A generalized Jaeger $\mathscr{I}(0 \quad 1; \quad)$ integral, resulting from mathematical modelling in electroanalytical chemistry

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Abstract: Eighty years ago J. C. Jaeger et al. introduced a class of improper integrals, currently called "Jaeger integrals" that occur in theoretical models of diverse physical phenomena characterized by cylindrical geometry. One application area is electroanalytical chemistry, where, in particular, the limiting Faradaic current in a potential step chronoamperometric experiment at a cylindrical electrode is described by the Jaeger $\mathscr{I}(0,1;t)$ integral. In a recently published paper the first author determined the Laplace transform of the nonlimiting Faradaic current for a reversible charge transfer between members of a redox couple characterized by different diffusion coefficients. In this study we invert the novel Laplace transform and observe that, while it cannot be expressed by any of the Jaeger integrals, it can be perceived as a generalization of the $\mathscr{I}(0,1;t)$ integral. We also describe how to compute this integral with the modulus of the relative error close to 10^{-16} or smaller, using a C++ code employing exclusively standard floating point variables, without resorting to quad precision or other external high precision libraries.
keywords: Jaeger integrals; Bessel functions; contour integration; Laplace transform; potential step chronoamperometry; cylindrical microelectrodes; computational electrochemistry
MSC 2020: 33C10, 33E20, 35C15, 35Q99, 44A10, 65D30, 92E99

$$\mathscr{I} \qquad \int \qquad \frac{\qquad}{\qquad} \; \frac{u^2 t}{\qquad}$$

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$$-\mathscr{I} \qquad \mathscr{L} \quad \left\{ \frac{\quad -}{\; - \qquad - \;} \right\}$$

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$\mathscr{I}$

$-\mathscr{I}$

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$$\mathscr{L} \quad \left\{ \quad \right\}$$

$$\mathscr{L} \quad \left\{ \frac{\quad -}{\; - \qquad - \;} \left[\quad - \quad \frac{\quad - \qquad -}{= \qquad =} \right] \right\}$$

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$\mathscr{I}$

$u^2 t$

$\mathscr{I}$ $\mathscr{I}$

$$\mathscr{I}(0\ \ 1;\ \ )$$

$$- \qquad -$$

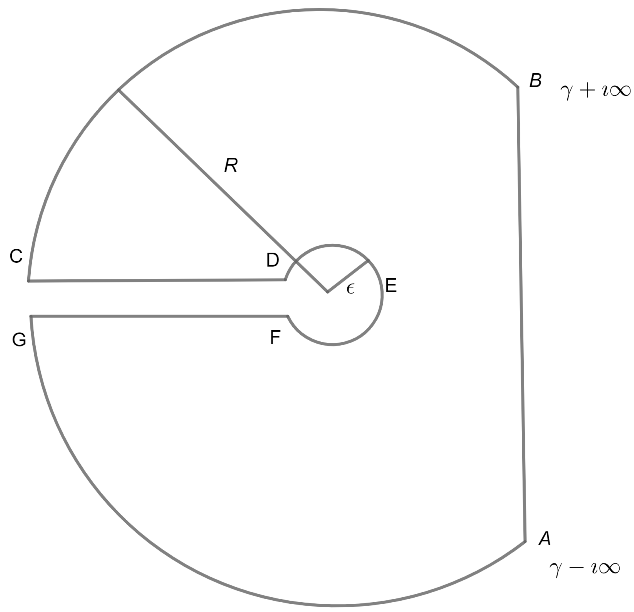
$$- \qquad -$$

$$- \qquad \frac{}{=}$$

$$\nu \quad - \quad \sqrt{\frac{}{=}} \quad - \left[\quad \frac{}{-} \quad \right]$$

$$-$$

$$-$$



Bromwich contour

$$\mathscr{L} \quad \Big\{ \qquad \Big\}$$

$$\overset{\epsilon}{R} \qquad \overline{} \int_{AB} \quad st$$

$$\overset{\epsilon}{R} \qquad \overline{} \left\{ \int_{BC} \quad \int_{CD} \quad \int_{DEF} \quad \int_{FG} \quad \int_{GA} \right\} \quad st$$

