Lambert W-Function

Problem: $W \cdot e^{W} = x$, find $W(x)$ - ?

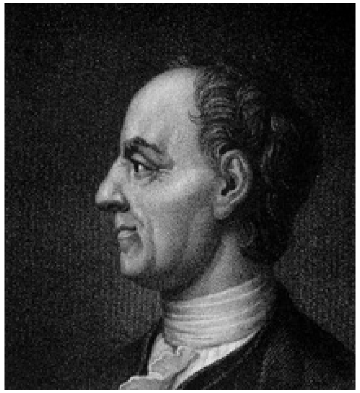
Solution: the *Lambert W-Function*

Lambert W-Function

Ref. :

Lambert, J. H. "Observationes variae in Mathes in Puram." *Acta Helvitica, physico-mathematico-anatomico-botanico-medica* **3**, 128-168, 1758.

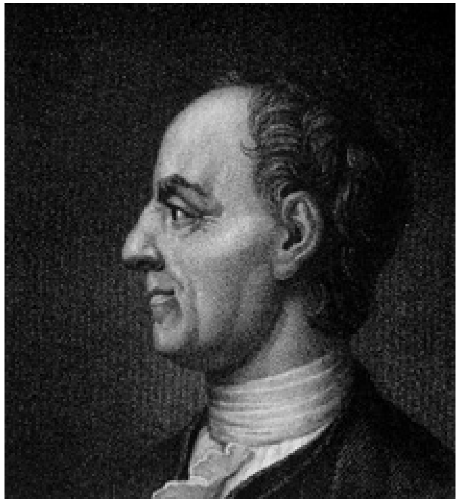
Euler, L. "De serie Lambertina plurimisque eius insignibus proprietatibus." *Acta Acad. Scient. Petropol.* **2**, 29-51, 1783. Reprinted in Euler, L. *Opera Omnia, Series Prima, Vol. 6: Commentationes Algebraicae.* Leipzig, Germany: Teubner, pp. 350-369, 1921.



Lambert W-Function

The Lambert ***W -function***, also called the ***omega function*** or the ***product log*** function , is the inverse function of $W(x)e^{W(x)} = x,$ discovered by:

and



Johann Lambert,

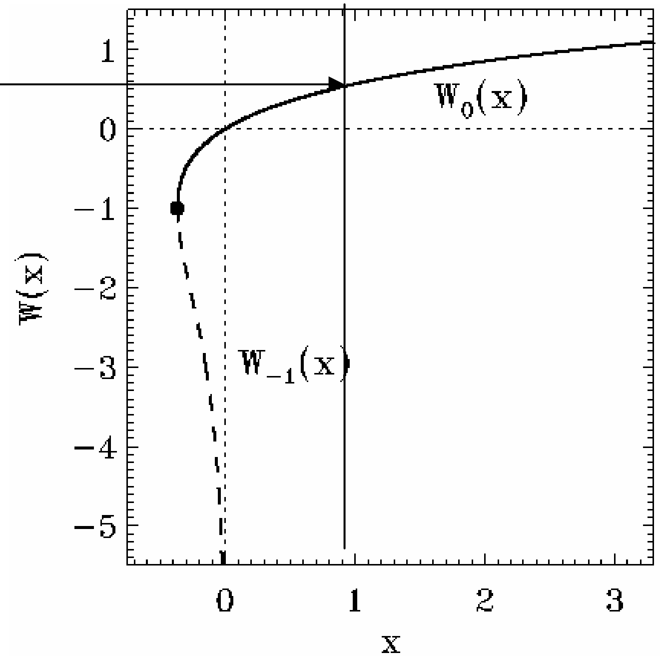
Zurich/Berlin, 1758

Leonhard Euler,

St.-Petersburg Academy Academy of Science, 1783

Lambert W-Function

W(1) = 0.56714 is called the omega constant and can be considered a sort of "golden ratio" of exponents.

