C. R. Acad. Sci. Paris, Ser. I 350 (2012) 917–920

Contents lists available at SciVerse ScienceDirect

C. R. Acad. Sci. Paris, Ser. I

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Differential Geometry/Dynamical Systems

On the kinetic equations of a lithium-ion battery model

Sur les équations cinétiques d'un modèle de la batterie lithium-ion

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A R T I C L E I N F O

Article history:
Received 18 July 2012
Accepted after revision 8 October 2012
Available online 22 October 2012

Presented by the Editorial Board

A B S T R A C T

In this Note we provide a Hamilton–Poisson realization of the system obtained from the kinetic equations of a well known lithium-ion battery model, explicitly integrate the Poincaré compactification of this system and give a Lax formulation.

R É S U M É

Dans cette Note, on donne une réalisation Hamilton–Poisson d'un système obtenu à partir des équations cinétiques d'un modèle bien connu pour la batterie lithium-ion, on intègre explicitement la compactification de Poincaré de ce système et on donne une formulation de Lax.

1. Hamilton–Poisson realizations of a battery model

In this Note, we are taking as a reference the kinetic equations describing the transport of active species (electrons and ions) based on charge and mass conservation constraints in case of lithium-ion batteries [2,3]. After some transformations in which we consider $q = ux + vt$, $x = \frac{1}{n_{Li}}$, $y = n'_{Li}$, $z = \Phi$ (with u and v being real constants while n_{Li} and Φ are defined in [3] as molar concentration and electric potential), one can obtain the system:

$$\begin{cases} \dot{x} = -x^2 y, \\ \dot{y} = -\frac{x^2 y - bx^2 yz + bdxy^2}{bd}, \\ \dot{z} = \frac{xy - bxyz}{b}, \end{cases} \tag{1}$$

where $b, d \in \mathbb{R}^*$ are real constants.

The following theorem gives a Hamilton–Poisson realization of the system (1):

Theorem 1.1. *The dynamics* (1) *has the following Hamilton–Poisson realization*:

$$\big((0,\infty) \times \mathbb{R}^2, \Pi_C, H\big),$$

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1631-073X/$ – see front matter
http://dx.doi.org/10.1016/j.crma.2012.10.008

where

$$\Pi_C(x,y,z)=\frac{1}{bd}\begin{bmatrix}0 & -bx^3y & 0\\ bx^3y & 0 & x^2y(bz-1)\\ 0 & -x^2y(bz-1) & 0\end{bmatrix}$$

is the Poisson structure generated by the smooth function $C(x,y,z):=\frac{bz-1}{x}$, *and the Hamiltonian* $H\in C^\infty((0,\infty)\times\mathbb{R}^2,\mathbb{R})$ *is given by* $H(x,y,z):=\frac{dy}{x}+z$.

The Poisson structure generated by the smooth function C, *is the Poisson structure generated by the Poisson bracket* $\{f,g\}:=\nabla C\cdot(\nabla f\times\nabla g)$, *for any smooth functions* $f,g\in C^\infty((0,\infty)\times\mathbb{R}^2,\mathbb{R})$.

Proof. It is not hard to see that $\Pi_C(x,y,z)\cdot\nabla H(x,y,z)=\begin{bmatrix}\dot{x}\\ \dot{y}\\ \dot{z}\end{bmatrix}$, as required. □

Let us now give other Hamilton–Poisson realizations of the system (1).

Proposition 1.1. *The dynamics* (1) *admits a family of Hamilton–Poisson realizations parameterized by the group* $SL(2,\mathbb{R})$. *More exactly,* $((0,\infty)\times\mathbb{R}^2,\{\cdot,\cdot\}_{\alpha,\beta},H_{\gamma,\delta})$ *is a Hamilton–Poisson realization of the dynamics* (1) *where the bracket* $\{\cdot,\cdot\}_{\alpha,\beta}$ *is defined by*

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

for any $f,g\in C^\infty((0,\infty)\times\mathbb{R}^2,\mathbb{R})$, *and the functions* $C_{\alpha,\beta}$ *and* $H_{\gamma,\delta}$ *are given by*:

$$C_{\alpha,\beta}(x,y,z)=\frac{\alpha xz+d\alpha y+b\beta z-\beta}{x},\qquad H_{\gamma,\delta}(x,y,z)=\frac{\gamma xz+d\gamma y+b\delta z-\delta}{x},$$

respectively, the matrix of coefficients $\alpha,\beta,\gamma,\delta$ *is* $\left[\begin{smallmatrix}\alpha & \beta\\ \gamma & \delta\end{smallmatrix}\right]\in SL(2,\mathbb{R})$.

