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► **To cite this version:**

François Dubois, Olivier Lafitte, Clair Poignard. Analytic solutions of two problems of Biology and Physics using the Jacobi elliptic functions. 16th International Symposium on Orthogonal Polynomials, Special Functions and Applications, Centre de recherches Mathématiques, Jun 2022, Montréal, Canada. hal-04004709

HAL Id: hal-04004709

<https://hal.science/hal-04004709>

Submitted on 25 Feb 2023

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Analytic solutions of two problems of Biology and Physics using the Jacobi elliptic functions

Francois Dubois, Olivier Lafitte, Clair Poignard

LE CNAM-Université Sorbonne Paris Nord (LAGA)-IRL-CRM-CNRS, Centre de Recherches Mathématiques (U de Montréal)-Inria Bordeaux Sud Ouest

June 17th, 2022

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Coupling thermohydraulics and neutronics (O.L., F. Dubois *et al*)

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Special functions in this presentation

Jacobi elliptic function

$$F_m(\varphi) = \int_0^\varphi \frac{d\theta}{\sqrt{1 - m \sin^2 \theta}}$$

Modified Jacobi elliptic function

$$K_m(\varphi) = \int_0^\varphi \sqrt{1 - m \sin^2 \theta} d\theta.$$

Solutions of $(y')^2 = R(y)$, R rational function.

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Model coupling the electrostatic potential and the distribution of ions

In Ω : ρ_k is the concentration of ions of species k , of valence z_k , ψ is the electrostatic potential, e is the charge of the proton, ε_s is the dielectric constant of the cell, k_b is the Boltzmann constant and T is the temperature:

$$\begin{cases} -\nabla_x \cdot \left(D_k \left(\nabla_x \rho_k + \frac{e z_k}{k_b T} \rho_k \nabla_x \psi \right) \right) = 0 \\ -\nabla_x \cdot (\varepsilon_s \nabla_x \psi) = e \sum_k z_k \rho_k \end{cases}$$

Inhomogeneous Dirichlet boundary condition for the potential on $\partial\Omega$ and no flux condition for each species of ions.

Reduction to a 1D model: $\Omega = [-L, L]$. Boundary conditions

- for the potential: $\psi(\pm L) = \pm\psi_D$
- for the concentration of ions: $(\rho'_k + \frac{e z_k}{k_b T} \rho_k \psi')(\pm L) = 0$.

Reduction of the model to a single ODE

For ion concentrations $\rho_k(x) = \rho_k(-L)e^{-\frac{ez_k}{k_b T}\psi(x)}$.

Electrostatic equation:

$$-\psi'' = \frac{e}{\varepsilon_s} \sum_k z_k \rho_k(-L) e^{-\frac{ez_k}{k_b T}\psi(x)}.$$

Notation $\varphi(X) = \frac{e}{k_b T}\psi(XL)$, $X \in [-1, 1]$. Equation

$$-\varphi'' = \frac{e^2 L^2}{k_b T \varepsilon_s} \sum_k z_k \rho_k(-L) e^{-z_k \varphi}.$$

Number of ions of each species given

$$n_k = \int_{-L}^L \rho_k(-L) e^{-\frac{ez_k}{k_b T}\psi(x)} dx \Leftrightarrow \rho_k(-L) = \frac{n_k}{\int_{-L}^L e^{-\frac{ez_k}{k_b T}\psi(x)} dx}.$$

Reduction to a elliptic equation

Equation: $-\varphi'' = \frac{e^2 L}{k_b T \varepsilon_s} \sum_k n_k z_k \frac{e^{-z_k \varphi}}{\int_{-1}^1 e^{-z_k \varphi(X)} dX}$. Boundary conditions $\varphi(\pm 1) = \pm \varphi_D$.

Lemma

This problem has a unique solution in $H^1([-1, 1])$.

Proof: one observes that it is the Euler equation for

$$J(\varphi) = \int_{-1}^1 \frac{1}{2} [(\varphi'(X))^2 + \frac{e^2 L}{k_b T \varepsilon_s} \sum_k n_k \ln(\int_{-1}^1 e^{-z_k \varphi(X)} dX)] dX.$$

$$\frac{1}{2}(\varphi')^2 - \frac{1}{2}(\varphi'(X_0))^2 = \frac{e^2 L}{k_b T \varepsilon_s} \sum_k n_k \frac{e^{-z_k \varphi} - e^{-z_k \varphi(X_0)}}{\int_{-1}^1 e^{-z_k \varphi(X)} dX}. \quad (1)$$

$f(X) = e^{-\varphi(X)}$ yields $(f')^2 = (\varphi')^2 f^2 \Rightarrow (f')^2 = R(f)$, where R is a rational fraction \Rightarrow elliptic equation.

