\alpha\alpha\alpha\alpha\beta\alpha|, \quad D_{28} = |\beta\alpha\alpha\alpha\alpha\alpha\alpha\beta|.$$



The relating eigenfunctions are as follows:

$$n = 4$$

$$\Phi_1^4 = A.$$

$$n = 6$$

$$\Phi_1^6 = O_{X_1 X_2} B_1 = \frac{1}{\sqrt{30}} [5B_1 - (B_2 + B_3 + B_4 + B_5 + B_6)];$$

$$\Phi_2^6 = O_{X_1 X_2 X_3} B_2 = \frac{1}{\sqrt{20}} [4B_2 - (B_3 + B_4 + B_5 + B_6)];$$

$$\Phi_3^6 = O_{X_1 X_2 X_3} B_3 = \frac{1}{\sqrt{12}} [3B_3 - (B_4 + B_5 + B_6)];$$

$$\Phi_4^6 = O_{X_1 X_2 X_3} B_4 = \frac{1}{\sqrt{6}} [2B_4 - (B_5 + B_6)];$$

$$\Phi_5^6 = O_{X_1 X_2 X_3} B_5 = \frac{1}{\sqrt{2}} (B_5 + B_6).$$

$$n = 8$$

$$\begin{aligned} \Phi_1^8 = O_{X_1 X_2} D_1 = & \frac{\sqrt{35}}{210} [30D_1 + 2(D_4 + D_7 + D_{10} + D_{11} + D_{14} + D_{15} + D_{18} + \\ & + D_{19} + D_{20} + D_{21} + D_{22} + D_{23} + D_{24} + D_{26}) - \\ & - 5(D_2 + D_3 + D_5 + D_6 + D_8 + D_9 + D_{12} + D_{13} + D_{16} + D_{17} + D_{27} + D_{28})]; \end{aligned}$$

$$\begin{aligned} \Phi_2^8 = O_{X_1 X_2 X_3} D_2 = & \frac{\sqrt{6}}{30} [10D_2 + D_7 + D_{11} + D_{15} + D_{19} + D_{20} + \\ & + D_{21} + D_{22} + D_{23} + D_{24} + D_{25} - 2(D_4 + D_6 + D_9 + D_{10} + \\ & + D_{13} + D_{14} + D_{17} + D_{18} + D_{26} + D_{27})]; \end{aligned}$$

$$\begin{aligned} \Phi_3^8 = O_{X_1 \dots X_4} D_3 = & \frac{1}{30} [25D_3 + 2(D_7 + D_{11} + D_{15} + D_{19} + D_{20} + D_{21} + D_{22} + \\ & + D_{23} + D_{24} + D_{25}) + D_4 + D_6 + D_9 + D_{10} + D_{13} + D_{14} + D_{17} + D_{18} + D_{26} + \\ & + D_{27} - 5(D_2 + D_4 + D_5 + D_8 + D_{10} + D_{12} + D_{14} + D_{16} + D_{18} + D_{26} + D_{28})]; \end{aligned}$$

$$\begin{aligned} \Phi_4^8 = O_{X_1 X_2 X_3} D_4 = & \frac{\sqrt{15}}{60} [15D_4 + D_{11} + D_{20} + D_{21} + D_{22} + D_{23} + D_{24} - \\ & - (D_7 + D_{10} + D_{14} + D_{15} + D_{18} + D_{19} + D_{25} + D_{26})]; \end{aligned}$$

$$\begin{aligned}\Phi_5^8 &= O_{X_1 \dots X_4} D_5 = \frac{\sqrt{6}}{60} [20D_5 + 2(D_{11} + D_{20} + D_{21} + D_{22} + D_{23} + D_{24}) + \\ &\quad + D_9 + D_{10} + D_{13} + D_{14} + D_{17} + D_{18} + D_{26} + D_{27} - 5(D_8 + D_{12} + D_{16} + D_{28}) - \\ &\quad - 4(D_4 + D_6) - 3(D_7 + D_{15} + D_{19} + D_{25})];\end{aligned}$$

