

Field to thermo-field to thermionic electron emission: A practical guide to evaluation of the Murphy-Good formalism

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Abstract

These are technical notes written during implementation of the method described in [1]. The notes have been written for internal use and not were not intended to be read by other people, however some colleagues who have read them found them useful.

1 The Richardson-Schottky formula

$$j(T, F, \phi) = A_{em} T^2 \exp\left(-\frac{\phi - \Delta A}{kT}\right) \quad (1)$$

where T is the surface temperature, F is the electric field at the surface of the emitter, ϕ is the work function, Schottky correction to the work function is

$$\Delta A = \sqrt{\frac{e^3 F}{4\pi\epsilon_0}} = \sqrt{\frac{(1.60217733 \times 10^{-19} \text{ C})^3}{4\pi 8.854187817 \times 10^{-12} \text{ F m}^{-1}}} \text{ V m}^{-1} \frac{1}{\text{eV}} \sqrt{\frac{F}{\text{V m}^{-1}}} \text{ eV} \quad (2)$$

$$= 3.794\,687\,303 \times 10^{-5} \sqrt{\frac{F}{\text{V m}^{-1}}} \text{ eV}, \quad (3)$$

and

$$A_{em} = \frac{4\pi m_e k^2 e}{h^3} = \frac{4\pi 9.1093897 \times 10^{-31} \text{ kg} (1.3806568 \times 10^{-23} \text{ J K}^{-1})^2 1.60217733 \times 10^{-19} \text{ C}}{(6.6260755 \times 10^{-34} \text{ J s})^3} \quad (4)$$

$$= 1.201\,744\,270 \times 10^6 \text{ A m}^{-2} \text{ K}^{-2} \quad (5)$$

2 Field emission

Tunnelling from a cold metal is described by the Fowler-Nordheim formula. The latter may be viewed as a limiting case of the Murphy-Good formalism; see equation (56) and

subsequent material in Sec. IV of [2]. Transforming the latter equation from Hartree units to dimensional ones and then replacing e , F , and j by, respectively, $e(4\pi\epsilon_0)^{-1/2}$, $F(4\pi\epsilon_0)^{1/2}$, and $j(4\pi\epsilon_0)^{-1/2}$ in order to obtain SI units, one finds

$$j = \frac{aF^2}{\phi t^2} \exp\left(-bv\frac{\phi^{3/2}}{F}\right), \quad (6)$$

where

$$a = \frac{e^3}{8\pi h} = \frac{(1.60217733 \times 10^{-19} \text{ C})^3}{8\pi 6.6260755 \times 10^{-34} \text{ J s}} \frac{(\text{V/m})^2}{\text{eV A m}^{-2}} \frac{\text{eV}}{(\text{V/m})^2} \frac{\text{A}}{\text{m}^2} \quad (7)$$

$$= 1.541434 \times 10^{-6} \frac{\text{A eV}}{\text{V}^2} \quad (8)$$

and

$$b = \frac{8\pi\sqrt{2m_e}}{3he} = \frac{8\pi\sqrt{2 \times 9.1093897 \times 10^{-31} \text{ kg}}}{3 \times 6.6260755 \times 10^{-34} \text{ J s} \times 1.60217733 \times 10^{-19} \text{ C}} \frac{\text{eV}^{3/2}}{\text{V m}^{-1}} \frac{\text{V eV}^{3/2}}{\text{m}} \quad (9)$$

$$= 6.830888 \times 10^9 \frac{\text{V}}{\text{eV}^{3/2} \text{ m}} \quad (10)$$

are the first and second Fowler–Nordheim constants and v and t are functions of the argument $y = \Delta A/\phi$.

The validity of equation (6) as a limiting case of the Murphy–Good formalism is limited by the inequality (57) of [2]. The latter may be written as

$$\frac{\phi}{\Delta A} - 1 > q\sqrt{\Delta A}, \quad (11)$$

where

$$q = \frac{2h\epsilon_0}{\pi\sqrt{m_e}e^2} = \frac{2 \times 6.6260755 \times 10^{-34} \text{ J s} \times 8.854187817 \times 10^{-12} \text{ F m}^{-1}}{\pi\sqrt{9.1093897 \times 10^{-31} \text{ kg}} (1.60217733 \times 10^{-19} \text{ C})^2} (\text{eV})^{1/2} \frac{1}{\sqrt{\text{eV}}} \quad (12)$$

$$= 6.102035 \times 10^{-2} \frac{1}{\sqrt{\text{eV}}}. \quad (13)$$

For $\phi = 4.5 \text{ eV}$, inequality (11) is satisfied for $\Delta A < 4.010 \text{ eV}$. This value is slightly below ϕ , which should have been expected (in the range $0 \leq \Delta A \leq \phi$, where the lhs of the inequality (11) is non-negative, the rhs does not exceed approximately $0.06\sqrt{\phi/\text{eV}}$, i.e., is rather small). The corresponding limitation for the electric field reads $F < 1.116 \times 10^{10} \text{ V m}^{-1}$. As expected, the value on the rhs is somewhat lower than the value of $1.406 \times 10^{10} \text{ V m}^{-1}$, at which ΔA equals ϕ .

The function $t(y)$ in equation (6) may be estimated by means of equations (5) and (9) of [3]:

$$v(y) = 1 - y^2\left(1 - \frac{1}{3}\ln y\right), \quad (14)$$

$$t(y) = 1 + \frac{y^2}{9}(1 - \ln y). \quad (15)$$

3 Murphy-Good formalism

Emission current, equation (19) [2]

$$j(T, F, \phi) = e \int_{-W_a}^{\infty} N(T, W, \phi) D(F, W) dW, \quad (16)$$

where W has the meaning of the part of the electron energy for the motion normal to the surface measured from zero for a free electron outside the metal.

The Fermi-Dirac distribution, equation (1) [2]:

$$N(T, W, \phi) = \frac{4\pi m_e kT}{h^3} \ln \left[1 + \exp \left(-\frac{W + \phi}{kT} \right) \right]. \quad (17)$$

The tunnelling probability is set equal to unity, $D = 1$, for $W > W_l$, where

$$W_l = -\sqrt{\frac{e^3 F}{8\pi\epsilon_0}} = -\frac{\Delta A}{\sqrt{2}}. \quad (18)$$

For $W < W_l$, the WKB-approximation is used, equation (5) of [2] (cf. Ch. 9 of my lectures on Quantum Mechanics, file QM09.tex):

$$D = \left\{ 1 + \exp \left[-\frac{2i}{\hbar} \int_{x_1}^{x_2} p(x) dx \right] \right\}^{-1}, \quad (19)$$

where

$$p(x) = \sqrt{2m_e} [W - V(x)]^{1/2}, \quad V(x) = -\frac{e^2}{16\pi\epsilon_0 x} - eFx. \quad (20)$$

In order to evaluate the integral in equation (19), let us write

$$p(x) = \sqrt{2m_e} \left(W + \frac{e^2}{16\pi\epsilon_0 x} + eFx \right)^{1/2} = \sqrt{m_e (-W)} \left(-2 - \frac{2}{W} \frac{e^2}{16\pi\epsilon_0 x} - \frac{2}{W} eFx \right)^{1/2} \quad (21)$$