First application: the electroneutral case for two species of ions $z_k = \pm 1$

Notation $n_+ = n_- = n$ and introduce $\alpha = \frac{e^2 L n}{k_b T \epsilon_s}$. Equation

$$-\varphi'' = \alpha \left[\frac{e^{-\varphi}}{\int_{-1}^1 e^{-\varphi(X)} dX} - \frac{e^{\varphi}}{\int_{-1}^1 e^{\varphi(X)} dX} \right].$$

One proves φ odd. Thanks to

$$\int_{-1}^1 e^{-\varphi(X)} dX = \int_{-1}^1 e^{\varphi(X)} dX = 2 \int_0^1 e^{-\varphi(X)} dX, \text{ reduce the}$$

equation on $(0, 1)$ to

$$(f')^2 = 2f^2 \alpha \frac{f+f^{-1}-2K}{\int_{-1}^1 e^{-\varphi(X)} dX} = \beta f(f^2 - 2Kf + 1),$$

$$\beta = \frac{2\alpha}{\int_{-1}^1 e^{-\varphi(X)} dX}, \quad K = 1 - \frac{(\varphi'(0))^2}{2\beta} < 1, \quad f(0) = 1, \quad f(1) = e^{-\varphi_D}.$$

$$\int_1^{e^{-\varphi(X)}} \frac{df}{\sqrt{f(f^2 - 2Kf + 1)}} = \sqrt{\beta} X. \quad (2)$$

Equations for determining β and K :

$$\int_1^{e^{-\varphi_D}} \frac{df}{\sqrt{f(f^2 - 2Kf + 1)}} = \sqrt{\beta}, \quad \int_1^{e^{-\varphi_D}} \frac{fdf}{\sqrt{f(f^2 - 2Kf + 1)}} = \frac{\alpha}{\sqrt{\beta}}.$$

Expression of the solution

Case $K < -1$. Polynomial $f(f + q)(f + \frac{1}{q})$, $q > 1$. New unknown

$$\sin^2 \varphi = \frac{e^{-\varphi(X)}}{e^{-\varphi(X)} + \frac{1}{q}}, \text{ new variable } \sin^2 \theta = \frac{f}{f + \frac{1}{q}} = 1 - \frac{1}{q} \frac{1}{f + \frac{1}{q}},$$

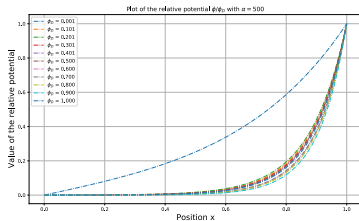
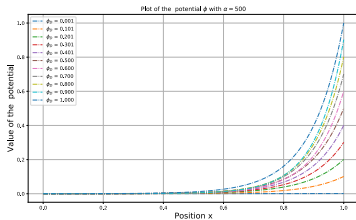
$$2 \sin \theta \cos \theta d\theta = \frac{1}{q} \frac{df}{(f + \frac{1}{q})^2}, \quad \cos^2 \theta = \frac{1}{q} \frac{1}{(f + \frac{1}{q})^2},$$

$$f(f + q)(f + \frac{1}{q}) = \frac{1}{q^2} \frac{\sin^2 \theta}{\cos^6 \theta} (q + (\frac{1}{q} - q) \sin^2 \theta).$$

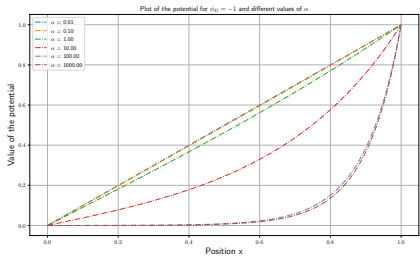
With $m = 1 - \frac{1}{q^2}$

$$\frac{df}{\sqrt{f(f + q)(f + \frac{1}{q})}} = \frac{2}{\sqrt{q}} \frac{d\theta}{\sqrt{1 - m \sin^2 \theta}},$$

$$F_m(\arcsin \sqrt{\frac{e^{-\varphi(X)}}{e^{-\varphi(X)} + \frac{1}{q}}}) - F_m(\arcsin \sqrt{\frac{1}{1 + \frac{1}{q}}}) = \sqrt{\beta} X \quad (3)$$



Boundary layer on the potential near the charged interface.
The potential in the Gouy-Chapman-Stern is described exactly.