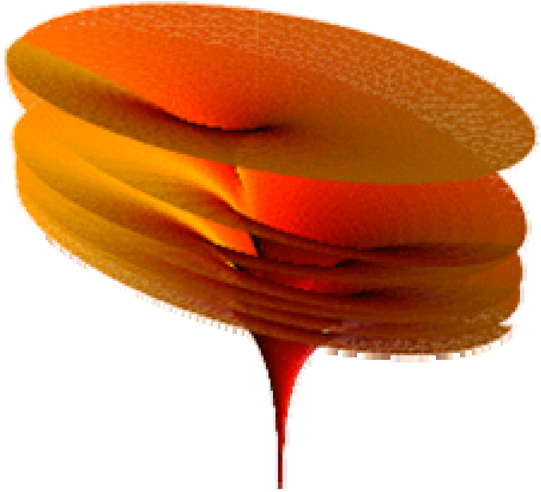


The Lambert W -function has the series expansion!

$$W(x) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1} n^{n-2}}{(n-1)!} x^n = x - x^2 + \frac{3}{2} x^3 - \frac{8}{3} x^4 + \frac{125}{24} x^5 - \frac{54}{5} x^6 + \frac{16807}{720} x^7 + \ldots$$

Lambert W-Function

(x,y) Re: (x,y) Im:



The real (left) and imaginary (right) parts of the analytic continuation of over the complex plane are illustrated above.

Euler, L. "De serie Lambertina plurimisque eius insignibus proprietatibus." *Acta Acad. Scient. Petropol.* **2**, 29-51, 1783. Reprinted in Euler, L. *Opera Omnia, Series Prima, Vol. 6: Commentationes Algebraicae.* Leipzig, Germany: Teubner, pp. 350-369, 1921.

Lambert W-Function

The General Problem : $\ln(A + Bx) + Cx = \ln D$

The General Solution : $x = \dfrac{1}{C} W\left[\dfrac{CD}{B}\exp\left(\dfrac{AC}{B}\right)\right] - \dfrac{A}{B}$

Lambert W-Function has numerous applications:

1) Banwell and Jayakumar (2000) showed that a W-function describes the relation between *voltage, current and resistance in a diode*
2) Packel and Yuen (2004) applied the W -function to a *ballistic projectile* in the presence of air resistance.
3) Other applications have been discovered in:

statistical mechanics, quantum chemistry, combinatorics, enzyme kinetics,

physiology of vision, engineering of thin films, hydrology,

analysis of algorithms (Hayes 2005) , and solar wind.

Lambert W-Function

The Isothermal Solar Wind Problem :

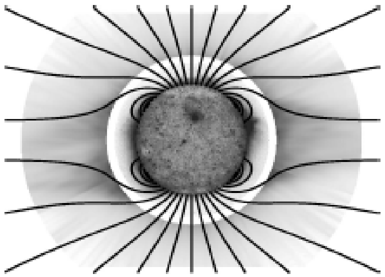


Fig. 1. The solar corona on 17 August 1996, with bright regions plotted as dark. The inner image was taken by the EIT (Extreme-ultraviolet Imaging Telescope) instrument on Solar and Heliospheric Observatory (SOHO), and is sensitive to the ultraviolet emission of Fe^{+11} ions at temperatures of about 10^6 K. The outer image was taken by the UVCS (Ultraviolet Coronagraph Spectrometer) instrument on SOHO by blocking out the bright disk to see the much dimmer ultraviolet emission of O^{+5} ions at temperatures exceeding 10^8 K. The magnetic field lines are from a model of the corona at the minimum of its 11 year activity cycle (Ref. 32).