Let us represent

$$-W = \sqrt{\frac{e^3 F}{4\pi\epsilon_0}} \frac{1}{y}, \quad x = \frac{-W}{2eF} \rho \quad (22)$$

(it follows that $y = \frac{\Delta A}{-W}$) and substitute these expressions into (21):

$$p(x) = \sqrt{\frac{m_e}{y}} \left(\frac{e^3 F}{4\pi\epsilon_0} \right)^{1/4} \sqrt{f(\rho, y)}, \quad (23)$$

where

$$f(\rho, y) = -2 + \frac{y^2}{\rho} + \rho. \quad (24)$$

Equation (19) assumes the form

$$D = \left\{ 1 + \exp \left[-\frac{2i}{\hbar} \sqrt{\frac{m_e}{y}} \left(\frac{e^3 F}{4\pi\epsilon_0} \right)^{1/4} \frac{-W}{2eF} \int_{1-\sqrt{1-y^2}}^{1+\sqrt{1-y^2}} \sqrt{f(\rho, y)} d\rho \right] \right\}^{-1} \quad (25)$$

$$= \left\{ 1 + \exp \left[a \frac{v(y)}{y^{3/2}} \right] \right\}^{-1}, \quad (26)$$

where

$$a = \frac{4\sqrt{2}}{3(4\pi\epsilon_0)^{3/4}} \left(\frac{m_e^2 e^5}{\hbar^4 F} \right)^{1/4} \quad (27)$$

$$= \frac{4\sqrt{2}}{3(4\pi \cdot 8.854187817 \times 10^{-12} \text{ F m}^{-1})^{3/4}} \quad (28)$$

$$\times \left(\frac{(9.1093897 \times 10^{-31} \text{ kg})^2 (1.60217733 \times 10^{-19} \text{ C})^5}{(6.5821220 \times 10^{-16} \text{ eV s})^4 \text{ V m}^{-1}} \right)^{1/4} \left(\frac{\text{V m}^{-1}}{F} \right)^{1/4} \quad (29)$$

$$= 1.596765526 \times 10^3 \left(\frac{\text{V m}^{-1}}{F} \right)^{1/4}, \quad (30)$$

$$v(y) = \frac{-3i}{4\sqrt{2}} \int_{1-\sqrt{1-y^2}}^{1+\sqrt{1-y^2}} \sqrt{f(\rho, y)} d\rho; \quad (31)$$

cf. equation (13) of [2].

Equation (16) assumes the form:

$$j(T, F, \phi) = \frac{4\pi m_e k T e}{h^3} \left\{ \int_{-W_a}^{W_i} \frac{\ln \left[1 + \exp \left(-\frac{W+\phi}{kT} \right) \right]}{1 + \exp \frac{av(y)}{y^{3/2}}} dW + \int_{W_i}^{\infty} \ln \left[1 + \exp \left(-\frac{W+\phi}{kT} \right) \right] dW \right\}. \quad (32)$$

If the factor $(4\pi\epsilon_0)^{-3/4}$ in equation (27) is dropped, equation (32) will coincide with equation (19) of [2]. Note that the value $5.15 \times 10^9 \text{ V cm}^{-1}$ for $m_e^2 e^5 \hbar^{-4}$, given in [2] after equation (19), is in agreement with the above equation (30):

$$a = \frac{4\sqrt{2}}{3} \left(5.15 \times 10^9 \frac{\text{V cm}^{-1}}{F} \right)^{1/4} = \frac{4\sqrt{2}}{3} \left(5.15 \times 10^9 \frac{\text{cm}^{-1}}{\text{m}^{-1}} \right)^{1/4} \left(\frac{\text{V m}^{-1}}{F} \right)^{1/4} \quad (33)$$

$$= 1.597 \times 10^3 \left(\frac{\text{V m}^{-1}}{F} \right)^{1/4} \quad (34)$$

On the other hand, equation (7) of [4] is likely to be erroneous: it would have been equivalent to (32) if 4 in the numerator of the first multiplier on the rhs of equation (27) were missing.

4 Function $v(y)$

Equation (24) may be rewritten as

$$f(\rho, y) = \frac{(\rho - 1)^2 + y^2 - 1}{\rho}. \quad (35)$$

For $-\infty < W \leq -\Delta A$, y varies in the range $0 < y \leq 1$ and the integration limits in equation (31) are real, so the integration can be performed along the real axis. Since $f(\rho, y)$ vanishes at the integration limits and $f(1, y) = y^2 - 1 < 0$, the integrand is imaginary in the whole interval. Hence the integral in equation (31) is imaginary and $v(y)$ real.

For $-\Delta A \leq W \leq W_l = -\Delta A/\sqrt{2}$, y varies in the range $1 \leq y \leq \sqrt{2}$ and the integration limits are complex. The integration can be performed along the interval $\rho = 1 + i\sqrt{y^2 - 1}t$, $-1 \leq t \leq 1$. On this interval,

$$f(\rho, y) = (y^2 - 1) \frac{1 - t^2}{1 + i\sqrt{y^2 - 1}t}. \quad (36)$$

The argument is odd with respect to t , hence $\text{Im} \sqrt{f}$ is odd as well and the integral in equation (31) is once again imaginary and $v(y)$ real.

Equation (16) of [2]:

$$v(y) = \sqrt{1 + y} \left[E\left(\frac{1 - y}{1 + y}\right) - yK\left(\frac{1 - y}{1 + y}\right) \right], \quad (37)$$

where $K = K(m)$ and $E = E(m)$ are complete elliptic integrals of the first and second kinds [5]:

$$K(m) = \int_0^{\pi/2} (1 - m \sin^2 \theta)^{-1/2} d\theta, \quad E(m) = \int_0^{\pi/2} (1 - m \sin^2 \theta)^{1/2} d\theta. \quad (38)$$

Equation (37) gives real values for any $y > 0$. However, functions $K(m)$ and $E(m)$ are normally tabulated only for $0 \leq m \leq 1$ (e.g., [5]), hence this equation, while being convenient for $0 < y \leq 1$, is better be transformed for $y \geq 1$. Let us use relations (see file *Properties_and_integrals_of_K(m).tex*)

$$K(-m) = \frac{1}{\sqrt{1 + m}} K\left(\frac{m}{m + 1}\right), \quad E(-m) = \sqrt{1 + m} E\left(\frac{m}{m + 1}\right). \quad (39)$$

Setting $m = -\frac{1-y}{1+y}$ in these relations and substituting them into equation (37), one obtains

$$v(y) = \sqrt{\frac{y}{2}} \left[2E\left(\frac{y-1}{2y}\right) - (y+1)K\left(\frac{y-1}{2y}\right) \right]. \quad (40)$$

This is equation (15) of [2].

5 Range of values of control parameters

The range of variables T and F considered in [6] was $10^3 \text{ K} \leq T \leq 10 \times 10^3 \text{ K}$, $5 \times 10^7 \text{ V m}^{-1} \leq F \leq 2 \times 10^{10} \text{ V m}^{-1}$. In my 2009 calculations for Siemens, the maximum value of F was $2.2 \times 10^9 \text{ V m}^{-1}$, which corresponds to $a \geq 7.37$.

