Logarithmic Integrals of Airy Functions

Bernard J. Laurenzi
Department of Chemistry
UAlbany, The State University of New York
1400 Washington Ave., Albany N.Y. 12222

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Abstract

Integrals arising in the Thomas-Fermi (TF) theory of atomic structure and which contain logarithms of the Airy functions have been expressed in terms of the incomplete Bell polynomials. In keeping with the spirit of TF theory closed forms for these integrals are sought.

1 Introduction

In the theory of atomic structure due to Thomas and Fermi [1] integrals arise [2] which contain the Airy function $Ai(x)$ and its derivative $Ai'(x)$ [3]. A typical example of these integrals being

$$I = \int_0^\infty A^2(x) \ln[A(x)] \, dx,$$

where $A(x)$ is given by

$$A(x) = \frac{Ai'(x)}{Ai'(0)}.$$

The value of the integral (to 8 figures) obtained by numerical methods is -0.26363171. However, it would be useful and within the spirit of Thomas Fermi (TF) theory if an exact or at least an analytic expression for this integral and others like it could be obtained. With this in mind, this paper presents methods which attempt to move towards that goal. In anticipation of the work which follows we set

$$z = 1 - A(x)$$

and rewrite the integral above as

$$I = \int_0^1 (1 - z)^2 \ln(1 - z) \frac{dz}{dz} \, dz.$$
Integration by parts gives

\[ I = \int_0^1 (1 - z)[1 + 2(1 - z) \ln(1 - z)] x(z) \, dz. \]  \hspace{1cm} (1)

Where we see that \( x(z) \) is the inverse function for \( A \) with argument \( 1 - z \). The latter function can be obtained using the Lagrange expansion formula \[4\] i.e.

\[ x(z) = \sum_{k=1}^{\infty} \frac{a_k}{k!} (\sqrt{z})^k, \]  \hspace{1cm} (2)

with the coefficients \( a_k \) given by

\[ a_k = \left. \frac{d^{k-1}}{dx^{k-1}} \left( \frac{1}{\sqrt{u(x)}} \right)^k \right|_{x=0}, \]

where \( u(x) = \frac{[1 - A(x)]}{x^2} \).

Using (2), the integrals on the right hand side of (1) are elementary and the integral \( I \) can be written as

\[ I = 8 \sum_{k=1}^{\infty} \frac{a_k}{k!} \left[ \psi(3) - \psi(k/2 + 3) \right] \frac{1}{(k+2)(k+4)}, \]

where \( \psi(k) \) is the Psi (digamma) function \[5\].

### 1.1 Evaluation of the \( a_k \)

The derivatives within \( a_k \) can in turn be given by the Faà di Bruno formula for the \((k-1)^{st}\) derivative of a composite function \[6\] as expressed in terms of the incomplete Bell polynomials \( B_{k,n}(x_1, x_2, \ldots, x_{k-n+1}) \) \[7\] i.e.

\[ a_k = \sum_{p=1}^{k-1} \left[ \frac{d^{p} u^{-k/2}}{d u^p} \right]_{x=0} B_{k-1,p}(u^{(1)}(0), u^{(2)}(0), \ldots, u^{(k-p)}(0)), \]

where

\[ u^{(i)}(0) = \left. \frac{d^i u(x)}{dx^i} \right|_{x=0}. \]

The expression for \( a_k \) can be quickly reduced to terms involving the Gamma function \( \Gamma(k) \) \[8\] to get

\[ a_k = \frac{1}{u(0)^{k/2}} \sum_{p=1}^{k-1} \left( -\frac{1}{u(0)} \right)^p \frac{\Gamma(k/2+p)}{\Gamma(k/2)} B_{k-1,p}(u^{(1)}(0), u^{(2)}(0), \ldots, u^{(k-p)}(0)). \]
The derivatives of the function $u(x)$ can easily be obtained since the power series for $Ai'(x)$ is well known i.e.

\[
Ai'(x)/Ai'(0) = 1 - \frac{2^{2/3} \Gamma(1/3)}{\pi} \sum_{n=0}^{\infty} \frac{\Gamma(n+4)}{(n+2)!} \sin\left(\frac{2}{3}(n+4)\pi\right) (3^{1/3}x)^n.
\]

Using the latter expression we get

\[
u(0) = \frac{\pi}{3^{5/6} \Gamma(2/3)},
\]
\[
u^{(i)}(0) = \left[\frac{2}{3^{5/6} \Gamma(2/3)}\right]^{i/3} \frac{\Gamma(i+1) \sin\left(\frac{2}{3}(i+1)\pi\right)}{\Gamma(i/2+1)}.
\]

Finally the integral is given by

\[
I = \frac{8}{3^{1/3}} \sum_{k=1}^{\infty} \frac{[\psi(3) - \psi(k/2+3)]}{(k+2)(k+4)} S_k,
\]

where $S_k$ is defined as

\[
S_k = \left(\frac{3^{3/4} \Gamma(2/3)}{\sqrt{\pi}}\right)^k \sum_{p=0}^{k-1} \left(\frac{-2 \Gamma(2/3)}{\pi}\right)^p \frac{\Gamma(k+2+p)}{\Gamma(k/2)} B_{k-1,p} \left(\tilde{u}^{(1)}(0), \tilde{u}^{(2)}(0), \ldots, \tilde{u}^{(k-p)}(0)\right),
\]

and the reduced quantities $\tilde{u}^{(i)}(0)$ are given by

\[
\tilde{u}^{(i)}(0) = \frac{\Gamma\left(\frac{i+1}{3}\right) \sin\left(\frac{2}{3}(i+1)\pi\right)}{\Gamma(i/2+1)}.
\]