Boundary layer on the potential near the charged interface.
 The potential in the Gouy-Chapman-Stern is described exactly.

Second application: the non electroneutral case for two species of ions $z_k = \pm 1$

With $\varphi_D = 0$, $n_+ \neq n_-$, **one proves that** the function φ is even, has its maximum (or its minimum) at $X = 0$ according to the sign of $n_+ - n_-$. Equation ($f_0 = e^{-\varphi(0)} := e^{-\varphi_0}$)

$$(f')^2 = 2\alpha f^2 \left[\beta_- \left(\frac{1}{f} - \frac{1}{f_0} \right) + \beta_+ (f - f_0) \right],$$

with $\beta_- = \frac{n_-}{\int_{-1}^1 f(X) dX}$, $\beta_+ = \frac{n_+}{\int_{-1}^1 f^{-1}(X) dX}$. Need three equations for

f_0, β_-, β_+ . Introduce $f_1 = \frac{\beta_+}{\beta_- f_0}$. Equation

$$(f')^2 = 2\alpha \beta_+ f_0^{-1} f (f - f_0) (f - f_1) = K^2 f (f - f_0) (f - f_1).$$

Two cases: $f_1 < f_0$ (f_0 is the point of minimum of f) or $f_1 > f_0$ (f_0 is the point of maximum of f).

Solution ($0 < f_1 < f_0$, $m_0 f_0 = f_1$)

$$K|X| = \int_{f_0}^{e^{-\varphi(X)}} \frac{df}{\sqrt{f(f-f_0)(f-m_0 f_0)}}$$

Conditions for the three constants ($K^2 f_0 = 2\alpha\beta_+$):

$$\begin{cases} K = \int_{f_0}^1 \frac{df}{\sqrt{f(f-f_0)(f-m_0 f_0)}}, \\ Kn_+ = 2\beta_+ \int_{f_0}^1 \frac{f df}{\sqrt{f(f-f_0)(f-m_0 f_0)}}, \\ Kn_- = 2\beta_- \int_{f_0}^1 \frac{df}{f \sqrt{f(f-f_0)(f-m_0 f_0)}}. \end{cases}$$

Change of variable in the integral $\sin^2 \varphi = \frac{f-f_0}{f-m_0 f_0}$

$$K|X| = 2(1-m_0)f_0^{\frac{1}{2}} F_{m_0}(\arcsin \sqrt{\frac{e^{-\varphi(X)} - f_0}{e^{-\varphi(X)} - m_0 f_0}}). \quad (4)$$

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The coupled 1d model

Diffusion equation for the neutrons: density of probability $\Phi(z, t)$ of neutrons in $[0, L]$ at time t (h : enthalpy (temperature), V : velocity of neutrons)

$$\frac{1}{V} \partial_t \Phi - \partial_z (D(h) \partial_z \Phi) + \Sigma_a(h) \Phi = \Sigma_f(h) \Phi$$

Boundary conditions: $\Phi(0, t) = 0, \Phi(L, t) = 0$. Condition on the density $\int_0^L \Phi(z, 0) dz = 1$.

Classical analysis: $\Phi(z, t) = e^{t\tau} \varphi(z)$. Sign of τ important.

Equation on φ

$$-\frac{d}{dz} (D(h) \frac{d\varphi}{dz}) + \Sigma_a(h) \varphi = (\Sigma_f(h) - \frac{\tau}{V}) \varphi$$

Definition $k_{eff} = \frac{\Sigma_f(h)}{\Sigma_f(h) - \frac{\tau}{V}}$. Eigenvalue problem:

$$\begin{cases} -\frac{d}{dz} (D(h) \frac{d\varphi}{dz}) + \Sigma_a(h) \varphi = \frac{\Sigma_f(h)}{k_{eff}} \varphi, \\ \varphi(0) = \varphi(L) = 0. \end{cases}$$

Coupled with the production of enthalpy $h' = Q \Sigma_f(h) \varphi$.