$$\begin{aligned}\Phi_6^8 &= O_{X_1 \dots X_5} D_6 = \frac{1}{20} [16D_6 + 2(D_{11} + D_{20} + D_{21} + D_{22} + D_{23} + D_{24}) + D_{10} + \\ &\quad + D_{14} + D_{18} + D_{26} - 4(D_4 + D_9 + D_{13} + D_{17} + D_{27}) - 3(D_7 + D_{15} + D_{19} + D_{25})];\end{aligned}$$

$$\begin{aligned}\Phi_7^8 &= O_{X_1 X_2 X_3} D_7 = \frac{\sqrt{2}}{6} [3D_7 + D_{21} + D_{22} + D_{27} - (D_{11} + D_{15} + D_{19} + \\ &\quad + D_{20} + D_{24} + D_{25})];\end{aligned}$$

$$\begin{aligned}\Phi_8^8 &= O_{X_1 \dots X_4} D_8 = \frac{\sqrt{10}}{60} [15D_8 + 2(D_{21} + D_{22} + D_{23}) + D_{13} + D_{14} + \\ &\quad + D_{15} + D_{17} + D_{18} + D_{19} + D_{25} + D_{26} + D_{27} - 5(D_{12} + D_{16} + \\ &\quad + D_{28}) - 3(D_7 + D_9 + D_{10}) - 2(D_{11} + D_{20} + D_{24})];\end{aligned}$$

$$\begin{aligned}\Phi_9^8 &= O_{X_1 \dots X_5} D_9 = \frac{\sqrt{15}}{60} [12D_9 + 2(D_{21} + D_{22} + D_{23}) + D_{14} + D_{15} + D_{18} + \\ &\quad + D_{19} + D_{25} + D_{26} - 4(D_{13} + D_{17} + D_{27}) - 3(D_7 + D_{10}) - 2(D_1 + D_{20} + D_{24})];\end{aligned}$$

$$\begin{aligned}\Phi_{10}^8 &= O_{X_1 \dots X_5} D_{10} = \frac{1}{12} [9D_{10} + 2(D_{21} + D_{22} + D_{23}) + D_{15} + D_{19} + \\ &\quad + D_{25} - 3(D_7 + D_{11} + D_{14} + D_{18} + D_{20} + D_{24} + D_{26})];\end{aligned}$$

$$\Phi_{11}^8 = O_{X_1 X_2 X_3} D_{11} = \frac{\sqrt{3}}{6} [2(D_{11} + D_{22}) - (D_{20} + D_{21} + D_{23} + D_{24})];$$

$$\begin{aligned}\Phi_{12}^8 &= O_{X_1 \dots X_4} D_{12} = \frac{\sqrt{5}}{30} [10D_{12} + 2D_{22} - 5(D_{16} + D_{28}) - (D_{21} + D_{23}) - \\ &\quad - 2(D_{11} + D_{13} + D_{14} + D_{15}) + D_{17} + D_{18} + D_{19} + D_{20} + D_{24} + D_{25} + D_{26} + D_{27}];\end{aligned}$$

$$\begin{aligned}\Phi_{13}^8 &= O_{X_1 \dots X_5} D_{13} = \frac{\sqrt{30}}{60} [8D_{13} + D_{18} + D_{19} + D_{20} + 2D_{22} + D_{24} + D_{25} + \\ &\quad + D_{26} - 4(D_{17} + D_{27}) - 2(D_{11} + D_{14} + D_{15}) - (D_{21} + D_{23})];\end{aligned}$$

$$\Phi_{14}^8 = O_{X_1 \dots X_5} D_{14} = \frac{\sqrt{2}}{12} [6D_{14} + D_{19} + D_{20} + 2D_{22} + D_{24} + D_{25} - 3(D_{18} + D_{26}) - 2(D_{11} + D_{15} - (D_{21} + D_{23}))];$$

$$\Phi_{15}^8 = O_{X_1 \dots X_5} D_{15} = \frac{1}{6} [4D_{15} + D_{20} + 2D_{22} + D_{24} - 2(D_{11} + D_{19} + D_{25}) - (D_{21} + D_{23})];$$

$$\Phi_{16}^8 = O_{X_1 \dots X_4} D_{16} = \frac{\sqrt{15}}{30} [5D_{16} + D_{23} + D_{24} + D_{25} + D_{26} + D_{27} - 5D_{28} - (D_{17} + D_{18} + D_{19} + D_{20} + D_{21})];$$