$F \text{ (V m}^{-1}\text{)}$	$\Delta A \text{ (eV)}$	a
5×10^7	0.268	19.0
2.2×10^9	1.780	7.37
2×10^{10}	5.366	4.25

6 Evaluating the integrals

Let us rewrite equation (32) as

$$\frac{j(T, F, \phi)}{A_{em} T^2} = I_1 + g I_2, \quad (41)$$

where

$$I_1 = \int_c^\infty \ln(1 + e^{-z}) dz, \quad c = \frac{\phi + W_l}{kT} = \frac{1}{kT} \left(\phi - \frac{\Delta A}{\sqrt{2}} \right), \quad (42)$$

$$I_2 = \int_{1/\sqrt{2}}^{W_a/\Delta A} \frac{\ln[1 + \exp(gz - b)]}{1 + \exp[az^{3/2}v(z^{-1})]} dz, \quad g = \frac{\Delta A}{kT}, \quad b = \frac{\phi}{kT}. \quad (43)$$

It is usual to set $W_a = \infty$ ([2] pp. 1468 and 1469).

6.1 Integral I_1

The function $I_1 = I_1(c)$ may readily be expressed in terms of dilogarithm (Spence's integral for $n = 2$): $I_1 = L(e^{-c})$, where $L = L(x)$ is dilogarithm as defined in [7], p. 67:

$$L(x) = \int_0^x \frac{\ln(1+t)}{t} dt. \quad (44)$$

Note that the definition used in [5] and SWP (Maple) is somewhat different: $f(x) = \text{dilog}(x) = -\int_1^x \frac{\ln t}{t-1} dt$, so $L(x) = -\text{dilog}(1+x)$ and $I_1(c) = -\text{dilog}(1+e^{-c})$.

The approach to evaluation of the function $L(x)$ proposed in [7], p. 67 consists in using a Chebyshev series in the interval $0 \leq x \leq 1$ (the relevant Chebyshev coefficients are given) and functional relations for x outside this interval. [Note that a Fortran subroutine based on this approach is mentioned on the Net:

<http://wwwasdoc.web.cern.ch/wwwasdoc/shortwrupsdir/c332/top.html>.] In our case, this procedure would amount to using the Chebyshev series for $c \geq 0$ and the functional relation

$$I_1(c) = \frac{\pi^2}{6} + \frac{c^2}{2} - I_1(-c) \quad (45)$$

for $c < 0$.

Note that the relation (45) may be derived from relations given in [5] as follows. Let us subtract equation (27.3.5) from (27.3.3):

$$f(1-x) - f\left(\frac{1}{x}\right) = -\ln x \ln(1-x) + \frac{\pi^2}{6} + \frac{1}{2} \ln^2 x. \quad (46)$$

Let us now subtract from this equation equation (27.3.5) with x replaced by $(1-x)$:

$$-f\left(\frac{1}{x}\right) - f\left(\frac{1}{1-x}\right) = \frac{\pi^2}{6} + \frac{1}{2} \ln^2 \frac{x}{1-x}. \quad (47)$$

Setting in this equation $x = 1/(1+e^c)$, one obtains relation (45). Note also that this relation may be readily verified in SWP by plotting the function $-\text{dilog}(1+e^{-x}) - \text{dilog}(1+e^x) - \frac{\pi^2}{6} - \frac{x^2}{2}$: it is of the order of 10^{-18} .

However, a much faster and sufficiently accurate way is to use for $c \geq 0$ a rational approximation (Padé approximant) over the variable $x = e^c$. The two-term expansions of the function $I_1(x)$ for $x \rightarrow 1$ and $x \rightarrow \infty$ read, respectively,

$$I_1 = \frac{\pi^2}{12} - (\ln 2)(x - 1) + \dots, \quad I_1 = \frac{1}{x} - \frac{1}{4x^2} + \dots \quad (48)$$

Note that the latter formula is obtained by expanding the logarithm in (44) in powers of t ; it may be obtained also from the expansion (27.7.2) of [5]. The simplest rational approximation which agrees with these expansions may be written as

$$I_1 = \frac{c_1 + c_2(x - 1)}{1 + c_3(x - 1) + c_2(x^2 - 1)} \quad (49)$$

with

$$c_1 = \frac{\pi^2}{12}, \quad c_2 = -\frac{1}{3} \frac{\pi^4 - 144 \ln 2}{-48 + 5\pi^2}, \quad c_3 = \frac{2}{3} \frac{-6\pi^2 + \pi^4 - 54 \ln 2}{-48 + 5\pi^2}. \quad (50)$$

Verification

Definitions

$$c_1 = \frac{\pi^2}{12}$$

$$c_2 = -\frac{1}{3} \frac{\pi^4 - 144 \ln 2}{-48 + 5\pi^2}$$

$$c_3 = \frac{2}{3} \frac{-6\pi^2 + \pi^4 - 54 \ln 2}{-48 + 5\pi^2}$$

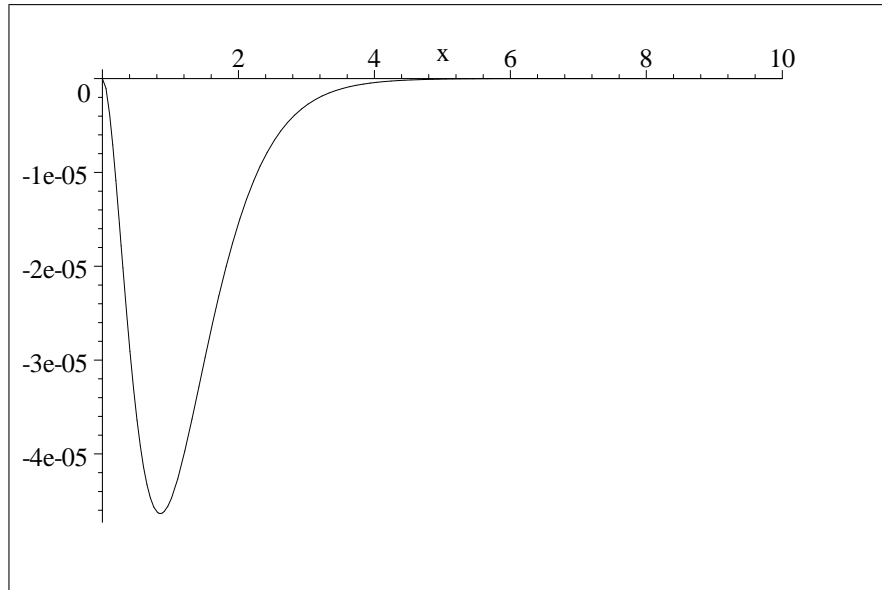
$$\text{Evaluation: } -\text{dilog}(1 + e^{-c}) - \frac{c_1 + c_2(e^c - 1)}{1 + c_3(e^c - 1) + c_2(e^{2c} - 1)} = 0c + O(c^2),$$

$$\left[-\text{dilog}(1 + e^{-c}) - \frac{c_1 + c_2(e^c - 1)}{1 + c_3(e^c - 1) + c_2(e^{2c} - 1)} \right]_{c = -\ln \varepsilon} = 0\varepsilon^2 + O(\varepsilon^3)$$

Error of this approximant does not exceed 4.6×10^{-5} for all $c > 0$, which is seen by plotting the function

$$\frac{\frac{c_1 + c_2(e^x - 1)}{1 + c_3(e^x - 1) + c_2(e^{2x} - 1)}}{-\text{dilog}(1 + e^{-x})} - 1 \quad (51)$$

in the range $0 \leq x \leq 10$. (If the plot below does not appear on the screen, try making any formal change in the plotted item and saving the plot.)



