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LETTER TO THE EDITOR

Letter to the Editor

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In this letter, I would like to comment on the main calculations presented in Sect. 3 of [1]. These calculations involved the following integral:

$$S = \exp(-\alpha) \int_{1}^{\infty} \left[\frac{\cos \mathrm{h}(\rho + \alpha\mu)}{\rho + \alpha\mu} - \frac{\sin \mathrm{h}(\rho + \alpha\mu)}{(\rho + \alpha\mu)^2} \right] \exp(-\rho\mu) d\mu. \tag{1}$$

Szalay and Surjan [1] stated that "the primitive function of this integrand cannot be found" and computed S by expanding the hyperbolic functions into Taylor series. Here, I would like to show that (1) can be reduced to an expression involving well known special functions. First, using the facts $\cos \mathrm{h}(x) = \{\exp(x) + \exp(-x)\}/2$ and $\sin \mathrm{h}(x) = \{\exp(x) - \exp(-x)\}/2$, rewrite (1) as

$$\begin{aligned} S = \exp(-\alpha) \Bigg[& \int_{1}^{\infty} \frac{\exp\{\rho - (\rho - \alpha)\mu\} + \exp\{-\rho - (\rho + \alpha)\mu\}}{2(\rho + \alpha\mu)} d\mu \\ & - \int_{1}^{\infty} \frac{\exp\{\rho - (\rho - \alpha)\mu\} - \exp\{-\rho - (\rho + \alpha)\mu\}}{2(\rho + \alpha\mu)^2} d\mu \Bigg]. \end{aligned}$$

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$$= \frac{\exp\left\{\rho^2/\alpha - \alpha\right\}}{2\alpha}\left[\int_{\rho+\alpha}^{\infty} \frac{\exp\{-(\rho-\alpha)x/\alpha\} + \exp\{-(\rho+\alpha)x/\alpha\}}{x}dx - \int_{\rho+\alpha}^{\infty} \frac{\exp\{-(\rho-\alpha)x/\alpha\} - \exp\{-(\rho+\alpha)x/\alpha\}}{x^2}dx\right]$$

$$= \frac{\exp\left\{\rho^2/\alpha - \alpha\right\}}{2\alpha}\left[\int_{(\rho^2-\alpha^2)/\alpha}^{\infty} \frac{\exp(-y)}{y}dy + \int_{(\rho+\alpha)^2/\alpha}^{\infty} \frac{\exp(-y)}{y}dy - \frac{\rho-\alpha}{\alpha}\int_{(\rho^2-\alpha^2)/\alpha}^{\infty} \frac{\exp(-y)}{y^2}dy + \frac{\rho+\alpha}{\alpha}\int_{(\rho+\alpha)^2/\alpha}^{\infty} \frac{\exp(-y)}{y^2}dy\right]. \quad (2)$$

The integrals in (2) can be expressed in terms of the well known exponential integral function $\mathrm{Ei}_\nu(z) = z^{\nu-1}\int_z^\infty t^{-\nu}\exp(-t)dt$ (see Sect. 8.21 of [2] for detailed properties), yielding the simple form

$$S = \frac{\exp\left\{\rho^2/\alpha - \alpha\right\}}{2\alpha}\left[\mathrm{Ei}_1\left(\frac{\rho^2-\alpha^2}{\alpha}\right) + \mathrm{Ei}_1\left(\frac{(\rho+\alpha)^2}{\alpha}\right) - \frac{1}{\rho+\alpha}\,\mathrm{Ei}_2\left(\frac{\rho^2-\alpha^2}{\alpha}\right) + \frac{1}{\rho+\alpha}\,\mathrm{Ei}_2\left(\frac{(\rho+\alpha)^2}{\alpha}\right)\right]. \quad (3)$$

In-built routines for the computation of the exponential integral function are available in every major computer package, including Maple and Mathematica (these in-built routines may be based on some well established series expansions or equivalent procedures). Hence, (3) provides a simple way to compute the integral in (1).

References

1. Z. Szalay, P.R. Surjan, Distorted s-type orbitals: the H_2^+ problem revisited. J. Math. Chem. **43**, 227–236 (2007)
2. I.S. Gradshteyn, I.M. Ryzhik, *Table of Integrals, Series, and Products*, 6th edn. (Academic Press, San Diego, 2000)