$$\Phi_{17}^8 = O_{X_1 \dots X_5} D_{17} = \frac{\sqrt{10}}{20} [4D_{17} + D_{23} + D_{24} + D_{25} + D_{26} - D_{27} - (D_{18} + D_{19} + D_{20} + D_{21})];$$

$$\Phi_{18}^8 = O_{X_1 \dots X_5} D_{18} = \frac{\sqrt{6}}{12} [3D_{17} + D_{23} + D_{24} + D_{25} - D_{26} - (D_{19} + D_{20} + D_{21})];$$

$$\Phi_{19}^8 = O_{X_1 \dots X_5} D_{19} = \frac{\sqrt{3}}{6} [2D_{19} + D_{23} + D_{24} - (D_{20} + D_{21} + D_{25})];$$

$$\Phi_{20}^8 = O_{X_1 \dots X_5} D_{20} = \frac{1}{2} [D_{20} + D_{23} - (D_{21} + D_{24})].$$

*The n-electron septets:*

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

$$n = 6$$

$$G = |\alpha\alpha\alpha\alpha\alpha\alpha|$$

$$n = 8$$

$$K_1 = |\alpha\alpha\alpha\alpha\alpha\alpha\beta|, \quad K_2 = |\alpha\alpha\alpha\alpha\alpha\beta\alpha|,$$

$$K_3 = |\alpha\alpha\alpha\alpha\beta\alpha\alpha|, \quad K_4 = |\alpha\alpha\alpha\beta\alpha\alpha\alpha|,$$

$$K_5 = |\alpha\alpha\beta\alpha\alpha\alpha\alpha|, \quad K_6 = |\alpha\alpha\beta\alpha\alpha\alpha\alpha|,$$

$$K_7 = |\alpha\beta\alpha\alpha\alpha\alpha\alpha|, \quad K_8 = |\beta\alpha\alpha\alpha\alpha\alpha\alpha|.$$

The relating eigenfunctions are as follows:

$$n = 6$$

$$\Psi_1^6 = G$$

$$n = 8$$

$$\Psi_1^8 = O_{X_1 X_2} K_1 = \frac{\sqrt{14}}{28} [7K_1 - (K_2 + K_3 + K_4 + K_5 + K_6 + K_7 + K_8)];$$

$$\Psi_2^8 = O_{X_1 X_2 X_3} K_2 = \frac{\sqrt{42}}{42} [6K_2 - (K_3 + K_4 + K_5 + K_6 + K_7 + K_8)];$$

$$\Psi_3^8 = O_{X_1 X_2 X_3} K_3 = \frac{\sqrt{30}}{30} [5K_3 - (K_4 + K_5 + K_6 + K_7 + K_8)];$$

$$\Psi_4^8 = O_{X_1 X_2 X_3} K_4 = \frac{\sqrt{5}}{10} [4K_4 - (K_5 + K_6 + K_7 + K_8)];$$

$$\Psi_5^8 = O_{X_1 X_2 X_3} K_5 = \frac{\sqrt{3}}{6} [3K_5 - (K_6 + K_7 + K_8)];$$

$$\Psi_6^8 = O_{X_1 X_2 X_3} K_6 = \frac{\sqrt{6}}{6} (K_7 + K_8);$$

$$\Psi_7^8 = O_{X_1 X_2 X_3} K_7 = \frac{\sqrt{2}}{2} (K_7 - K_8).$$

*The n-electron nonet:*

Let us denote the Slater determinant describing the state of  $n$ -electron system as follows:

$$n = 8$$

$$L = |\alpha\alpha\alpha\alpha\alpha\alpha\alpha\alpha|.$$

The relating eigenfunction is as follows:

$$\chi_1^8 = L.$$

## References

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 $n$ -ЭЛЕКТРОННЫЕ ( $n=4, 6, 8$ ) КВИНТЕТЫ, СЕПТЕТЫ И НОНЕТЫ  
КАК СОБСТВЕННЫЕ ФУНКЦИИ  $S^2$ *Ф. Беренц*

$n$ -электронные ( $n=4, 6, 8$ ) квинтеты, септеты и нонеты были созданы как собственные функции  $S^2$  методом спиновых операторов.