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Response to the Comment: "On the computation of molecular auxiliary functions A_n and B_n"

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Abstract. The Comment 'on the computation of auxiliary functions $A_n(p)$ and $B_n(pt)$' (F E Harris, *Pramana – J. Phys.* **61**, C779 (2003)) is analysed in the arbitrary range of parameters n, p and pt. It is shown that our downward recursion approach for $B_n(pt)$ in the range $(n/pt) > 1$ is more efficient than the well-known upward recursion method, and the upward recursion procedure for $A_n(p)$ does not have merit for smaller non-zero values of p $(p < 0.01)$.

Keywords. Molecular auxiliary functions; multicenter intergrals.

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1. Introduction

Evaluation of the auxiliary functions $A_n(p)$ and $B_n(pt)$ is one of the most important problems in electronic structure studies of molecules [1]. Numerical analysis of accuracy for the arbitrary range of parameters n, p and pt in these problems are naturally followed with interest [2]. In the Comment, Harris [3], claims that the upward recurrence for $A_n(p)$ is numerically stable for all positive values of p, and the downward recurrence method for $B_n(pt)$ introduced in our paper [4] is less effective than a straightforward procedure which has been known for many years; there is, however, a range of smaller pt for which the downward approach is competitive. In this reply, we present computer results that show that the upward recursion procedure is not numerically stable for the calculation of $A_n(p)$ and $B_n(pt)$ in the range $p < 0.01$ and $(n/pt) > 1$, respectively.

2. Accuracy of the computer results

The auxiliary functions $A_n(p)$ and $B_n(pt)$ satisfy the following recursive relations [5,6]:

Upward recurrences for $A_n(p)$

$$A_n(p) = (nA_{n-1}(p) + \mathrm{e}^{-p})/p, \tag{1}$$

$$C_n(p) = nC_{n-1}(p) + p^n. \tag{2}$$

Upward recurrences for $B_n(pt)$

$$B_n(pt) = \frac{1}{pt}(nB_{n-1}(pt) + (-1)^n e^{pt} - e^{-pt}). \tag{3}$$

Downward recurrences for $A_n(p)$

$$A_n(p) = \frac{1}{n+1}(pA_{n+1}(p) - e^{-p}), \tag{4}$$

$$C_n(p) = \frac{1}{n+1}(C_{n+1}(p) - p^{n+1}). \tag{5}$$

Downward recurrences for $B_n(pt)$

$$B_n(pt) = \frac{1}{n+1}(ptB_{n+1}(pt) + (-1)^n e^{pt} + e^{-pt}), \tag{6}$$

where [6]

$$A_n(p) = \frac{e^{-p}}{p^{n+1}} C_n(p). \tag{7}$$

Table 1. Numbers of correct decimal figures for $A_n(p)$ obtained from upward recurrences.

	$p = 0.01$		$p = 0.005$		$p = 30$		$p = 50$	
n	Eq. (1)	Eqs (2), (7)	Eq. (1)	Eqs (2), (7)	Eq. (1)	Eqs (2), (7)	Eq. (1)	Eqs (2), (7)
25	∞	∞	∞	∞	∞	∞	∞	∞
30	∞	∞	∞	∞	∞	∞	∞	43
35	∞	∞	∞	∞	∞	32	∞	∞
40	∞	∞	∞	∞	∞	31	∞	∞
50	∞	∞	∞	∞	∞	∞	∞	∞

Table 2. Numbers of correct decimal figures for $B_n(pt)$ obtained from upward and downward recurrences.

	$pt = 30$		$pt = 40$		$pt = 50$	
n	Eq. (3)	Eq. (6)	Eq. (3)	Eq. (6)	Eq. (3)	Eq. (6)
25	8	∞	3	∞	∞	∞
30	∞	∞	3	∞	∞	∞
35	∞	∞	3	∞	∞	∞
40	8	∞	3	∞	∞	∞
45	∞	∞	4	∞	-1	∞
50	9	∞	4	∞	-1	∞
55	∞	∞	4	∞	-1	∞
60	9	∞	5	∞	-1	∞

In eq. (6), we should start the downward recursion with an even value of n_{top} satisfying

$$n_{\text{top}} \geq \begin{cases} \dfrac{d}{|\log(n_{\max}/pt)|} + n_{\max} & \text{for } n_{\max} \neq pt, \quad (8a) \\ n_{\max}^2 & \text{for } n_{\max} = pt. \quad (8b) \end{cases}$$

One can determine the accuracy of the computer results obtained from the upward recurrences (downward recurrences) by the use of the downward recurrences (upward recurrences). The numbers of correct decimal figures m_u and m_d determined from $\Delta f_u = 10^{-m_u}$ and $\Delta f_d = 10^{-m_d}$ are given in tables 1 and 2, where $\Delta f = f^{\mathrm{L}} - f^{\mathrm{R}}$. Here, the values f^{L} and f^{R} are obtained from the left-hand side (LHS) and the right-hand side (RHS) respectivley of the above-mentioned equations.

As can be seen from the tables that eqs (1) and (3) for the upward recurrences are not numerically stable for $A_n(p)$ and $B_n(pt)$ in the range $p < 0.01$ and $(n/pt) > 1$, respectively. With the calculation of $A_n(p)$ for $p < 0.01$ we should use eqs (2) and (7) taken from [6].

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