Proof. Since the matrix formulation of the Poisson bracket $\{\cdot,\cdot\}_{\alpha,\beta}$ is given in coordinates by:

$$\Pi_{\alpha,\beta}(x,y,z)=\frac{1}{bd}\begin{bmatrix}0 & x^3y(\alpha x+b\beta) & -d(\alpha x^3y)\\ -x^3y(\alpha x+b\beta) & 0 & -x^2y(d\alpha y-\beta+b\beta z)\\ d(\alpha x^3y) & x^2y(d\alpha y-\beta+b\beta z) & 0\end{bmatrix},$$

we obtain the conclusion directly. □

For details on Poisson geometry and Hamiltonian dynamics see e.g. [4,5].

2. The behavior on the sphere at infinity

Now we explicitly integrate on the sphere the Poincaré compactification of the system (1) at infinity. Recall that using the Poincaré compactification of $\mathbb{R}^3$, the infinity of $\mathbb{R}^3$ is represented by the sphere $\mathbb{S}^2$ – the equator of the unit sphere $\mathbb{S}^3$ in $\mathbb{R}^4$. For details regarding the Poincaré compactification of polynomial vector fields in $\mathbb{R}^3$ see [1].

With the notations from [1] we put the system (1) in the following form: $\dot{x}=P^1(x,y,z)$, $\dot{y}=P^2(x,y,z)$, $\dot{z}=P^3(x,y,z)$ with $P^1(x,y,z)=-x^2y$, $P^2(x,y,z)=-\frac{x^2y-bx^2yz+bdxy^2}{bd}$, $P^3(x,y,z)=\frac{xy-bxyz}{b}$.

We study the Poincaré compactification of the system (1) in the local charts U_i and V_i, $i\in\{1,2,3\}$, of the manifold $\mathbb{S}^3$.

The Poincaré compactification ($p(X)$ in the notations from [1]) of the system (1) in the local charts U_1, U_2 and respectively U_3 is given in the corresponding local coordinates by

$$(U_1)\begin{cases}\dot{z}_1=\frac{z_1(bz_2-z_3)}{bd}\\ \dot{z}_2=\frac{z_1z_3^2}{b}\\ \dot{z}_3=z_1z_3^2\end{cases},\qquad (U_2)\begin{cases}\dot{z}_1=\frac{z_1^3(-bz_2+z_3)}{bd}\\ \dot{z}_2=\frac{z_1(-bz_1z_2^2+z_1z_2z_3+dz_3^2)}{bd}\\ \dot{z}_3=\frac{z_1z_3(-bz_1z_2+bdz_3+z_1z_3)}{bd}\end{cases},\qquad (U_3)\begin{cases}\dot{z}_1=-\frac{z_1^2z_2z_3^2}{b}\\ \dot{z}_2=\frac{z_1z_2(bz_1-z_1z_3-dz_2z_3^2)}{bd}\\ \dot{z}_3=\frac{z_1z_2(b-z_3)z_3^2}{b}\end{cases}. \tag{2}$$

The flow of the system (2) on the local chart V_1, V_2 and respectively V_3 is the same as the flow on the local chart U_1, U_2 and respectively U_3 reversing the time. It comes from the Poincaré compactification of the system in the local chart V_1, V_2 and respectively V_3, because the compactified vector field $p(X)$ in the local chart V_1, V_2 and respectively V_3 is the vector field $-p(X)$ in U_1, U_2 and respectively U_3.

