Advanced Engineering Forum *Online: 2013-06-27*
ISSN: 2234-991X, Vols. 8-9, pp 405-412
doi:10.4028/www.scientific.net/AEF.8-9.405

A geometric approach to a battery electrochemical model using specific tools from the Poisson geometry.

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Keywords: energy monitoring; battery models; differential geometry.

Abstract. Through this paper is presented a geometric approach of a battery electrochemical model using specific tools from the Poisson geometry.

Introduction

The area of remote sensing and controlling based on smart wireless sensors, is currently facing a trend from specific, highly customized applications, toward generic applications tailored for the use of a more general public. The new wireless motes are able to concurrently handle a variety of sensing units, but their flexibility is increasing the energy consumption and inevitable, the lifetime of the wireless sensors network will decrease dramatically when the motes will be equipped with several energy hungry sensors, as there is a limited energy that batteries can deliver. To overcome these limitations, different approaches are required for energy optimization like dynamic voltage and/or frequency scaling, powering off the sensing modules for the time intervals when they are not used, dynamic scaling of the radio transceiver power to limit the range of the transmitted signal to the actual communication partners and not waste energy, etc.

In this context, we are working on the energy optimization in wireless sensor networks through online monitoring of the energy consumption at a node level and runtime accounting of the battery state-of-charge based on accurate battery models. The mathematical models of battery are generally used in wireless sensor networks simulations or during the design and development phases of these networks for life-time estimation, to analyze the impact of various strategies on energy consumption, for sizing the batteries in terms of price and performance at the application level. A less common usage of the battery mathematical models is for online battery state-of-charge monitoring even though it was proven that using the battery state-of-charge information in decision making can lead to an extended network lifetime of three times than the case in which decisions are taken on the basis of probabilities [1].

There are several types of battery models available, each being characterized by a different accuracy – computational effort ratio. Differences between the actual battery models arise from the way in which the battery parameters are taken into account: the physical characteristics of the batteries (like material of the electrodes, electrolyte and separator, the size and the geometry of these electrodes, the distance between them and the internal resistance), the variations of load and of the temperature, etc.

Some other aspects that are covered by the battery mathematical models are related to the real batteries behavior like self-discharge (effect caused by internal resistance of the battery, as a reduction of the state-of-charge over time even when no load is connected), relaxation effect (at very low consumption rates, the concentration of electrons became homogeneous by the electrons diffusion across the electrolyte, this behavior being seen from outside the battery as a partial recovery of the capacity), rate capacity effect (at high consumption rates, the effective battery capacity is lower than the rated capacity, due to the poor electrons concentration in the area surrounding the electrodes as the electrons diffusion in the electrolyte is performed at a much lower rate than consumption rate), temperature effect (at higher temperatures, the reduction-oxidation electrochemical reactions are accelerated) and capacity fading (it is the battery aging when increasing number of charge-discharge cycles, as the reverse reaction is induced for a smaller amount of active material). Therefore, there are battery linear models (the worst precision but the best computational effort required as the actual battery capacity is obtained by extracting the consumed energy from a nominal value), stochastic models (are obtained based on observations and simulations that are calibrated with experimental data), electrical models (based on electrical circuit with an equivalent behavior as that of batteries), analytic models (are obtained, in general, as simplifications of electrochemical models and are less accurate, but involves less computational effort) and electrochemical models which are the most accurate battery models, being taken as reference for validation of other battery models.

The electrochemical models are based on systems of differential equations that describe the physical and chemical processes occurring at the anode, cathode and separator. As the solutions of these models are very close to the real system behavior, we took these models as the basis in our attempt to obtain a model which implies a computational effort similar to the electric battery models based on characteristic tables but with precision very close to the electrochemical models. In other words, our goal is to obtain interpolation tables similar to the characteristic tables using exclusively an analytic approach in order to preserve the models precision, as opposed to the actual characteristic tables that are obtained experimentally. To achieve this goal, we are using the tools offered by the differential geometry, analyzing the battery electrochemical models as Hamilton-Poisson systems.

