COMPUTATION OF INTEGRALS OVER ls GAUSSIAN BASIS FUNCTIONS

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Computing the energy of a wave function constructed from a Gaussian basis involves the evaluation of many integrals of the form (Shavitt 1963).

$$F_m(z) = \int_0^1 u^{2m} e^{-zu^2} du. \tag{1}$$

If only (ls) $= \exp(-ar^2)$ Gaussian functions are used (Whitten 1963, Schwartz 1965), then only the $F_o(z)$ appear. Rapid computation of these basic integrals pays off in substantial savings on overall computing time. We report here a fast method for computing $F_o(z)$ using a standard, but often overlooked technique.

$F_o(z)$ has been computed by recurring downward with (Shavitt 1963)

$$F_m(z) = \frac{1}{(2m+1)} \left[2z\, F_{m+1}(z) + e^{-z}\right] \tag{2}$$

or using the series

$$F_o(z) = e^{-z} \sum_{i=0}^{\infty} \frac{(2z)^i}{(2i+1)!!}\,. \tag{3}$$

The transformation

$$F_o(z) = \tfrac{1}{2} (\pi/z)^{\frac{1}{2}} \operatorname{erf}(z^{\frac{1}{2}}) \tag{4}$$

is useful for checking computational accuracy since 15-place tables of the error function are available (Lowan 1954). Further, for $z > 17.1$, erf $(z^{\frac{1}{2}}) = 1$ to eight digits. We have therefore used

$$F_o(z) = 0.8862\ 2693\ z^{-\frac{1}{2}}\ ; \quad z > 17.1\,. \tag{5}$$

This takes only 1 millisecond per F_o on an IBM 7072 which was used for all computations in this note. In the range $0 < z < 17.1$, use of (2) requires about the same computing time as (3); but (3) gives somewhat better accuracy. For convergence to 8 figures, the series (3)—which must be summed starting with smallest terms for best accuracy—requires 12 terms and 9 milliseconds for $z = 1$, to 60 terms and 40 milliseconds for $z = 17$. This time can be cut by a factor of about 10 on the average by using (4) with a Hastings approximation for the error function (Hastings 1955).

$$\operatorname{erf}(X) = 1 - \Big[1 + 0.7052\ 3078 \cdot 10^{-1} X + 0.4228\ 2012 \cdot 10^{-1} X^2 + 0.9270\ 5272 \cdot 10^{-2} X^3 + 0.1520\ 1430 \cdot 10^{-3} X^4 + 0.2765\ 6720 \cdot 10^{-3} X^5 + 0.4306\ 3800 \cdot 10^{-4} X^6\Big]^{-16}. \tag{6}$$

This is not satisfactory below $z = 1$ since $\operatorname{erf}(z^{\frac{1}{2}})$ and $z^{\frac{1}{2}}$ both go to 0 as z goes to 0 while $F_o(z)$ goes to 1. The best arrangement seems to be to use the series (3) for $0 < z \leqslant 1$, (4) and (6) for $1 < z \leqslant 17.1$, and (5) for $z > 17.1$.

As an example of the overall time savings to be expected, an earlier SCF calculation of H^+_4 with ls Gaussian basis functions (Schwartz 1965) was rerun. This required 71,592 electron repulsion integrals. With F_o's by (3) and (5) the total computation took 31 minutes and gave $E = -1.7442693$ au. Using (6) instead for $1 < z \leqslant 17.1$ took 17 minutes and gave $E = -1.7442694$ au.

We are now developing Hastings approximations for the $F_m(z)$ directly.

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