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***Annotatio et Erratum***

# A Physical Interpretation of the Cusp Conditions for Molecular Wave Functions

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W. A. BINGEL

Lehrstuhl für Theoretische Chemie der Universität Göttingen

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The third term in Eq. (21), page 60, should be

$$\left(-\tfrac{1}{4}\Delta_0 - \sum_\alpha \frac{2Z_\alpha}{r_{0\alpha}}\right) \qquad \text{instead of} \qquad \left(-\tfrac{1}{2}\Delta_0 - \sum_\alpha \frac{Z_\alpha}{r_{0\alpha}}\right). \tag{1}$$

The following remark may be added.

The expansion (22) can be simplified for 2-electron systems. If $S = 0$, the spatial wave function must be symmetric with respect to a permutation of electrons 1 and 2. This means, that the second term in (22) must vanish ($c \equiv 0$). If $S = 1$, the spatial wave function must be antisymmetric, with the result that the first term in (22) vanishes identically [$\Psi(\boldsymbol{r}_0, \boldsymbol{r}_0, \ldots) \equiv 0$].

PACK and BYERS-BROWN (Ref. [3] of my paper) state, that this *alternative* still obtains for $n$-electron systems with any $n > 2$. This statement needs some clarification. Only in the case of maximal spin $S = n/2$, where $\Psi$ must be antisymmetric in *all* electrons, we can still say that the first term in Eq. (22) must always vanish identically. For $S < n/2$, there are $f_S^n$ different spatial wave functions $\Psi_i$ for the same energy, which span their reducible representation $\mathfrak{D}_S^n$ of the permutation group. They can indeed be so chosen, that the matrix representation of the special permutation $P_{12}$ is diagonal and has diagonal elements equal to $+1$ or $-1$. For those $\Psi_i$ which belong to rows with $-1$ the first term and for those which belong to rows with $+1$ the second term in their expansion (22) must vanish. However, there is no longer any alternative, since both cases occur in the expression

$$\Phi_{S,M_S} = \sum_{i=1}^{f_S^n} \Psi_i \, \Theta_{S,M_S,i} \tag{2}$$

for the complete wave function of a single state including spin. Moreover, any other choice of the degenerate basis, while leaving (2) invariant, would lead to a situation, where the $\Psi_i$ are neither symmetric nor antisymmetric with respect to interchange of electrons 1 and 2.

Prof. Dr. W. A. BINGEL
Lehrstuhl für Theoretische Chemie
der Universität Göttingen
3400 Göttingen
Bürgerstr. 50a