To ease the battery models analysis it is necessary to represent the solution of the Hamilton-Poisson system as an intersection of two surfaces in a three dimensional space. As the number of parameters used in the electrochemical battery models is quite large, and we need to obtain the variation in time of the state-of-charge based on terminal voltage, temperature and load, while not all the combinations between these variables will admit a Hamilton-Poisson realization, it is necessary to obtain as much as possible combinations of variables that will conduct to such systems with exact solutions. The next step is to extract the battery characteristics using the previously obtained solutions and finally, the model implementation on battery powered devices with high computational constraints. This paper is part of the first step in this achievement, by presenting some of the Hamilton-Poisson realizations for a Lithium-ion electrochemical model. The previous results in this stage are presented in [2,3,4,5].

In this paper we consider a special case of the Li-ion battery system derived from the model presented in [6,7]. In one particular case we write the system as a Hamiltonian system of Poisson type. More exactly, we write the Li-ion battery system as a Hamilton-Poisson system, and also find a SL(2, **R**) parameterized family of Hamilton-Poisson realizations.

In the last part of the article we give a Lax formulations of the system. For details on Poisson geometry and Hamiltonian dynamics see e.g. [8,9,10,11]..

Hamilton-Poisson realizations of a Li-ion battery system

The Li-ion battery system that was considered for this study is derived from the equations given in [6,7] where

$$= \quad + \quad , \; x_1(q) = n_{Li}, \quad x_2(q) = \nabla n_{Li}, \quad x_3(q) = \nabla \varphi, \qquad (1)$$

with u,v real parameters.

It is governed by the equations:

$$\begin{cases} \dot{x_1} = x_2 \\ \dot{x_2} = \frac{x_2 - b\, x_2 x_3 + c\, e\, x_1\, x_2^2}{a \quad d \quad {}^2_1} \\ \dot{x_3} = \frac{x_2\, (-d\, x_1 - a\, e\, x_2 + b\, d\, x_1\, x_3)}{a \quad d \quad {}^2_1} \end{cases} \tag{2}$$

with

$$a = \frac{D_{Li}}{v}, \quad b = \frac{D_{Li} zF}{vRT}(u^2 + v^2), c = i\,\frac{D_{Li} zF}{vRT}(u^2 + v^2), d = \frac{D_{Li} zF}{k_T RT}, e = j\,\frac{D_{Li} zF}{k_T RT} \tag{3}$$

where

n_{Li} - concentration of lithium
D_{Li} - the intrinsic diffusivity
φ - electric potential
F - Faraday constant
i,j - real numbers
R - universal gas constant
T - absolute temperature
k_T - total electrical conductivity
z - charge valence.

We study the system in one particular case when c=0; e= d, a,b,d∈**R**, a,b,d>0. Then the system (2) is given by:

$$\begin{cases} \dot{x_1} = x_2 \\ \dot{x_2} = \frac{1}{a} x_2 - \frac{b}{a} x_2 x_3 \\ \dot{x_3} = \frac{d}{a} x_2\, (-\, x_1 - a x_2 + b\, x_1\, x_3) \end{cases} \tag{4}$$

Proposition 1. The following smooth real functions H are constants of the motion defined by the system (4)

$$H(x_1,x_2,x_3) = d\, x_1\, x_2 + x_3, \quad d>0. \tag{5}$$

Proof.

$$\begin{aligned} \mathbf{d}H &= d x_2 \dot{x_1} + d x_1 \dot{x_2} + \dot{x_3} \\ &= d x_2^2 + \frac{d}{a} x_1 x_2 - \frac{bd}{a} x_1 x_2 x_3 + \frac{d}{a} x_2\, (-\, x_1 - a x_2 + b\, x_1\, x_3) \\ &= 0. \end{aligned} \tag{6}$$

□

The next step is to find a Hamilton-Poisson structure for system (4). For this, let us consider the skew-symmetric matrix given by:

$$\Pi = \begin{bmatrix} 0 & p_1(x_1, x_2, x_3) & p_2(x_1, x_2, x_3) \\ -p_1(x_1, x_2, x_3) & 0 & p_3(x_1, x_2, x_3) \\ -p_2(x_1, x_2, x_3) & -p_3(x_1, x_2, x_3) & 0 \end{bmatrix}. \tag{7}$$