$$(v^2 - a^2) - a^2 \ln\left(\frac{v^2}{a^2}\right) = 4a^2 \ln\left(\frac{r}{r_c}\right) + 2GM_\odot\left(\frac{1}{r} - \frac{1}{r_c}\right)$$

where v is the outflow velocity of the wind, which is the quantity we wish to solve for, r is the distance (measured here from the center of the Sun), a is the speed of sound in the outer solar atmosphere, which is proportional to the temperature of the gas, and which we assume to be constant. Also, r_c is the so-called ``Parker critical-point distance'' where the wind accelerates past the sound speed:

$$r_c = \frac{GM_\odot}{2a^2}$$

$$v = \begin{cases} a\sqrt{-W_0(-f)}\ , & \text{if } r \le r_c \\ a\sqrt{-W_{-1}(-f)}\ , & \text{if } r \ge r_c \end{cases} \qquad f = \left(\frac{r_c}{r}\right)^4 \exp\left[4\left(1 - \frac{r_c}{r}\right) - 1\right]$$

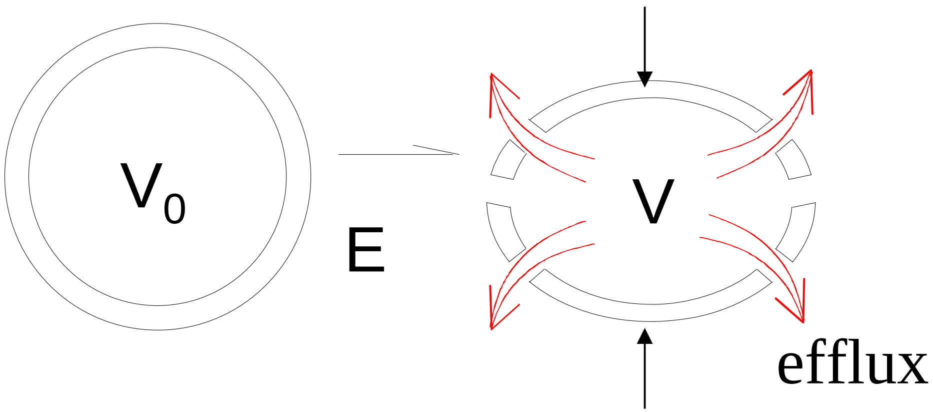
Steven R. Cranmer, **New views of the solar wind with the Lambert W function,** Am. J. Phys., 2005, Vol. 72, No. 11, 1397-1403.

Some applications of the Lambert W Function to Physical Chemistry

1) The kinetics of the electromechanical vesicle elongation

Kakorin, S. and Neumann, E. (1998) Kinetics of the electroporative deformation of lipid vesicles. *Ber. Bunsenges. Phys. Chem.* 102: 670-675.

Kakorin, S., Redeker, E. and Neumann, E. (1998) Electroporative deformation of salt filled vesicles. *Eur. Biophys. J.* 27: 43-53.



Cell volume $V_0 > V$

Some applications of the Lambert W Function to Physical Chemistry

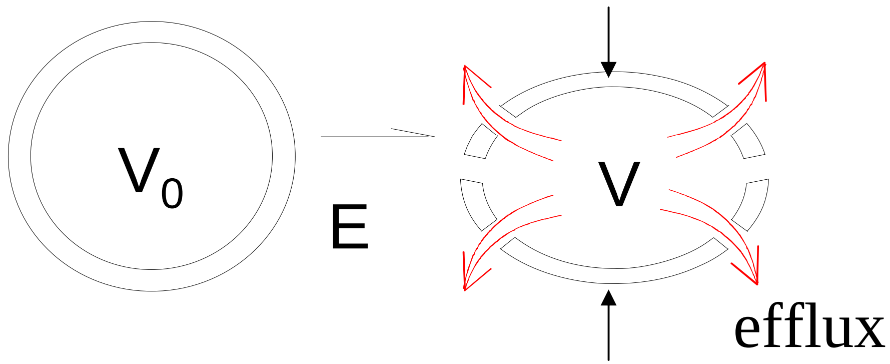
1) The kinetics of the electromechanical vesicle elongation