$\imath\theta$ $\qquad \overline{R^{1/2}}$

k

$\imath\theta$

$$\left| \int_{DEF} \quad st \quad \right| \quad \left|_{\epsilon} \int_{\pi \quad \epsilon}^{\pi \quad \epsilon} \quad \imath\theta \quad \imath\theta \quad \epsilon e^{\imath\theta} t \right|$$

$$\left|_{\epsilon} \int_{\pi \quad \epsilon}^{\pi \quad \epsilon} \frac{/ \quad \imath\theta/ \quad \imath\theta \quad \epsilon e^{\imath\theta} t}{/ \quad \imath\theta/ \quad / \quad \imath\theta/} \right|$$

$$\epsilon \int_{\pi \quad \epsilon}^{\pi \quad \epsilon} \left| \frac{}{/ \quad \imath\theta/} \right|$$

$$\imath\pi \qquad - \quad - \quad \imath\pi/ \qquad -$$

$$\frac{}{} \int_{CD} st \qquad \overset{\epsilon}{R} \quad \frac{}{} \int_{R}^{\epsilon} \frac{/ \quad st}{/ \quad /}$$

$$\overset{\epsilon}{R} \quad \frac{}{} \int_{R}^{\epsilon} \frac{- \quad xt}{- \quad -}$$

$$\frac{}{} \int \frac{- \quad xt}{- \quad -}$$

$$\imath\pi \qquad - \quad - \quad \imath\pi/ \qquad -$$

$$\frac{}{} \int_{FG} st \qquad \frac{}{} \int \frac{-}{-} \frac{xt}{-}$$

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$$\nu \qquad - \quad \tfrac{1}{2}\nu\pi\imath \quad \nu \quad \nu$$

$$\frac{\pi^2}{\ }\qquad\frac{\ }{\pi^2}$$

$$\nu \qquad \nu$$

$$\mathscr{L}\left\{\ \right\} \quad \int \quad xt$$

$$\int \quad u^2 t$$

$$\mathscr{L}$$

$$\mathscr{L}\left\{\ \right\} \quad \int \quad \pi \quad u^2 t$$

$$-\int \quad u^2 t \quad \frac{}{}$$

$$\frac{}{} \quad \mathscr{L}\left\{ -\int \frac{\pi}{} \frac{u^2 t}{} \right\}$$

$$\mathscr{L} \quad -\int \frac{\pi}{} \frac{u^2 t}{}$$

$$\frac{}{}$$

$$\left(\frac{}{\bar{\delta} \quad \bar{s}} \right)$$

$\mathbb{C}$

$\imath\theta$

$$\left| \quad \right| \quad k$$

$\imath\theta$

$$\mathscr{L}\left\{ \quad \right\} -\int \left[\quad \right] \frac{xt}{}$$

$$\frac{}{}$$

$$\mathscr{L}\{\quad\} \int \quad ^{xt}$$

$$\mathscr{L}\left\{\quad\right\} \; -\int \frac{\quad}{\quad} \; \frac{xt}{\quad}$$

$$\mathscr{L}\left\{\quad\right\} \; -\int \frac{\quad}{\quad} \; \frac{u^2t}{\quad}$$

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$$\mathscr{L}\left\{\quad\right\} \; -\int \frac{\quad}{\quad} \; \frac{u^2t}{\quad}$$

$$-\int \frac{\quad}{\quad} \; \frac{u^2t}{\quad}$$

$\mathscr{I}$

$$\Big[\quad\Big]\Big[\quad\Big]$$

$$\mathscr{L}\left\{\quad\right\}\ \frac{\quad}{\quad}\int_{\mathscr{I}}\frac{\quad}{\quad}\frac{u^2t}{\quad}$$