In obtaining the expression in (3,4) we have used the homogeneous scaling properties of the incomplete Bell polynomials i.e.

\[
\alpha^n B_{k,n}(x_1, x_2, \ldots) = B_{k,n}(\alpha x_1, \alpha x_2, \ldots),
\]
\[
\alpha^k B_{k,n}(x_1, x_2, \ldots) = B_{k,n}(\alpha x_1, \alpha^2 x_2, \ldots),
\]

to rewrite the Bell polynomials in terms of the reduced quantities $\tilde{u}^{(i)}(0)$.

### 1.2 The Rate of Convergence of the $I$ Integral

The infinite sum representation for the integral $I$ in (3) is a slowly varying function of $k$. For example, the value of $I$ given by a partial sum containing the first ten terms is only 91% of the value obtained by numerical evaluation of the integral. Although a complete analysis (or estimate) of the convergence behavior of this sum does not appear to be possible, it is likely that (3) is an asymptotic series representation of the integral $I$. Nevertheless, in an attempt to increase the rate of convergence i.e. accelerate the assumed convergence of the sum, we note that the magnitudes (Figure 1) of the summands $I_k$

\[
I_k = \frac{8}{3^{1/3}} \frac{[\psi(3) - \psi(k/2+3)]}{(k+2)(k+4)} S_k,
\]
in (3) are small for values of $k$ greater than 10.

Furthermore, when $S_k$ is plotted (Figure 2) versus $k$ for values of $k \geq 10$, it can be seen to vary like powers of $1/k$ i.e.

$$S_k = a/k + b/k^2 + c/k^3,$$

where regression analysis yields $a = 0.751653834$, $b = 2.25325549$, $c = -6.815672901$.

Using the curve fitted expression for $S_k$ the expression for $I$ becomes

$$I = \frac{8}{3\sqrt{\pi}} \sum_{k=1}^{10} \frac{[\psi(3) - \psi(k/2+3)]}{(k+2)(k+4)} S_k + I_{\text{remainder}},$$
where

\[ I_{\text{remainder}} = \frac{8}{3\pi^2} \left\{ a \left( \sigma_1 - \sum_{k=1}^{10} \frac{\psi(3) - \psi(k/2+3)}{k^2 (k+2) (k+4)} \right) + b \left( \sigma_2 - \sum_{k=1}^{10} \frac{\psi(3) - \psi(k/2+3)}{k^3 (k+2) (k+4)} \right) \right\} + c \left\{ \sigma_3 - \sum_{k=1}^{10} \frac{\psi(3) - \psi(k/2+3)}{k^4 (k+2) (k+4)} \right\}. \]

The sums \( \sigma_i \) appearing in (5) can be calculated in terms of known \([12]\), closed forms i.e.

\[ \sigma_1 = \sum_{k=1}^{\infty} \frac{\psi(3) - \psi(k/2+3)}{k^2 (k+2)(k+4)} = -\frac{89}{576} + \frac{1}{6} \ln(2), \]

\[ \sigma_2 = \sum_{k=1}^{\infty} \frac{\psi(3) - \psi(k/2+3)}{k^3 (k+2)(k+4)} = \frac{349}{1152} - \frac{11}{16} \zeta(3) - \frac{1}{6} \ln(2), \]

\[ \sigma_3 = \sum_{k=1}^{\infty} \frac{\psi(3) - \psi(k/2+3)}{k^4 (k+2)(k+4)} = -\frac{2423}{9216} + \frac{5}{384} \pi^2 - \frac{11}{2880} \pi^2 \ln^2(2) + \frac{5 \ln(2)}{48} + \ln^3(2) + \left( \frac{7 \ln(2)}{32} + \frac{31}{256} \right) \zeta(3) + \frac{1}{4} Li_4(1/2), \]

where \( Li_4 \) is the 4th order polylogarithm function \([11]\) and \( \zeta(z) \) is the Riemann zeta function. The value of the sums given above are small with magnitudes \(-0.0389893588 \), \(-0.0191766714 \), \(-0.0146522682 \) respectively. Using these values \( I_{\text{remainder}} = -0.004280449344 \) yielding a value of \(-0.2637166702 \) for \( I \). The latter value of \( I \) having an error of 0.03 \%, this procedure is seen to produce the best estimate for an “analytic” representation the integral thus far.

In order to make further progress in obtaining a closed form expression for integrals of the kind sought here, closed form sums of the type

\[ \left( \frac{1}{2} \right)^{k-1} \sum_{p=0}^{k} (k/2)_p B_{k-1-p}(\hat{u}^{(1)}(0), \hat{u}^{(2)}(0), \ldots, \hat{u}^{(k-p)}(0)), \]

where \((a)_n\) is the Pochhammer polynomial symbol and the \( \hat{u}^{(i)}(0) \) terms have been given above, must be found. Expressions for closed form sums similar (6) have been given by Mihoubi \([13]\) and Brauchart \([10]\) albeit with simpler arguments of the Bell polynomials.

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