$$\frac{d\Delta V}{dt} = -\frac{3\pi \cdot r_p^4 \cdot N_p}{160 \cdot d \cdot \eta}\left(\varepsilon_0 \cdot \varepsilon_w \cdot E^2 - 32 \cdot \kappa \cdot \sqrt{\frac{-\Delta V}{\pi a^9}}\right)$$

$$\Delta V(t=0) = 0$$

$$\Delta V(t) = -\pi a \cdot \left(\frac{m}{n}\right)^2 \cdot \left\{1 + \mathrm{LambertW}\left[-\frac{1}{m} \cdot \exp[\frac{n^2}{m} \cdot (C-t) - 1]\right]\right\}^2$$

$$m = \frac{3}{320} \cdot \frac{\varepsilon_0 \cdot \varepsilon_w \cdot E^2 \cdot N \cdot r_p^4}{d \cdot \eta \cdot a} \qquad n = \frac{3}{10} \cdot \frac{N \cdot r_p^4 \cdot \kappa \cdot (1 - \bar{c}_0 / 6)}{d \cdot \eta \cdot a^5} \qquad C = (m/n^2) \cdot \ln|m|$$



Cell volume $V_0 > V$

Some applications of the Lambert W Function to Physical Chemistry

2) Conductivity of electroporated lipid bilayer membranes

Kakorin, S. and Neumann, E. (2002) Ionic conductivity of electroporated lipid bilayer membranes, Bioelectrochem., 56: 163-166.

Griese, T., Kakorin, S. and Neumann, E. (2002) Conductometric and electrooptic relaxation spectrometry of lipid vesicle electroporation at high fields, *Phys. Chem. Chem. Phys.* 4: 1217-1227.

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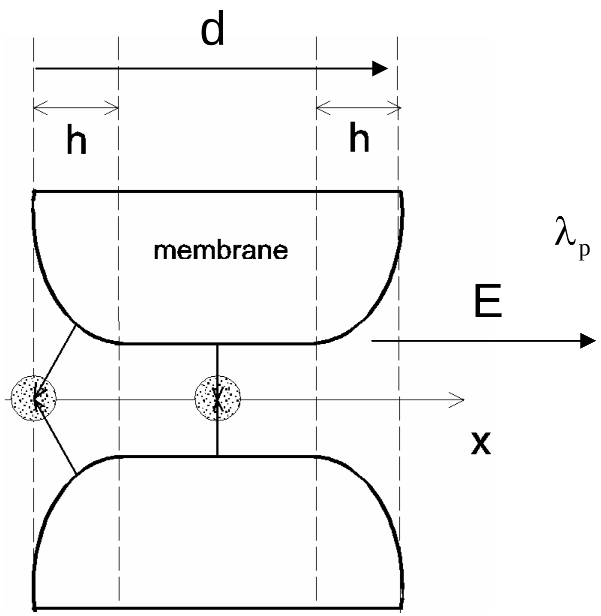

$$\lambda_p = \frac{F^2 \cdot D \cdot \left(c(0) + c(d)\right)}{RT} \cdot \exp\left[\left((1 - \frac{RT}{F \cdot \varphi_{im}^0}) \cdot \frac{h}{d} \cdot |\Delta\varphi| - \varphi_{im}^0\right) \cdot \frac{F}{RT}\right]$$

Some applications of the Lambert W Function to Physical Chemistry

2) Conductivity of electroporated lipid bilayer membranes

Integrated Nernst-Planck equation for the membrane conductivity:

$$\lambda_p = \lambda^0 \cdot \exp\left[\left(\alpha \cdot n \cdot |\Delta\varphi_0| \cdot (1-\lambda_p \cdot f_p \cdot \frac{a}{2d\lambda_{ex}}) - \varphi_{im}^0\right) \cdot \frac{F}{RT}\right]$$

$\lambda^0 = F^2 \cdot D \cdot \left(c(0)+c(d)\right)/RT$ $\alpha = (1 - RT/(F\varphi_{im}^0))$ n = h / d