Coupled problem and its integration

$$\text{Nonlinear system} \begin{cases} -\frac{d}{dz}(D(h)\frac{d\varphi}{dz}) + \Sigma_a(h)\varphi = \frac{\Sigma_f(h)}{k_{eff}}\varphi, \\ h' = Q\Sigma_f(h)\varphi, \\ \varphi(0) = \varphi(L) = 0, \\ h(0) = h_e, h(L) = h_s. \end{cases}$$

Four boundary conditions, problem of order 3: yields $k_{eff} := \lambda^{-1}$.

Exact integration

$$-\frac{d}{dz}(D(h)\frac{d\varphi}{dz}) + \left(\frac{\Sigma_a(h)}{\Sigma_f(h)} - \lambda\right)\frac{h'}{Q} = 0$$

$$-D(h)\frac{d\varphi}{dz} + \frac{F(h) - \lambda h + C_0}{Q} = 0$$

$$-\frac{d\varphi}{dz}\varphi + \frac{F(h) - \lambda h + C_0}{\Sigma_f(h)D(h)Q^2}h' = 0$$

Finally (with $X(h_e) = X(h_s) = Y(h_e) = Y(h_s) = 0$)

$$-Q^2\frac{\varphi^2}{2} + X(h) - \lambda Y(h) = 0 \Rightarrow (h')^2 = R(h). \quad (5)$$

When Σ_a, Σ_f and D are known only at given points

$h_i, 1 \leq i \leq p$, R is a rational fraction: elliptic integrals again.

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First example: $X(h) \simeq (h - h_e)(h_s - h)(a_X h + b_X)$,
 $Y(h) \simeq (h - h_e)(h_s - h)(a_Y h + b_Y)$.

Obtain a_X, a_Y, b_X, b_Y by projection of solutions of certain ODEs.

$$(h')^2 = \mu^2 (h - h_e)(h_s - h)((a_X - \lambda a_Y)h + (b_X - \lambda b_Y)).$$

New unknown $h(z) = h_e + (h_s - h_e) \sin^2 \theta(z)$, $\theta(0) = 0, \theta(L) = \frac{\pi}{2}$:

$$(\theta'(z))^2 = \frac{\mu^2}{4} [(a_X - \lambda a_Y)h_e + (b_X - \lambda b_Y) + (a_X - \lambda a_Y)(h_s - h_e) \sin^2 \theta(z)].$$

Define $m(\lambda) = -\frac{(a_X - \lambda a_Y)(h_s - h_e)}{(a_X - \lambda a_Y)h_e + (b_X - \lambda b_Y)}$. Equality

$$\int_0^{\theta(z)} \frac{d\theta}{\sqrt{1 - m \sin^2 \theta}} = \frac{\mu}{2} \sqrt{(a_X - \lambda a_Y)h_e + (b_X - \lambda b_Y)} z. \quad (6)$$

Equation for determining λ :

$$F_{m(\lambda)}\left(\frac{\pi}{2}\right) = \frac{\mu}{2} \sqrt{(a_X - \lambda a_Y)h_e + (b_X - \lambda b_Y)} L.$$

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New unknown $h(z) = h_e + (h_s - h_e) \sin^2 \theta(z)$, $\theta(0) = 0, \theta(L) = \frac{\pi}{2}$:

$$(\theta'(z))^2 = \frac{\mu^2}{4} [(a_X - \lambda a_Y)h_e + (b_X - \lambda b_Y) + (a_X - \lambda a_Y)(h_s - h_e) \sin^2 \theta(z)].$$

Define $m(\lambda) = -\frac{(a_X - \lambda a_Y)(h_s - h_e)}{(a_X - \lambda a_Y)h_e + (b_X - \lambda b_Y)}$. Equality

$$\int_0^{\theta(z)} \frac{d\theta}{\sqrt{1 - m \sin^2 \theta}} = \frac{\mu}{2} \sqrt{(a_X - \lambda a_Y)h_e + (b_X - \lambda b_Y)} z. \quad (6)$$