For $c < 0$, equation (45) will be used. In this connection, it is appropriate to rewrite equation (49) as

$$I_1(c) = \frac{c_1 e^{-c} + c_2 (1 - e^{-c})}{e^{-c} + c_3 (1 - e^{-c}) + c_2 (e^c - e^{-c})} \quad (52)$$

in order to avoid overflow which may occur in evaluation of the last term of the denominator while evaluating $I_1(-c)$ on the rhs of equation (45) for very high F and low T , when $-c$ is very high.

Verification: $\frac{c_1 + c_2(e^c - 1)}{1 + c_3(e^c - 1) + c_2(e^{2c} - 1)} = \frac{c_1 e^{-c} + c_2(1 - e^{-c})}{e^{-c} + c_3(1 - e^{-c}) + c_2(e^c - e^{-c})}$ is true

6.2 Evaluating $v(y)$ by means of Padé approximants

A straightforward numerical evaluation of the function $v(y)$ requires an evaluation of complete elliptic integrals $K(m)$ and $E(m)$. The latter can be performed, e.g., by means of the numerical method described in [8] or of polynomial approximations given in [5]. However, simple analytical formulas for $v(y)$ are desirable in order for numerical evaluation of the integral (43) to be fast. Note that since $v(y)$ greatly affects the calculated current density, derivation of such formulas requires careful treatment [9]. There are several works in which simple fit formulas of different degrees of accuracy for the function $v(y)$ are suggested; e.g., [3, 4, 6, 10–12]. In this work, simple and accurate formulas are derived by means of Padé approximants with the use of results [12] elucidating the character of the dependence $v(y)$.

Let us consider first the interval $0 \leq y \leq 1$. The expansion of function $v(y)$ for $y \rightarrow 0$ reads [12]:

$$v(y) = \left[1 - \left(\frac{9}{8} \ln 2 + \frac{3}{16} \right) w + \dots \right] + \ln w \left[\frac{3}{16} w + \dots \right], \quad (53)$$

where $w = y^2$ and the series in the square brackets involve integer powers of w . The series expansion for $y \rightarrow 1$ can be found with the use of series expansions of functions $K(m)$ and $E(m)$ in powers of m (e.g., [5]) and reads

$$v(y) = \frac{3\pi\sqrt{2}}{8} (1 - y) + \dots \quad (54)$$

Verification

Definitions

$$K(m) = \int_0^{\pi/2} (1 - m \sin^2 \theta)^{-1/2} d\theta$$

$$E(m) = \int_0^{\pi/2} (1 - m \sin^2 \theta)^{1/2} d\theta$$

$$v(y) = \sqrt{\frac{y}{2}} \left(2E\left(\frac{y-1}{2y}\right) - (y+1)K\left(\frac{y-1}{2y}\right) \right)$$

$$\text{Evaluation: } v(1 + \varepsilon) = \left(-\frac{3}{8}\pi\sqrt{2}\right)\varepsilon + O(\varepsilon^2)$$

In view of the structure of the expansion (53), it is natural to represent $v(y)$ in the interval $0 \leq y \leq 1$ as $v(y) = v^{(1)}(w) + v^{(2)}(w) \ln w$ and approximate dependences $v^{(1)}(w)$ and $v^{(2)}(w)$ by rational functions of w , i.e., to find their Padé approximants. Making use of the simplest approximants which agree with the expansions (53) and (54), one obtains

$$v(y) = \frac{1 - w}{1 + c_4 w} + \frac{3w \ln w}{16(1 + c_5 w)} \quad (55)$$

with

$$c_4 = \frac{9}{8} \ln 2 - \frac{13}{16}, \quad c_5 = \frac{13 - 3c_4 - 3\pi\sqrt{2}(1 + c_4)}{3\pi\sqrt{2}(1 + c_4) - 16}. \quad (56)$$

Verification

Definitions

$$c_4 = \frac{9}{8} \ln 2 - \frac{13}{16}$$

$$c_5 = \frac{13 - 3c_4 - 3\pi\sqrt{2}(1 + c_4)}{3\pi\sqrt{2}(1 + c_4) - 16}$$

$$\text{Evaluation: } \frac{1-w}{1+c_4w} + \frac{3w \ln w}{16(1+c_5w)} - \left(1 - \left(\frac{9}{8} \ln 2 + \frac{3}{16}\right) w\right) - \ln w \left(\frac{3}{16} w\right)$$

$$= \left[\frac{1-w}{1+c_4w} - \left(1 - \left(\frac{9}{8} \ln 2 + \frac{3}{16}\right) w\right) \right] + \left[\frac{3w}{16(1+c_5w)} - \left(\frac{3}{16} w\right) \right] \ln w = [O(w^2)] + [O(w^2)] \ln w,$$

$$\left[\frac{1-w}{1+c_4w} + \frac{3w \ln w}{16(1+c_5w)} - \frac{3\pi\sqrt{2}}{8} (-\varepsilon) \right]_{w=(1+\varepsilon)^2} = 0\varepsilon + O(\varepsilon^2)$$

The error of the approximate formula (55) does not exceed 3.7×10^{-4} over the whole range $0 \leq y \leq 1$, which is significantly smaller than that of previously reported simple formulas; an unsurprising result reflecting the power of Padé approximants. The next best is the formula [3, 11, 12], which, while being simple and elegant, is by happy accident close to the best fit [3] and possesses the maximum error of 3.3×10^{-3} . It should be stressed that the approximate formula (55) ensures correct asymptotic behavior of the function $v(y)$ for both $y \rightarrow 0$ and $y \rightarrow 1$, the latter being important for deriving a smooth approximation on the whole interval $0 \leq y \leq \sqrt{2}$ which is needed for evaluation of thermo-field emission.

Let us consider now the interval $1 \leq y \leq \sqrt{2}$. A series expansion of $v(y)$ for $y \rightarrow \sqrt{2}$ reads

$$v(y) = \frac{1}{2^{1/4}} \left[2E(m_0) - (\sqrt{2} + 1) K(m_0) \right] - \frac{3}{2^{5/4}} K(m_0) (y - \sqrt{2}) - \frac{3}{2^{13/4}} [2E(m_0) - K(m_0)] (y - \sqrt{2})^2 + \dots, \quad (57)$$

where $m_0 = \frac{2-\sqrt{2}}{4}$. (Verification not possible.) The simplest approximant that agrees with the expansions (54) and (57) may be written as

$$v(y) = -\frac{3\pi}{2^{5/2}} \frac{(y-1) + c_6(y-1)^2}{1 + c_7(y-1) + c_8(y-1)^2} \quad (58)$$

with coefficients c_6 , c_7 , and c_8 being expressed in terms of $K(m_0)$ and $E(m_0)$ (these expressions are skipped for brevity) and having numerical values $c_6 = 0.51470654$, $c_7 = 0.20232890$, and $c_8 = -0.01341007$. The error of this approximant does not exceed 4.8×10^{-6} over the whole range $1 \leq y \leq \sqrt{2}$, which again is significantly smaller than that of previously reported simple formulas.