,

Solution:

$$\lambda_p = \beta \cdot \lambda_{ex} \cdot \mathrm{LambertW}\left(\frac{\lambda^0}{\beta \cdot \lambda_{ex}} \exp\left[\frac{F \cdot (\sqrt{3} \cdot \alpha \cdot a \cdot E \cdot n/2 - \varphi_{im}^0)}{RT}\right]\right)$$

$\beta = 4 \cdot d^2 \cdot RT/(F \cdot \sqrt{3} \cdot \alpha \cdot a \cdot E \cdot h)$

Lambert W-Function

2) Enzyme Kinetics:

A.R. Tzafriri, E.R. Edelman, **The total quasi-steady-state approximation is valid for reversible enzyme kinetics**,
Journal of Theoretical Biology 226 (2004) 303–313.

A.R. Tzafriri, **Michaelis–Menten Kinetics at High Enzyme Concentrations,**
Bulletin of Mathematical Biology (2003) **65**, 1111–1129.

S. Schnell and C. Mendoza,
Enzyme kinetics of multiple alternative substrates,
Journal of Mathematical Chemistry 27 (2000) 155–170.

Lambert W-Function

Das Michaelis-Menten-Modell:
(Enzym - Reaktion mit einem Fließgleichgewicht)

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} (ES) \xrightarrow{k_{cat}} E + P$$

Enzym - Substrat – Komplex

Die Nährung des fluss-stationären Zustandes:

$$\frac{d[(ES)]}{dt} = \underset{\text{Bildung aus E und S}}{k_1 \cdot [E] \cdot [S]} - \underset{\text{Zerfall in E und S}}{k_{-1} \cdot [(ES)]} - \underset{\text{Zerfall in P}}{k_{cat} \cdot [(ES)]} = 0$$

$$k_1 \cdot [E] \cdot [S] = (k_{-1} + k_{cat}) \cdot [(ES)]$$

Michaelis-Menten-Modell

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} (ES) \xrightarrow{k_{cat}} E + P$$

$$k_1 \cdot [E] \cdot [S] = (k_{-1} + k_{cat}) \cdot [(ES)]$$

Die Gesamtkonzentration an Enzym ist konstant:

$$[E]_0 = [E] + [(ES)]; \quad [E] = [E]_0 - [(ES)] = \text{const.}$$

Nach der Umformung: $k_1 \cdot ([E]_0 - [(ES)]) \cdot [S] = (k_{-1} + k_{cat}) \cdot [(ES)]$

$$k_1 \cdot [E]_0 \cdot [S] = (k_{-1} + k_{cat}) \cdot [(ES)] + k_1 \cdot [S] \cdot [(ES)] = (k_{-1} + k_{cat} + k_1 \cdot [S]) \cdot [(ES)]$$

$$K_M \equiv \frac{k_{cat} + k_{-1}}{k_1}$$ (M = mol/L, Michaelis – Konstante)

$$[(ES)] = \frac{k_1 \cdot [E]_0 \cdot [S]}{k_{-1} + k_{cat} + k_1 \cdot [S]} = \frac{[E]_0 \cdot [S]}{\frac{k_{-1} + k_{cat}}{k_1} + [S]} = \frac{[E]_0 \cdot [S]}{K_M + [S]}$$

Michaelis-Menten-Modell

Die Bildungsgeschwindigkeit des Produktes:

$$v = \frac{d[P]}{dt} = k_{cat} \cdot [(ES)] = k_{cat} \cdot [E]_0 \cdot \frac{[S]}{K_M + [S]} = k_{cat} \cdot [E]_0 \cdot \frac{[S_0] - [P]}{K_M + [S_0] - [P]}$$

$$v_0 = k_{cat} \cdot [E]_0 \cdot \frac{[S_0]}{K_M + [S_0]}; \quad [P(t=0)] = 0 \quad ???$$