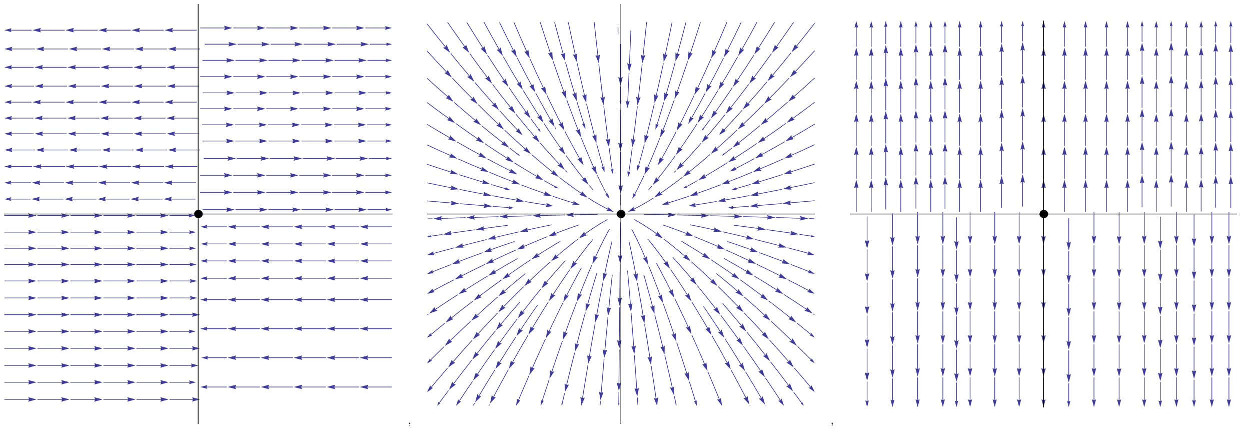

Fig. 1. Phase portrait of the systems (3) on the local charts U_1, U_2 and U_3, respectively, on the infinity sphere.

Fig. 1. Portrait de phase des systèmes (3) sur les cartes locales U_1, U_2 et U_3, respectivement, sur la sphère infinie.

The points on the sphere $\mathbb{S}^2$ at infinity are characterized by $z_3 = 0$. As the plane $z_1 z_2$ is invariant under the flow of the system (2), the compactified system (1) on the local charts U_i $(i \in \{1,2,3\})$ on the infinity sphere is reduced to integrable systems and the solutions are given by:

$$(U_1)\begin{cases} z_1(t) = k_2 e^{\frac{tk_1}{d}} \\ z_2(t) = k_1 \end{cases}, \qquad (U_2)\begin{cases} z_1(t) = \sqrt[3]{\frac{d}{3(tk_1 - dk_2)}} \\ z_2(t) = \sqrt[3]{\frac{dk_1}{3(tk_1 - dk_2)}} \end{cases}, \qquad (U_3)\begin{cases} z_1(t) = k_1 \\ z_2(t) = k_2 e^{\frac{tk_1^2}{d}} \end{cases}, \tag{3}$$

where k_1, k_2 are arbitrary real constants.

The phase portrait on the local charts U_i $(i \in \{1,2,3\})$ on the infinity sphere is given in Fig. 1 where the black lines are the equilibrium lines.

3. Lax formulation

In this section we present a Lax formulation of the system (1).

Let us first note that the system (1) restricted to a regular symplectic leaf, gives rise to a symplectic Hamiltonian system that is completely integrable in the sense of Liouville and consequently it has a Lax formulation.

The next proposition shows that the unrestricted system also admits a Lax formulation:

Proposition 3.1. *The system (1) can be written in the Lax form $\dot{L} = [L, B]$, where the matrices L and respectively B are given by*:

$$L = \begin{bmatrix} 0 & \frac{1+bz}{x} & \frac{dy}{x} + z \\ -\frac{1+bz}{x} & 0 & \frac{-i\sqrt{2}}{x} \\ -\frac{dy+xz}{x} & -\frac{-i\sqrt{2}}{x} & 0 \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & 0 & i\sqrt{2}xy \\ 0 & 0 & 0 \\ -i\sqrt{2}xy & 0 & 0 \end{bmatrix}, \quad i^2 = -1.$$

Acknowledgements

The work of Anania Gîrban was supported by the project "Development and support of multidisciplinary postdoctoral programmes in major technical areas of national strategy of Research – Development – Innovatio" 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.

The work of Gabriel Gîrban was supported by the strategic grant POSDRU/88/1.5/S/50783, Project ID50783 (2009), co-financed by the European Social Fund "Investing in People", within the Sectoral Operational Programme Human Resources Development 2007–2013.

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