Verification

Definitions

$$m_0 = \frac{2-\sqrt{2}}{4}$$

$$c_9 = \frac{1}{2} 2^{\frac{3}{4}} (2E(m_0) - (\sqrt{2} + 1) K(m_0))$$

$$c_{10} = -\frac{3}{4} 2^{\frac{3}{4}} K(m_0)$$

$$c_{11} = -\frac{3}{8} \frac{\sqrt{2}}{\sqrt{2}-1} \left((-2 + \sqrt{2}) K(m_0) + 2 \frac{\sqrt{2}}{\sqrt{2}+1} E(m_0) \right)$$

$$c_6 = -\frac{1}{3} \frac{3c_{11}\pi c_9 - 192c_9^3 - 6\pi c_{10}^2 - 6\pi c_{10}^2 \sqrt{2} + 3\pi \sqrt{2} c_{11} c_9 - 136c_9^3 \sqrt{2}}{(c_{11}c_9 - 2c_{10}^2 + 2c_9c_{10} + 2c_9c_{10}\sqrt{2})\pi}$$

$$\begin{aligned}
c_7 &= -\frac{1}{8} \frac{-32c_{10}^2 - 32c_{10}^2\sqrt{2} + 3c_{11}\pi\sqrt{2} + 16c_{11}c_9 + 16c_{11}c_9\sqrt{2} + 12\pi c_{10} + 6\pi c_{10}\sqrt{2} + 144c_9c_{10} + 96c_9c_{10}\sqrt{2}}{c_{11}c_9 - 2c_{10}^2 + 2c_9c_{10} + 2c_9c_{10}\sqrt{2}} \\
c_8 &= \frac{1}{8} \frac{224c_9c_{10} + 6c_{11}\pi - 272c_9^2 + 24c_{11}c_9 - 48c_{10}^2 + 16c_{11}c_9\sqrt{2} - 32c_{10}^2\sqrt{2} + 160c_9c_{10}\sqrt{2} + 3c_{11}\pi\sqrt{2} - 192c_9^2\sqrt{2}}{c_{11}c_9 - 2c_{10}^2 + 2c_9c_{10} + 2c_9c_{10}\sqrt{2}} \\
\text{Evaluation: } &\left[-\frac{3\pi}{2^{5/2}} \frac{(y-1) + c_6(y-1)^2}{1 + c_7(y-1) + c_8(y-1)^2} - \frac{3\pi\sqrt{2}}{8} (1-y) \right]_{y=1+\varepsilon} = O(\varepsilon^2), \\
&\left[-\frac{3\pi}{2^{5/2}} \frac{(y-1) + c_6(y-1)^2}{1 + c_7(y-1) + c_8(y-1)^2} - \left(\frac{1}{2^{1/4}} (2E(m_0) - (\sqrt{2} + 1) K(m_0)) - \frac{3}{2^{5/4}} K(m_0) (y - \sqrt{2}) - \frac{3}{2^{13/4}} (2E(m_0) - (\sqrt{2} + 1) K(m_0)) \right) \right]_{y=1+\varepsilon} \\
&= 0 + 0\varepsilon + 0\varepsilon^2 + O(\varepsilon^3)
\end{aligned}$$

6.3 Integral I_2

Integral (43) cannot be expressed in terms of conventional special functions. On the other hand, I_2 is governed by three dimensionless parameters (a, b, g) , so it is hardly possible to devise an accurate uniformly valid approximate formula. Therefore, the integral needs to be evaluated numerically.

Under conditions of practical interest, one or more parameters governing the integrand in equation (43) are large and the integrand represents a multi-scale function. Therefore, an efficient numerical evaluation of the integral must include an adaptive choice of the numerical grid. A suitable method is Romberg integration [8]. First, let us transform the integral to the integration variable $y = 1/z$,

$$I_2 = \int_0^{\sqrt{2}} \frac{r_1 r_2}{y^2} dy, \quad (59)$$

where

$$r_1 = \ln \left[1 + \exp \left(\frac{g}{y} - b \right) \right], \quad r_2 = \left[1 + \exp \frac{av(y)}{y^{3/2}} \right]^{-1}. \quad (60)$$

In order to avoid overflow which may occur in evaluation of the exponential functions for small y , it is advisable to rewrite equation (60) as

$$r_1 = \ln \left[1 + \exp \left(b - \frac{g}{y} \right) \right] - \left(b - \frac{g}{y} \right), \quad r_2 = \frac{\exp \left[-\frac{av(y)}{y^{3/2}} \right]}{\exp \left[-\frac{av(y)}{y^{3/2}} \right] + 1}. \quad (61)$$

In cases where $\exp \left(\frac{g}{y} - b \right)$ is very small, the use of the first expression in equation (61) causes accumulation of errors and the Romberg integration (or, more precisely, Richardson's deferred approach to the limit) may fail. The same happens if the first expression in equation (60) is used; in particular, the argument of the logarithm evaluated by the code will be exactly 1 and the logarithm exactly 0 for $\exp \left(\frac{g}{y} - b \right)$ sufficiently small while still above the underflow limit. Therefore, in cases where $\exp \left(\frac{g}{y} - b \right)$ is small, say, smaller than 0.01, the quantity r_1 should be evaluated by means of a series in powers of $\exp \left(\frac{g}{y} - b \right)$ which is obtained by expanding the logarithm in the first expression in equation (60).

In this framework, the Romberg integration in its standard form [8] works nicely for (at least) $10 \text{ V m}^{-1} \leq F \leq 10^{11} \text{ V m}^{-1}$ and $300 \text{ K} \leq T \leq 6000 \text{ K}$.

7 Computations with SWP (Maple)

Evaluation by means of SWP gives

$$\int_0^{\pi/2} (1 - m \sin^2 \theta)^{-1/2} d\theta = \text{EllipticK}(\sqrt{m}), \quad \int_0^{\pi/2} (1 - m \sin^2 \theta)^{1/2} d\theta = \text{EllipticE}(\sqrt{m}), \quad (62)$$

but SWP does not understand designations EllipticE and EllipticK (it considers EllipticK(m) to be a product!!!) However, it can work with the integrals on the lhs of equation (62). In particular, one can define

$$v_1(y) = \sqrt{1+y} \left(\int_0^{\pi/2} \left(1 - \frac{1-y}{1+y} \sin^2 \theta \right)^{1/2} d\theta - y \int_0^{\pi/2} \left(1 - \frac{1-y}{1+y} \sin^2 \theta \right)^{-1/2} d\theta \right), \quad (63)$$

$$v_2(y) = -\sqrt{\frac{y}{2}} \left((y+1) \int_0^{\pi/2} \left(1 - \frac{y-1}{2y} \sin^2 \theta \right)^{-1/2} d\theta - 2 \int_0^{\pi/2} \left(1 - \frac{y-1}{2y} \sin^2 \theta \right)^{1/2} d\theta \right), \quad (64)$$

(SWP gives equal numerical values for these functions). These definitions can be used for evaluation but, unfortunately, not for plotting.