Equation for determining λ :

$$F_{m(\lambda)}\left(\frac{\pi}{2}\right) = \frac{\mu}{2} \sqrt{(a_X - \lambda a_Y)h_e + (b_X - \lambda b_Y)} L.$$

Second example (joint work with F. Dubois):

$$D = 1, \Sigma_a = 1, \Sigma_f \text{ known at three values } h_1, h_2, h_3$$

Possible choice of solutions for the coupled problem

1. Σ_f interpolation polynomial of degree 2 $\rightarrow Y$ polynomial of degree four \rightarrow elliptic function as solutions (see A-S formulae 17.4.41 to 17.4.57), after transformation of the polynomial to $(t^2 - a^2)(b^2 - t^2)$ or $(a^2 - t^2)(t^2 + b^2)$ by homographic transform of the roots of Y into $\pm a, \pm b$ or $\pm a, \pm ib$.
2. Σ_f continuous, piecewise linear on intervals $[h_e, h_1], [h_1, h_2], [h_2, h_3], [h_3, h_s] \rightarrow Y \in C^1$ piecewise cubic polynomial h piecewise an inverse incomplete elliptic function.

In the first case, equation on λ of the form $F_{m(\lambda)}(g(\lambda)) = L$.

In the second case, one has a more complicated equation.

Main result for applications: the values of λ are quite different, though the solutions are extremely similar.

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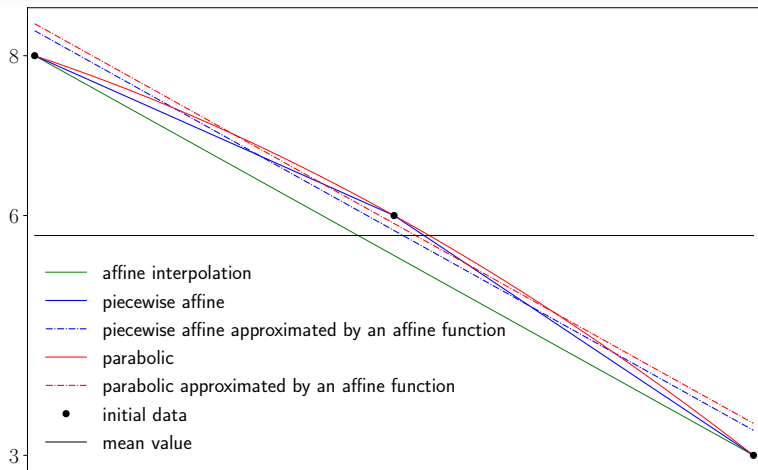


Figure: Function $h \mapsto \Sigma(h)$.

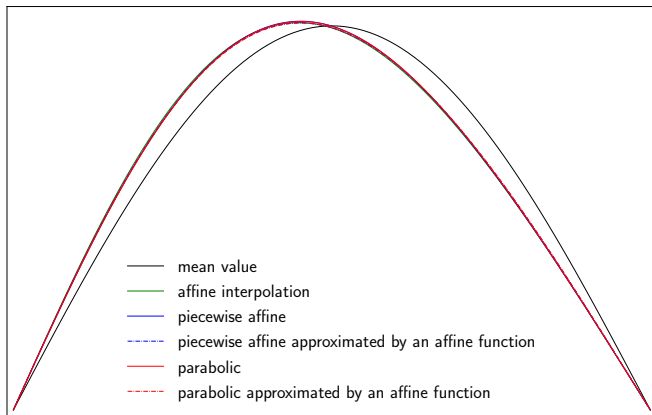
φ and λ 

Figure: Functions $z \mapsto \varphi(z) : \lambda$:
1.01722, 1.07373, 1.0043, 1.01991, 1, 01507.

Contents

Potential in a cell generated by a density of ions (O.L.-C. Poignard)

Coupling thermohydraulics and neutronics (O.L., F. Dubois *et al*)

Why it is interesting to have analytic formulae and special functions?

Why does one need analytic formulae?

- Quick and accurate calculations and graphical representation thanks to the presence of the special functions in packages.
- In the study of the potential inside a cell: link with models of exchanges of ions: dependency in terms of L and of φ_D or of number of ions.
- Uncertainty and sensitivity analysis (one has a dependency on parameters, n and L in the case of the first problem, n_-, n_+, L in the case of the second problem, given values of $D(h), \Sigma_a(h), \Sigma_f(h)$ in the third problem)