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$$\mathscr{L}$$

$$\mathscr{L}\ \frac{\quad}{\quad}\left[\Big(\quad\Big)\mathscr{L}\left\{\quad\right\}\ \frac{\quad}{\quad}\right]$$

$$\mathscr{L}\left\{\quad\right\}$$

$$\mathscr{L}\left\{\quad\right\}$$

$$\mathscr{L}\ \frac{\quad}{\quad}$$

$$\left\{\ \frac{\quad}{\quad}\int\frac{\quad}{\quad}\frac{u^2t}{\quad}\ \frac{\quad}{\quad}\right\}$$

$$\frac{\quad}{\quad}$$

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$$\left.\frac{\quad}{\quad}\int\ u^2t\ \right\}$$

$$\frac{\quad}{\quad}\frac{\quad}{\quad}$$

$$\left\{\int\frac{\quad\pi\quad}{\quad}\frac{u^2t}{\quad}\right\}$$

$$\mathscr{L} \qquad - \left(\frac{-}{} \right)$$

$$\int \frac{-}{} \, \frac{u^2 t}{}$$

$$\left[\quad - \quad - \quad \right] - \left[\quad - \quad - \quad \right] [\quad]$$

$$\left[\quad - \quad - \quad \right] \frac{}{=} [\quad]$$

$$- \left\{ \frac{}{-} \right.$$

$$\left. \left[\quad - \quad - \quad - \quad - \quad \right] \right\}$$

$$\frac{}{=} [\quad] - \left[\quad - \quad - \quad \right] [\quad]$$

$$\mathscr{L} \qquad \frac{-}{}$$

$$- \int \frac{-}{} \, \frac{u^2 t}{}$$

Mathematica

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$$-\int \frac{\left(\sqrt{\frac{w}{t}}\right) \quad \left(\sqrt{\frac{w}{t}}\right) \quad \left[\ \left(\sqrt{\frac{w}{t}}\right) \quad \left(\sqrt{\frac{w}{t}}\right)\ \right]}{\left(\sqrt{\frac{w}{t}}\right)} \frac{w}{}$$

$$\frac{\left(\sqrt{\quad \frac{w}{t}}\right) \qquad \left(\sqrt{\quad \frac{w}{t}}\right) \qquad \left[\quad \left(\sqrt{\frac{w}{t}}\right) \qquad \left(\sqrt{\frac{w}{t}}\right)\right]}{\left(\sqrt{\frac{w}{t}}\right)} \quad \frac{w}{\quad}$$

$$\frac{\quad}{\left\{ \qquad \left(\frac{w}{t}\right) \qquad \left[\quad \left(\frac{w}{t}\right)\right] \right\}}$$

$$\left[\qquad \right] \qquad {}^{-}\left[\qquad {}^{-}\right]$$

$$\left[\qquad {}^{-}\right]$$

$$\int^{w_\mathrm{b}} \frac{\quad}{\left\{ \qquad \left(\frac{w}{t}\right) \qquad \left[\quad \left(\frac{w}{t}\right)\right] \right\}}$$

$$\frac{\quad}{\quad} \qquad \left\{ \frac{\left(\frac{w_\mathrm{b}}{t}\right) \qquad \left[\qquad \frac{\delta}{\delta} \qquad {}^{-}\right]}{\quad} \right\}$$