Quantity on the rhs of definition (63) can be plotted. However, these plots are capricious, as well as, apparently, any other plots in SWP5.5. For example, the plot below normally does not appear on the screen immediately after it has been open. You should make any formal change in any of the plotted items and save the plot, after which it will appear.

8 Derivation of (57) and (58)

Definitions:

$$K(m) = \int_0^{\pi/2} (1 - m \sin^2 \theta)^{-1/2} d\theta$$

$$E(m) = \int_0^{\pi/2} (1 - m \sin^2 \theta)^{1/2} d\theta$$

$$v(y) = \sqrt{\frac{y}{2}} \left(2E\left(\frac{y-1}{2y}\right) - (y+1)K\left(\frac{y-1}{2y}\right) \right)$$

Derivatives:

$$\frac{dv(y)}{dy} + \frac{3\sqrt{2y}}{4} K\left(\frac{y-1}{2y}\right) \text{ (two times Simplify) : } 0 \iff \frac{dv(y)}{dy} = -\frac{3\sqrt{2y}}{4} K\left(\frac{y-1}{2y}\right)$$

$$\frac{d}{dy} \left(-\frac{3\sqrt{2y}}{4} K\left(\frac{y-1}{2y}\right) \right) + \frac{3}{8} \frac{\sqrt{2}}{\sqrt{y(y-1)}} \left((y-2)K\left(\frac{y-1}{2y}\right) + \frac{2y}{(y+1)}E\left(\frac{y-1}{2y}\right) \right) \text{ (two times Simplify) : } 0 \iff \frac{d^2v(y)}{dy^2} = -\frac{3}{8} \frac{\sqrt{2}}{\sqrt{y(y-1)}} \left[(y-2)K\left(\frac{y-1}{2y}\right) + \frac{2y}{(y+1)}E\left(\frac{y-1}{2y}\right) \right]$$

Values for $y = \sqrt{2}$:

$$m_0 = \left[\frac{y-1}{2y} \right]_{y=\sqrt{2}} = \frac{2-\sqrt{2}}{4}$$

Definition:

$$m_0 = \frac{2-\sqrt{2}}{4}$$

$$[v(y)]_{y=\sqrt{2}} - \frac{1}{2} 2^{\frac{3}{4}} (2E(m_0) - (\sqrt{2}+1)K(m_0)) \stackrel{\text{Simplify}}{=} 0$$

$$\iff [v(y)]_{y=\sqrt{2}} = \frac{1}{2} 2^{\frac{3}{4}} (2E(m_0) - (\sqrt{2}+1)K(m_0)) = c_9$$

$$\left[-\frac{3\sqrt{2y}}{4} K\left(\frac{y-1}{2y}\right) \right]_{y=\sqrt{2}} + \frac{3}{4} 2^{\frac{3}{4}} K(m_0) \stackrel{\text{Simplify}}{=} 0 \iff \left[\frac{dv(y)}{dy} \right]_{y=\sqrt{2}} = -\frac{3}{4} 2^{\frac{3}{4}} K(m_0) = c_{10}$$

$$\left[-\frac{3}{8} \frac{\sqrt{2}}{\sqrt{y}(y-1)} \left((y-2) K \left(\frac{y-1}{2y} \right) + \frac{2y}{(y+1)} E \left(\frac{y-1}{2y} \right) \right) \right]_{y=\sqrt{2}} + \frac{3}{8} \frac{\sqrt[4]{2}}{\sqrt{2}-1} \left((-2+\sqrt{2}) K(m_0) + 2 \frac{\sqrt{2}}{\sqrt{2}+1} E(m_0) \right)$$

Simplify $\frac{0}{\left[\frac{d^2 v(y)}{dy^2} \right]_{y=\sqrt{2}}} \iff -\frac{3}{8} \frac{\sqrt[4]{2}}{\sqrt{2}-1} \left[(-2+\sqrt{2}) K(m_0) + 2 \frac{\sqrt{2}}{\sqrt{2}+1} E(m_0) \right] = c_{11}$

Approximant: $v(y) = -\frac{3\pi}{2^{5/2}} \frac{(y-1)+c_6(y-1)^2}{1+c_7(y-1)+c_8(y-1)^2}$

$$v = \left[-\frac{3\pi}{2^{5/2}} \frac{(y-1)+c_6(y-1)^2}{1+c_7(y-1)+c_8(y-1)^2} \right]_{y=\sqrt{2}+\varepsilon} = \left(-\frac{3}{8} \pi \sqrt{2} \frac{\sqrt{2}-1+c_6(\sqrt{2}-1)^2}{1+c_7(\sqrt{2}-1)+c_8(\sqrt{2}-1)^2} \right) + \left(-\frac{3}{8} \frac{\pi \sqrt{2}(1+c_6(2\sqrt{2}-2)) - \pi}{1+c_7(\sqrt{2}-1)+c_8(\sqrt{2}-1)^2} \right)$$

$$\varepsilon + \left(-\frac{3}{8} \frac{\pi \sqrt{2} c_6 - \pi \sqrt{2} \frac{-\sqrt{2}+1-3c_6+2c_6\sqrt{2}}{-1-c_7\sqrt{2}+c_7-3c_8+2c_8\sqrt{2}} c_8 - \sqrt{2} \pi \frac{1-3c_8+2c_8\sqrt{2}+2c_6\sqrt{2}+3c_6c_7-2c_6\sqrt{2}c_7-2c_6}{(-1-c_7\sqrt{2}+c_7-3c_8+2c_8\sqrt{2})^2} (c_7+c_8(2\sqrt{2}-2))}{1+c_7(\sqrt{2}-1)+c_8(\sqrt{2}-1)^2} \right) \varepsilon^2 + O(\varepsilon^3)$$

$$\left(-\frac{3}{8} \pi \sqrt{2} \frac{\sqrt{2}-1+c_6(\sqrt{2}-1)^2}{1+c_7(\sqrt{2}-1)+c_8(\sqrt{2}-1)^2} \right) = c_9$$

$$\left(-\frac{3}{8} \frac{\pi \sqrt{2}(1+c_6(2\sqrt{2}-2)) - \pi \sqrt{2} \frac{-\sqrt{2}+1-3c_6+2c_6\sqrt{2}}{-1-c_7\sqrt{2}+c_7-3c_8+2c_8\sqrt{2}} (c_7+c_8(2\sqrt{2}-2))}{1+c_7(\sqrt{2}-1)+c_8(\sqrt{2}-1)^2} \right) = c_{10}$$

$$\left(-\frac{3}{8} \frac{\pi \sqrt{2} c_6 - \pi \sqrt{2} \frac{-\sqrt{2}+1-3c_6+2c_6\sqrt{2}}{-1-c_7\sqrt{2}+c_7-3c_8+2c_8\sqrt{2}} c_8 - \sqrt{2} \pi \frac{1-3c_8+2c_8\sqrt{2}+2c_6\sqrt{2}+3c_6c_7-2c_6\sqrt{2}c_7-2c_6}{(-1-c_7\sqrt{2}+c_7-3c_8+2c_8\sqrt{2})^2} (c_7+c_8(2\sqrt{2}-2))}{1+c_7(\sqrt{2}-1)+c_8(\sqrt{2}-1)^2} \right) = \frac{c_{11}}{2}$$

