We have, as a simple trial case, applied the expressions to the results of a small very limited C.I. wavefunction obtained, for another purpose, for the beryllium atom [6]. Three optimized excited orbitals $2p$, $3s$ and $3p$ are used and consequently only three double excitations Φ_{2s}^{2p}, Φ_{1s}^{3s} and Φ_{1s}^{3p} are considered. We have carried out the exact calculation with and without inclusion of quadruple excitations so as to compare the estimate given by the present method with the exact values. The results are given in the table which is self-explanatory.

The formulae given so far are all derived on the assumption that a given excited orbital is only used in association with a given ground state orbital. If this restriction is relaxed, it is not clear whether the second term in (10) would be small compared with unity. If it is assumed to be, the formulae become of rather greater complexity as can be seen in Eqs. (13) and (14).

$$\Psi^{(2)} = \sum_{p,q>p,r,s>r} (c_p^r c_q^s + c_p^s c_q^r)\, \Phi_{pq}^{rs} + \text{double excitations}\,. \tag{13}$$

$$E^{(4)} = \sum_{p,q\neq p,r,s\neq r} (c_p^{r2} c_q^s + c_p^r c_p^s c_q^r)\, K_{qs}\,. \tag{14}$$

The expression for $E^{(5)}$ is so awkward as not to be worth presenting.

Table. *Comparison of estimated and exact effects of quadruple excitations in beryllium*

	Exact	Using 1st order $c_p^{p'}$	Using exact $c_p^{p'}$
c_{1s2s}^{3s2p}	$-4.07 \cdot 10^{-3}$	$-4.64 \cdot 10^{-3}$	$-3.86 \cdot 10^{-3}$
c_{1s2s}^{3p2p}	$+4.83 \cdot 10^{-3}$	$+5.42 \cdot 10^{-3}$	$+4.52 \cdot 10^{-3}$
$E^{(4)}$ (a.u.)	—	$-6.43 \cdot 10^{-4}$	$-4.70 \cdot 10^{-4}$
$E^{(5)}$ (a.u.)	—	$+4.6 \cdot 10^{-6}$	$+3.0 \cdot 10^{-6}$
Total energy increment (a.u.)	$-5.00 \cdot 10^{-4}$	$-6.38 \cdot 10^{-4}$	$-4.67 \cdot 10^{-4}$

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Erratum

Homochiralität als Klassifizierungsprinzip von Molekülen spezieller Molekülklassen

ERNST RUCH

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Bei den Formeln auf S. 190 unten sind die Indizes 2 und 3 vertauscht. Die Formeln lauten richtig:

$$\lambda_1, \lambda_3 < \lambda_2, \lambda_4$$

$$\lambda_1 \to \lambda_1' = \lambda_3\,; \quad \lambda_3 \to \lambda_3' = \lambda_1\,; \quad \lambda_2 \to \lambda_2' = \lambda_4\,; \quad \lambda_4 \to \lambda_4' = \lambda_2\,.$$