We have to find the real smooth functions p_1, p_2, p_3: $\mathbf{R}^3 \rightarrow \mathbf{R}$ such that:

$$\begin{bmatrix} \dot{x_1} \\ \dot{x_2} \\ \dot{x_3} \end{bmatrix} = \Pi \cdot \nabla H \tag{8}$$

and the Jacobi identity should be satisfied:

$$-p_3\left(\frac{\partial p_2}{\partial x_3}+\frac{\partial p_1}{\partial x_2}\right)+p_2\left(\frac{\partial p_3}{\partial x_3}+\frac{\partial p_1}{\partial x_1}\right)+p_1\left(\frac{\partial p_3}{\partial x_2}+\frac{\partial p_2}{\partial x_1}\right)=0 \tag{9}$$

Under these assumptions, using eventually MATHEMATICA 8.0, the above equation has the following solutions:

$$p_1(x_1,x_2,x_3)=\frac{\sqrt{b}e^{\frac{bdx_1^2}{2a}}x_2}{2\sqrt{ad}}\left[4adf(u,v)-\sqrt{2\pi}efr\left(\frac{\sqrt{bd}x_1}{\sqrt{2a}}\right)\right]$$

$$p_2(x_1,x_2,x_3)=x_2-\frac{\sqrt{bd}e^{\frac{bdx_1^2}{2a}}x_1x_2}{2\sqrt{a}}\left[4adf(u,v)-\sqrt{2\pi}efr\left(\frac{\sqrt{bd}x_1}{\sqrt{2a}}\right)\right] \tag{10}$$

$$p_3(x_1,x_2,x_3)=\frac{x_2-bx_2x_3}{a}+\frac{\sqrt{bd}e^{\frac{bdx_1^2}{2a}}x_2^2}{2\sqrt{a}}\left[4adf(u,v)-\sqrt{2\pi}efr\left(\frac{\sqrt{bd}x_1}{\sqrt{2a}}\right)\right]$$

where $f\in C^1(\mathbf{R}^2,\mathbf{R})$ is an arbitrary real function and

$$u=-\frac{b(dx_1x_2+x_3)}{a}$$

$$v=\frac{\sqrt{\pi}(bdx_1x_2+bx_3-1)efr\left(\frac{\sqrt{bd}x_1}{\sqrt{2a}}\right)}{\sqrt{2abd}}+e^{-\frac{bdx_1^2}{2a}}x_2, \tag{11}$$

where *erf*(z) is the error function,

$$erf(z)=\frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2}\,dt. \tag{12}$$

As a consequence, we obtain the next result:
Proposition 2. The system (4) has the Hamilton-Poisson realization:

$$(\mathbf{R}^3,\ \Pi:=[\Pi^{ij}],\ H), \tag{13}$$

where

$$\Pi=\begin{bmatrix}0 & p_1(x_1,x_2,x_3) & p_2(x_1,x_2,x_3)\\ -p_1(x_1,x_2,x_3) & 0 & p_3(x_1,x_2,x_3)\\ -p_2(x_1,x_2,x_3) & -p_3(x_1,x_2,x_3) & 0\end{bmatrix} \tag{14}$$

whith the functions p_1, p_2, $p_3:\mathbf{R}^3\to\mathbf{R}$ given in (10), $f\in C^1(\mathbf{R}^2,\mathbf{R})$, $f=f(u,v)$, is an arbitrary real function with u, v given in (11)

$$H(x_1,x_2,x_3)=d\,x_1\,x_2+x_3,\qquad d\in\mathbf{R}_+. \tag{15}$$

□

Let us now pass to find the Casimir of the configuration described by the Proposition 2. Since the rank of Π is constant and equal to 2, there exists only one functionally independent Casimir associated to our structure.