Solution is: $\left\{ c_6 = -\frac{1}{3} \frac{3c_{11}\pi c_9 - 192c_9^3 - 6\pi c_{10}^2 - 6\pi c_{10}^2 \sqrt{2} + 3\pi \sqrt{2} c_{11} c_9 - 136c_9^3 \sqrt{2}}{(c_{11}c_9 - 2c_{10}^2 + 2c_9c_{10} + 2c_9c_{10}\sqrt{2})\pi}, c_7 = -\frac{1}{8} \frac{-32c_{10}^2 - 32c_{10}^2 \sqrt{2} + 3c_{11}\pi \sqrt{2} + 16c_{11}\pi c_9}{c_{11}c_9 - 2c_{10}^2 + 2c_9c_{10} + 2c_9c_{10}\sqrt{2}} \right\}$

Definitions

$$c_9 = \frac{1}{2} 2^{\frac{3}{4}} (2E(m_0) - (\sqrt{2}+1) K(m_0))$$

$$c_{10} = -\frac{3}{4} 2^{\frac{3}{4}} K(m_0)$$

$$c_{11} = -\frac{3}{8} \frac{\sqrt[4]{2}}{\sqrt{2}-1} \left((-2+\sqrt{2}) K(m_0) + 2 \frac{\sqrt{2}}{\sqrt{2}+1} E(m_0) \right)$$

Evaluate numerically: $c_6 = 0.514\,706\,537\,019\,658\,0$, $c_7 = 0.202\,328\,904\,291\,161\,5$,

$$c_8 = -1.341\,007\,278\,577\,611 \times 10^{-2}$$

Definitions:

$$c_6 = 0.514\,706\,54$$

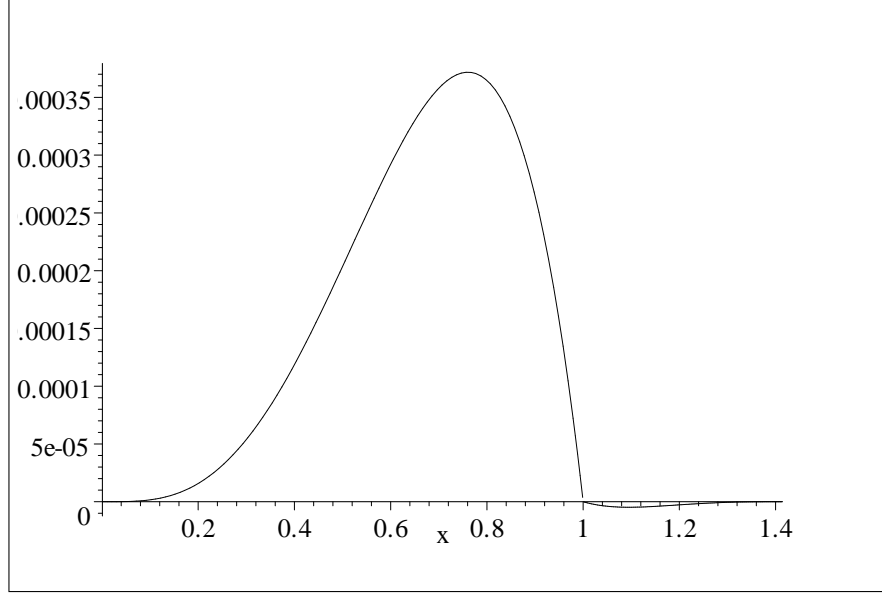
$$c_7 = 0.202\,328\,90$$

$$c_8 = -0.013\,410\,07$$

The relative errors have been estimated by magnifying the following graph, where the functions

$$\frac{\frac{1-x^2}{1+c_4x^2} + \frac{3x^2 \ln(x^2)}{16(1+c_5x^2)}}{\sqrt{x+1} \left(\int_0^{\frac{1}{2}\pi} \sqrt{1-\frac{-x+1}{x+1} \sin^2 \theta} d\theta - x \int_0^{\frac{1}{2}\pi} \frac{1}{\sqrt{1-\frac{-x+1}{x+1} \sin^2 \theta}} d\theta \right)} - 1 \text{ and}$$

$$\frac{-\frac{3\pi}{2^{5/2}} \frac{(x-1)+c_6(x-1)^2}{1+c_7(x-1)+c_8(x-1)^2}}{\sqrt{x+1} \left(\int_0^{\frac{1}{2}\pi} \sqrt{1-\frac{-x+1}{x+1} \sin^2 \theta} d\theta - x \int_0^{\frac{1}{2}\pi} \frac{1}{\sqrt{1-\frac{-x+1}{x+1} \sin^2 \theta}} d\theta \right)} - 1 \text{ are plotted:}$$



Error of Pade approximants (55) and (58).

9 Formulas for $v(y)$ from preceding publications

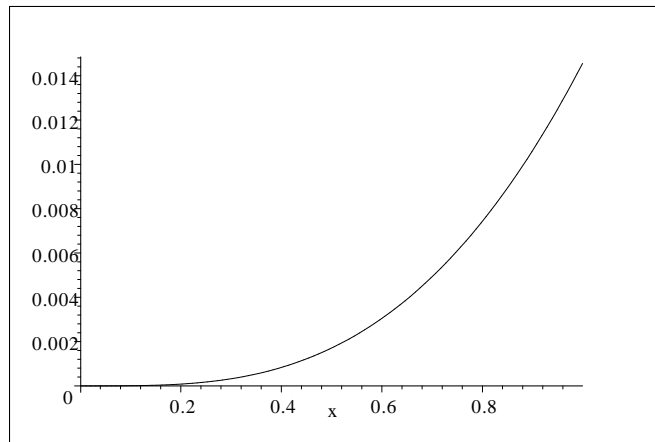
9.1 Hantzsche 1982

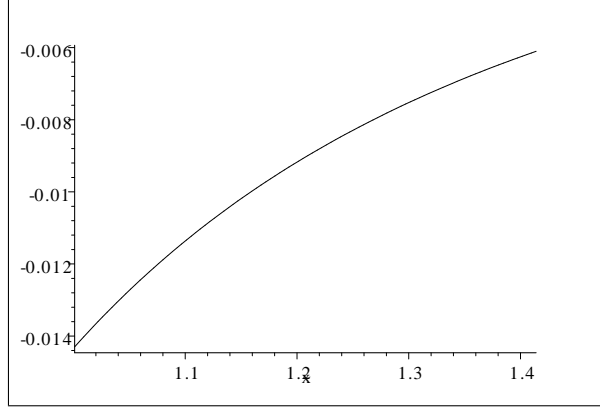
[6], equation (3e):

$$v(y) = \begin{cases} 1 - y^2 (0.9673 - 0.3750 \ln y) - 0.0327 y^4 & \text{for } y \leq 1 \\ -1.3110 y^{3/2} + 0.8986 y^{1/2} + 0.4936 y^{-1/2} - 0.0812 y^{-3/2} & \text{for } y \geq 1 \end{cases} \quad (65)$$