$^{-}$ $\mathscr{L}$

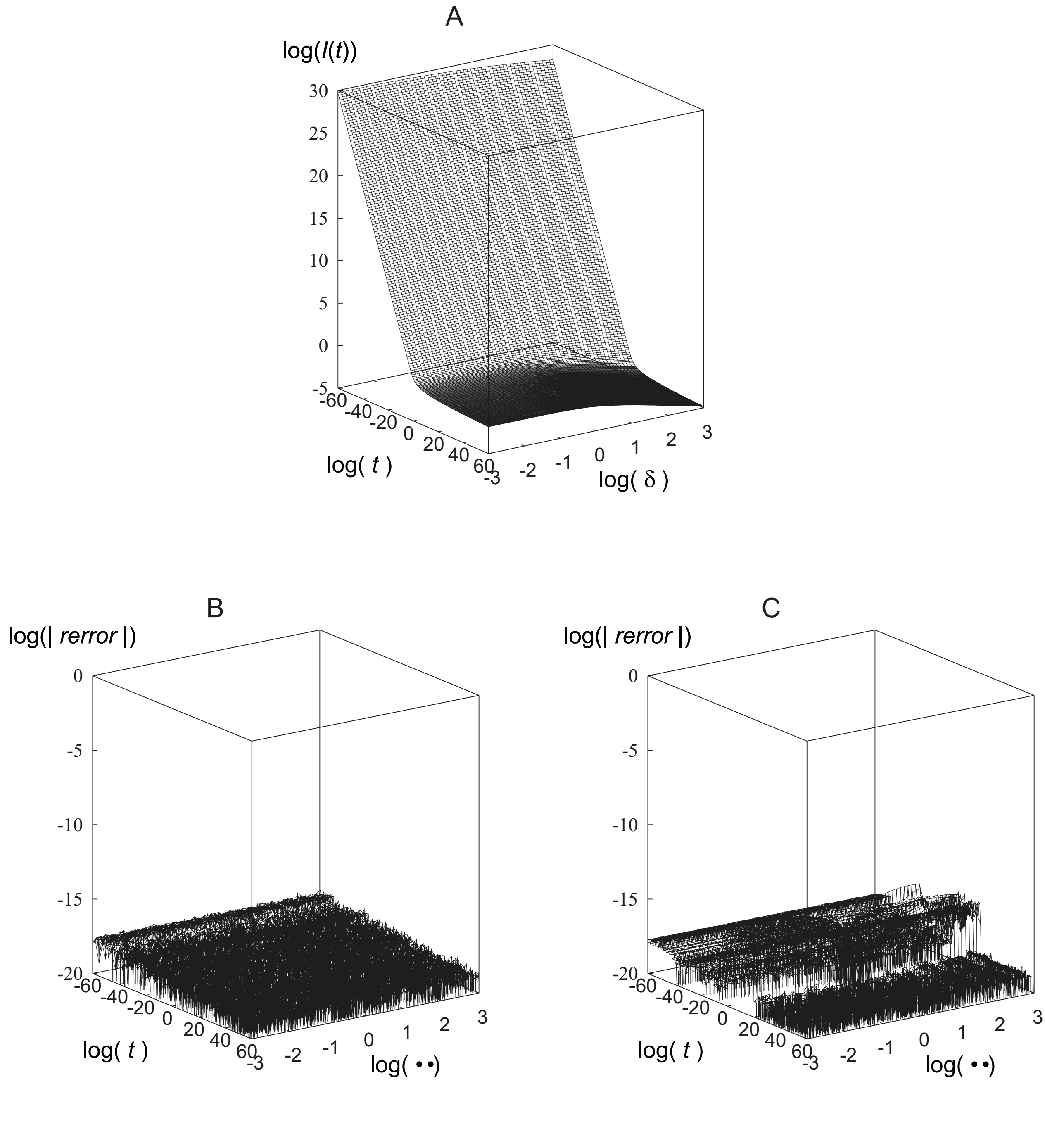

Figure 2: Current $I(t)$ for $\Theta = 1$ ($U = 0$), evaluated numerically by the double exponential quadrature (A); and corresponding moduli of the relative errors (B). Errors obtainable by using the hybrid algorithm from Ref. [18] are shown in subfigure C, for comparison.