For the determination of a Casimir in a finite dimensional Hamilton-Poisson system we use the algebraic method of Bermejo-Fairen (see [12]):
(i) First we compute explicitly the components of the matrix given by

$$\Gamma=(\Pi_1\cdot\Pi_2^{-1})^t, \tag{16}$$

where

$$\Pi_1 = [-p_2(x_1,x_2,x_3) \quad -p_3(x_1,x_2,x_3)] \tag{17}$$

and

$$\Pi_2 = \begin{bmatrix} 0 & p_1(x_1,x_2,x_3) \\ -p_1(x_1,x_2,x_3) & 0 \end{bmatrix}. \tag{18}$$

We obtain:

$$\Gamma = \begin{bmatrix} -\frac{p_3(x_1,x_2,x_3)}{p_1(x_1,x_2,x_3)} \\ \frac{p_2(x_1,x_2,x_3)}{p_1(x_1,x_2,x_3)} \end{bmatrix}. \tag{19}$$

(ii) Next we associate the Pffafian system

$$\mathbf{d}x_3=\Gamma_1\mathbf{d}x_1+\Gamma_2\mathbf{d}x_2, \tag{20}$$

i.e.

$$\mathbf{d}x_3 = -\frac{p_3(x_1,x_2,x_3)}{p_1(x_1,x_2,x_3)}\mathbf{d}x_1 + \frac{p_2(x_1,x_2,x_3)}{p_1(x_1,x_2,x_3)}\mathbf{d}x_2, \tag{21}$$

where p_1,p_2,p_3 are given by the formulas (10).

Consequently we have derived the following result.

Proposition 3. The real smooth function C:$\mathbf{R}^3\to\mathbf{R}$,

$$C(x_1,x_2,x_3) = \sqrt{2abd}e^{-\frac{bdx_1^2}{2a}}x_2 + \sqrt{\pi}(bdx_1x_2 + bx_3 - 1)efr\left(\frac{\sqrt{bd}x_1}{\sqrt{2a}}\right) \tag{22}$$

is the only one functionally independent Casimir of the Hamilton-Poisson realization

$$\left((0,\infty)\times\mathbf{R}^2, \Pi = \begin{bmatrix} 0 & p_1 & p_2 \\ -p_1 & 0 & p_3 \\ -p_2 & -p_3 & 0 \end{bmatrix}, H\right) \tag{23}$$

of the system (4), where p_1,p_2, p_3,H **:**$\mathbf{R}^3\to\mathbf{R}$ are respectively given by

$$p_1(x_1,x_2,x_3) = -\frac{\sqrt{b\pi}e^{\frac{bdx_1^2}{2a}}x_2 efr\left(\frac{\sqrt{bd}x_1}{\sqrt{2a}}\right)}{\sqrt{2ad}}$$

$$p_2(x_1,x_2,x_3) = \frac{\sqrt{bd\pi}e^{\frac{bdx_1^2}{2a}}x_1x_2 efr\left(\frac{\sqrt{bd}x_1}{\sqrt{2a}}\right)}{\sqrt{2a}} + x_2 \tag{24}$$

$$p_3(x_1, x_2, x_3) = -\frac{x_2\left[\sqrt{2abd\pi}e^{\frac{bdx_1^2}{2a}}x_2 efr\left(\frac{\sqrt{bd}x_1}{\sqrt{2a}}\right) + 2bx_3 - 2\right]}{2a}$$

and

$H(x_1,x_2,x_3)=d\, x_1\, x_2 + x_3,$ (25)

$d \in R_+$ being a parameter.

Note that, by Poisson structure generated by the smooth function C, we mean the Poisson structure generated by the Poisson bracket $\{f,g\}:=\nabla C\cdot(\nabla f\times\nabla g)$, for any smooth functions $f,g \in C^1(\mathbf{R}^3,\mathbf{R})$.

Proof. Indeed, we have successively:

$$\Pi_C(x_1, x_2, x_3)\cdot\nabla H(x_1, x_2, x_3) = \begin{bmatrix}\dot{x_1}\\ \dot{x_2}\\ \dot{x_3}\end{bmatrix}, \tag{26}$$

as required.

□

Next proposition gives others Hamilton-Poisson realizations of the Li-ion battery system (4).