According to [6], the relative error of these formulas $\leq 1.4\%$ in the whole range of y values. My evaluation of this formula confirms this estimate. This is seen from the following graphs, where of the functions

and $\frac{1 - x^2(0.9673 - 0.3750 \ln x) - 0.0327 x^4}{\sqrt{x+1} \left(\int_0^{\frac{1}{2}\pi} \sqrt{1 - \frac{-x+1}{x+1} \sin^2 \theta} d\theta - x \int_0^{\frac{1}{2}\pi} \frac{1}{\sqrt{1 - \frac{-x+1}{x+1} \sin^2 \theta}} d\theta \right)} - 1$
 $\frac{-1.3110 x^{3/2} + 0.8986 x^{1/2} + 0.4936 x^{-1/2} - 0.0812 x^{-3/2}}{\sqrt{x+1} \left(\int_0^{\frac{1}{2}\pi} \sqrt{1 - \frac{-x+1}{x+1} \sin^2 \theta} d\theta - x \int_0^{\frac{1}{2}\pi} \frac{1}{\sqrt{1 - \frac{-x+1}{x+1} \sin^2 \theta}} d\theta \right)}$, respectively, are plotted:





9.2 Forbes 2006

A simple, elegant, and a bit more accurate formula for the range $0 \leq y \leq 1$ was proposed in [3] (see also [11, 12]):

$$v(y) = 1 - y^2 + \frac{1}{3}y^2 \ln y \quad (66)$$

According to [3], this formula, when assessed over the whole range $0 \leq y \leq 1$, has absolute error $< 0.33\%$. My evaluation of this formula confirms this estimate.

Formula (66) can be obtained from (55) by setting $c_4 = c_5 = 0$ and replacing the numerical coefficient $3/16$ in the second term by a slightly smaller coefficient $1/6$. Since absolute values of the coefficients c_4 and c_5 are rather small, $c_4 \approx -3.270 \times 10^{-2}$ and $c_5 \approx -6.612 \times 10^{-2}$, the formulas are not dramatically different.

All the above formulas give $v(1) = 0$, which is the exact value. The derivatives at $y = 1$ are

$$\left. \frac{dv}{dy}(1-0) \right|_{\text{Eq. (65)}} = -1.6904, \quad \left. \frac{dv}{dy}(1-0) \right|_{\text{Eq. (66)}} = -\frac{5}{3}, \quad \left. \frac{dv}{dy}(1+0) \right|_{\text{Eq. (65)}} = -1.6422 \quad (67)$$

The discontinuity in the derivative at $y = 1$ is around 3% if equation (65) is used for both $y \leq 1$ and $y \geq 1$ and around 1.5% if equation (65) is used for $y \geq 1$ and equation (66) is used for $y \leq 1$.

9.3 Jensen 2008

Formula from [13] (last para of Appendix A): $v(y) = 0.93869 - y^2$. The error at $y = 1$ exceeds 6%.

9.4 Jensen 2007

Eq. (18) of [14]:

$$v(y) = \frac{3}{8}y^2 \ln y + (1 - y^2) (1 + y^2 (A_1 - A_2 y^2 + A_3 y^4)) \quad (68)$$

Eq. (17) of [14]:

$$A_1 = \frac{9897}{16384}\pi\sqrt{2} - \frac{85}{32}, \quad A_2 = \frac{5145}{8192}\pi\sqrt{2} - \frac{89}{32}, \quad A_3 = 0.0021112 \quad (69)$$

There is an error in the third equation (17) since $\frac{15}{16384}\pi\sqrt{2} - \frac{15}{16} = -0.9334324191850357 \neq 0.0021112$. Apparently, $A_3 = 0.0021112$ is correct.

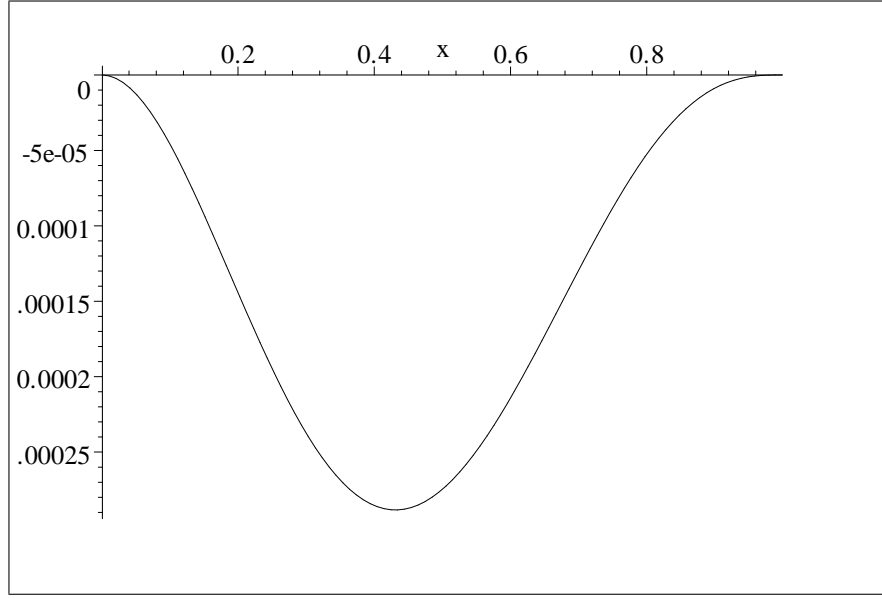
Verification of derivative at $y = 1$: $\left[\frac{3}{8}y^2 \ln y + (1 - y^2)(1 + y^2(A_1 - A_2y^2 + A_3y^4))\right]_{y=1+\varepsilon} - \frac{1}{-\frac{3\pi\sqrt{2}}{8}}$
 $1.000000038105277\varepsilon + O(\varepsilon^2)$

Verification of expansion for small y :

$$(1 - y^2)(1 + y^2(A_1 - A_2y^2 + A_3y^4)) = 1 - 0.9724601782865387y^2 + O(y^4)$$

$$\frac{0.9724601782865387}{\frac{9}{8}\ln 2 + \frac{3}{16}} = 1.005344412809845$$

Plot $\frac{\frac{3}{8}x^2 \ln x + (1-x^2)(1+x^2(A_1 - A_2x^2 + A_3x^4))}{\sqrt{x+1}\left(\int_0^{\frac{1}{2}\pi} \sqrt{1-\frac{-x+1}{x+1}\sin^2\theta} d\theta - x \int_0^{\frac{1}{2}\pi} \frac{1}{\sqrt{1-\frac{-x+1}{x+1}\sin^2\theta}} d\theta\right)} - 1$:



10 NOT USED

$\frac{v(y)}{y^{3/2}}$ on the interval $1 \leq y \leq \sqrt{2}$ to the accuracy of 6% coincides with the first term of its series expansion for $z \rightarrow 0$, which is $-\frac{3\sqrt{2}\pi z}{8}$. Plot $\frac{-3\sqrt{2}\pi x}{8(1-x)^{3/2}v((1-x)^{-1})} - 1$.

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