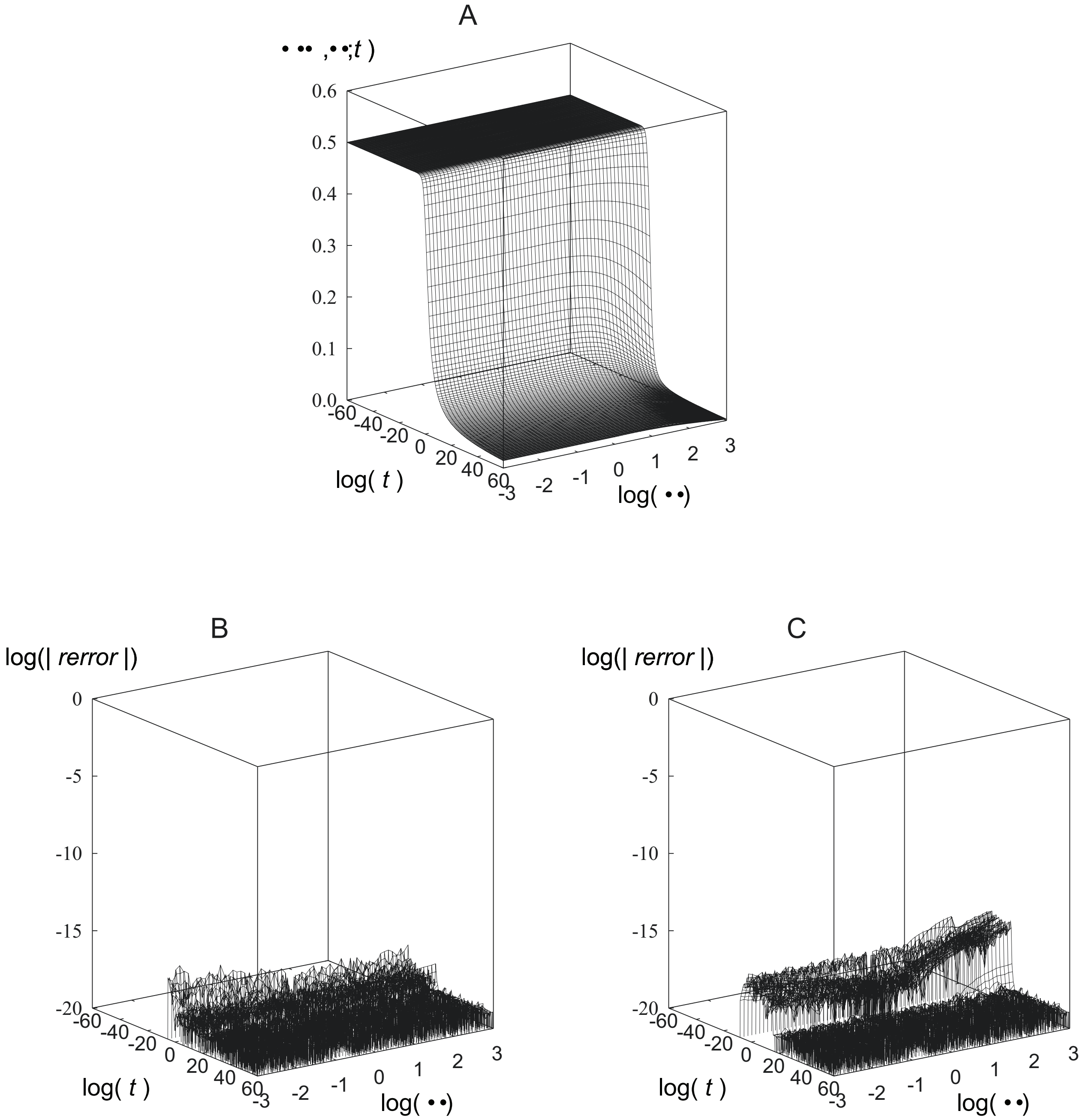

Figure 3: Function $\Xi(\Theta, \delta; t)$ for $\Theta \approx 0.00674$ ($U = -5$), evaluated numerically by the hybrid procedure from Ref. [18], with the Stehfest method replaced by the double exponential quadrature for integral (40) (A); and corresponding moduli of the relative errors (B). Errors obtainable by using the unmodified hybrid algorithm from Ref. [18] are shown in subfigure C, for comparison.

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