Proposition 4. The dynamics (4) admits a family of Hamilton-Poisson realizations parameterized by the group $SL(2,\mathbf{R})$. More exactly, $(\mathbf{R}^3,\{\cdot,\cdot\}_{\alpha,\beta},H_{\gamma,\delta})$ is a Hamilton-Poisson realization of the dynamics (4) where the bracket $\{\cdot,\cdot\}_{\alpha,\beta}$ is defined by

$$\{f,g\}_{\alpha,\beta}:=\nabla C_{\alpha,\beta}\cdot(\nabla f\times\nabla g), \tag{27}$$

for any $f,g \in C^1(\mathbf{R}^3,\mathbf{R})$, and the functions $C_{\alpha,\beta}$ and $H_{\gamma,\delta}$ are given by:

$$C_{\alpha,\beta}(x_1, x_2, x_3) = \sqrt{2abd}e^{-\frac{bdx_1^2}{2a}}\alpha x_2 + \beta d x_1 x_2 + \beta x_3 + \sqrt{\pi}\alpha(bdx_1x_2 + bx_3 - 1)efr\left(\frac{\sqrt{bd}x_1}{\sqrt{2a}}\right),$$

$$H_{\delta,\gamma}(x_1, x_2, x_3) = \sqrt{2abd}e^{-\frac{bdx_1^2}{2a}}\delta x_2 + \gamma d x_1 x_2 + \gamma x_3 + \sqrt{\pi}\delta(bdx_1x_2 + bx_3 - 1)efr\left(\frac{\sqrt{bd}x_1}{\sqrt{2a}}\right), \tag{28}$$

respectively, the matrix of coefficients α, β, δ, γ is $\begin{bmatrix}\alpha & \beta\\ \gamma & \delta\end{bmatrix} \in SL(2,\mathbf{R})$.

Proof. The conclusion follows directly by taking into account that the matrix formulation of the Poisson bracket ,$\{\cdot,\cdot\}_{\alpha,\beta}$ is given in coordinates by:

$$\Pi_{\alpha,\beta}(x_1, x_2, x_3) = \begin{bmatrix}0 & p_{1\alpha,\beta} & p_{2\alpha,\beta}\\ -p_{1\alpha,\beta} & 0 & p_{3\alpha,\beta}\\ -p_{2\alpha,\beta} & -p_{3\alpha,\beta} & 0\end{bmatrix} \tag{29}$$

where

$$p_{1\alpha,\beta}(x_1, x_2, x_3) = e^{\frac{bdx_1^2}{2a}} x_2 \frac{\beta + \alpha b\sqrt{\pi} efr\left(\frac{\sqrt{bd}x_1}{\sqrt{2a}}\right)}{\sqrt{2abd}}$$

$$p_{2\alpha,\beta}(x_1, x_2, x_3) = -x_2 \frac{\alpha\sqrt{2ab} + \beta\sqrt{d}e^{\frac{bdx_1^2}{2a}} x_1 + \alpha b\sqrt{d\pi} e^{\frac{bdx_1^2}{2a}} x_1 efr\left(\frac{\sqrt{bd}x_1}{\sqrt{2a}}\right)}{\sqrt{2ab}} + x_2$$

(30)

$$p_{3\alpha,\beta}(x_1, x_2, x_3) = x_2 \frac{\left[-2\alpha\sqrt{b} + \beta\sqrt{2abd\pi} e^{\frac{bdx_1^2}{2a}} x_2 + 2\alpha\sqrt{b^3} + \alpha b\sqrt{2ad\pi} e^{\frac{bdx_1^2}{2a}} x_2 efr\left(\frac{\sqrt{bd}x_1}{\sqrt{2a}}\right)\right]}{2a\sqrt{b}}$$

□

Lax Formulation

In this section is described a Lax formulation of the system (4).

Let us first note that as the system (4) restricted to a regular symplectic leaf, give rise to a sypmlectic Hamiltonian system that is completely integrable in the sense of Liouville and consequently it has a Lax formulation.

It is a natural question to ask if the unrestricted system admit a Lax formulation. The answer is positive and is given by the following proposition:

Proposition 5. The system (4) can be written in the Lax form $\dot{L} = [L, B]$ where the matrices L and respectively B are given by:

$$\mathrm{L} = \begin{bmatrix} 0 & l_1 & l_2 \\ -l_1 & 0 & l_3 \\ -l_2 & -l_3 & 0 \end{bmatrix} \text{ with } l_1 = -\sqrt{\frac{d}{ab}}(x_1 - ax_2 - bx_1x_3), l_2 = -i\sqrt{\frac{d}{ab}}(x_1 + ax_2 - bx_1x_3)$$

$l_3 = -\frac{1}{b} - dx_1x_2 + x_3)$ and

$$\mathrm{B} = \begin{bmatrix} 0 & b_1 & b_2 \\ -b_1 & 0 & b_3 \\ -b_2 & -b_3 & 0 \end{bmatrix} \text{ with } b_1 = \frac{a-ibd}{a\sqrt{abd}}\left(x_1 - \frac{a(ia-bd)}{ia+bd}x_2 - bx_1x_3\right),$$

$$b_2 = \frac{bd+ia}{a\sqrt{abd}}(x_1 + ax_2 - bx_1x_3),\ b_3 = -\frac{i}{a} + \frac{1}{bd} + x_1x_2 + \left(\frac{ib}{a} + \frac{1}{d}\right)x_3,$$

where $i^2=-1$.

□

Acknowledgment

The paper was supported by the project "Development and support of multidisciplinary postdoctoral programmes in major technical areas of national strategy of Research - Development - Innovation" 4D-POSTDOC, contract no. POSDRU/89/1.5/S/52603, project co-funded by the European Social Fund through Sectoral Operational Programme Human Resources Development 2007-2013.

References

[1] R. Musunuri, and J.A. Cobb. Hierarchical-Battery Aware Routing in Wireless Sensor Networks. In Vehicular Technology Conference (VTC), IEEE, September 2005, pp. 2311-2315.

[2] A. Aron, G. Gîrban and C. Pop, "About the solution of a battery mathematical model", BSG Proceedings, Geometry Balkan Press, vol. 18, April 2011, pp. 1-10.

[3] Anania Aron, Gabriel Gîrban, Ştefan Kilyeni, A Geometric Approach of a Battery Mathematical Model for On-Line Energy Monitoring, Proceedings of EUROCON 2011, International Conference on Computer as a Tool, Lisbon, Portugal, April 2011, pp. 454 -457.

[4] Anania Aron, Ştefan Kilyeni, A Geometrical Point of View Over a Battery Mathematical Model, Proceedings of EUROCON 2011, International Conference on Computer as a Tool, Lisbon, Portugal, April 2011, pp. 458 - 461.

[5] Anania Gîrban, Gabriel Gîrban, On the kinetic equations of a lithium-ion battery model, Comptes Rendus Mathematique, Acad. Sci. Paris, Ser. I , Volume 350, Issue 19, (2012) 917-920.

[6] M. Doyle, T. F. Fuller, J. Newman, Modeling of galvanostatic charge and discharge of the lithium/polymer/insertion cell, J. Electrochem. Soc., 140(6) (1993), 15-26.

[7] R. E. Garcia, Y-M. Chiang, W. C. Carter, P. Limthongkul, C. M. Bishop, Microstructural modeling and design of rechargeable lithium-ion batteries, J. Electrochem. Soc. 152(1) (2005), A255.

[8] R.H. Cushman, L. Bates, Global aspects of classical integrable systems, Basel: Birkhauser, 1977.

[9] J.E. Marsden, Lectures on mechanics, London Mathematical Society Lecture Notes Series, vol. 174, Cambridge University Press, 1992.

[10] J.E. Marsden and T.S. Ratiu, Introduction to mechanics and symmetry, Texts in Applied Mathematics, vol. 17, second edition, second printing, Springer, Berlin, 1999.

[11] T.S. Ratiu, R.M. Tudoran, L. Sbano, E. Sousa Dias and G. Terra, Geometric Mechanics and Symmetry: the Peyresq Lectures; Chapter II: A Crash Course in Geometric Mechanics, London Mathematical Society Lecture Notes Series, vol. 306 Cambridge University Press, 2005, pp. 23-156.

[12] M. Puta, R. M. Tudoran and R. M. Tudoran, Poisson manifolds and Bermejo-Fairen construction of Casimirs, Tensor N.S., 66, (2005), 59-70.