Open Communications in Nonlinear Mathematical Physics]ocnmp[Vol.4 (2024) pp 13–21 Article

Simple Conditions for the Transformation of Dynamical Coordinates into Canonical Ones in Hamiltonian Dynamics

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Received January 18, 2024; Accepted February 18, 2024

Abstract

We obtain conditions, which when fulfilled, permit to transform the coordinates of a dynamical system into pairs of canonical ones for some Hamiltonian system. These conditions, restricted to the class of coordinate transformations which act on each coordinate independently, are greatly simplified. However, they are surprisingly successful in defining canonical coordinates and an associated Hamiltonian for several test examples. So, a method is proposed to exploit these simple transformations in a systematic manner.

1 Introduction

A Hamiltonian dynamical system has specific properties, which can be taken advantage of in its study [1]. General, N-dimensional, Poisson brackets permit to obtain generalized Hamiltonians [3]. However, quantization of the latter can be ambiguous [4]. Here, we will take the term "Hamiltonian" in the restricted sense of a function giving Hamilton equations for pairs of conjugate canonical coordinates. Such canonical Hamiltonian systems can be quantized by replacing Poisson brackets by commutators [2].

Darboux's theorem or its generalization [5] insures that locally there always exists a canonical representation of a Hamiltonian in the generalized sense. In this work, we aim at finding directly this canonical representation. It is well-known that it is not possible to change the canonical or non-canonical nature of a dynamical system with a linear transformation of the coordinates. In this work, we show how it is feasible with a non-linear but simple one, by just writing equalities [6], that must be satisfied according to Schwartz theorem after transformation. The method is applied succesfully to several classical models, in spite of the quite severe restriction we make, that the transformations act on each coordinate independently.

As straightforward and simple as the method might be, we have not found such proposal in the literature. For example, the Lotka-Volterra model in 2-dimension has been extensively studied and the Hamiltonian we obtain with our approach is known [7, 8]. However, the systematic derivation of an Hamiltonian by defining an appropriate generalized Poisson bracket [9] or by time rescaling [10], give different Hamiltonian functions as there is no change of the dynamical system coordinates. Volterra's own construction preserves the canonical Poisson bracket, but introduce extra-variables, and the Hamiltonian he obtained, though formally close to ours, gives more complicated Hamilton-Jacobi equations[11, 12]. In addition, it appears that our transformed coordinates can be of physical interest for the description of the system. So, we propose an algorithm based on Schwartz theorem equalities, to deal with general systems, which searches for, (at least,) a subset of coordinates amenable to be turned into canonically conjugate ones, satisfying a set of Hamilton's equations.

The article is organized as follows: First we present the method in two-dimension and illustrate its application on two case examples. Then, we generalize it to any finite dimension, and apply it to the Kermack-McKendrick model, before concluding.

2 Transformation of a dynamical system in $\mathbb{R}^2$

2.1 Theory

We consider a dynamical system in 2 real coordinates in an open set $U \subseteq \mathbb{R}^2$, defined by a mapping $f : U \longrightarrow \mathbb{R}^2$, that is to say, $f = (f_1, f_2)$, $\forall i \in \{1, 2\}$ $f_i : U \longrightarrow \mathbb{R}$ is smooth enough (often considered to be C^∞, however this is not necessay for our purpose, it may also depends upon the time variable, but we will omit this too), and, $\dot{x}_i = f_i(x_1, x_2)$.

We do not know *a priori* whether the system is Hamiltonian or not. Hoping it is Hamiltonian, we look for a diffeomorphism $h : U \longmapsto \mathbb{R}^2$, whose components h_1 and h_2 define two new coordinates,

$$q = h_1(x_1, x_2) \quad (1)$$
$$p = h_2(x_1, x_2). \quad (2)$$

that satisfy Hamilton's equations for some Hamiltonian function, H,

$$\dot{q} = \frac{\partial H}{\partial p}\ , \quad (3)$$
$$\dot{p} = -\frac{\partial H}{\partial q}\ . \quad (4)$$

We are going to obtain necessary conditions for this problem to admit solutions. Note that, if the system is Hamiltonian, then, there will be infinitely many solutions.
We denote the inverse mapping h^{-1} by $g = (g_1, g_2)$,

$$x_1 = g_1(q, p)\ , \quad (5)$$
$$x_2 = g_2(q, p)\,. \quad (6)$$

The local inversion theorem [6] insures that for $(x_1, x_2) = g(q, p)$ such that $(q, p) \in h(U)$, we have the relation between the differentials: $Dh(x_1,x_2) = [Dg(q,p)]^{-1}$, so that:

$$\frac{\partial h_1(x_1,x_2)}{\partial x_1} = \frac{\frac{\partial g_2}{\partial p}}{\frac{\partial g_1}{\partial q}\frac{\partial g_2}{\partial p} - \frac{\partial g_1}{\partial p}\frac{\partial g_2}{\partial q}} \; , \tag{7}$$

$$\frac{\partial h_1(x_1,x_2)}{\partial x_2} = \frac{-\frac{\partial g_1}{\partial p}}{\frac{\partial g_1}{\partial q}\frac{\partial g_2}{\partial p} - \frac{\partial g_1}{\partial p}\frac{\partial g_2}{\partial q}} \; , \tag{8}$$

$$\frac{\partial h_2(x_1,x_2)}{\partial x_1} = \frac{-\frac{\partial g_2}{\partial q}}{\frac{\partial g_1}{\partial q}\frac{\partial g_2}{\partial p} - \frac{\partial g_1}{\partial p}\frac{\partial g_2}{\partial q}} \; , \tag{9}$$

$$\frac{\partial h_2(x_1,x_2)}{\partial x_2} = \frac{\frac{\partial g_1}{\partial q}}{\frac{\partial g_1}{\partial q}\frac{\partial g_2}{\partial p} - \frac{\partial g_1}{\partial p}\frac{\partial g_2}{\partial q}} \; . \tag{10}$$

Injecting expressions (1) and (2) in Eq.(3) and using the chain rule, we obtain

$$\begin{aligned} \frac{\partial H}{\partial p} &= \frac{\partial h_1(x_1,x_2)}{\partial x_1}\dot{x}_1 + \frac{\partial h_1(x_1,x_2)}{\partial x_2}\dot{x}_2 \\ &= \frac{\partial h_1(x_1,x_2)}{\partial x_1} f_1(g_1(q,p),g_2(q,p)) + \frac{\partial h_1(x_1,x_2)}{\partial x_2} f_2(g_1(q,p),g_2(q,p)) \; , \end{aligned} \tag{11}$$

and similarly, using Eq.(4),

$$-\frac{\partial H}{\partial q} = \frac{\partial h_2(x_1,x_2)}{\partial x_1} f_1(g_1(q,p),g_2(q,p)) + \frac{\partial h_2(x_1,x_2)}{\partial x_2} f_2(g_1(q,p),g_2(q,p)) \; . \tag{12}$$

Substituting Eqs.(7)-(10) into Eqs. (11) and (12), we obtain the Hamilton equations,

$$\frac{\partial H}{\partial p} = \frac{f_1(g_1(q,p),g_2(q,p))\cdot\frac{\partial g_2}{\partial p} - \frac{\partial g_1}{\partial p}\cdot f_2(g_1(q,p),g_2(q,p))}{\frac{\partial g_1}{\partial q}\frac{\partial g_2}{\partial p} - \frac{\partial g_1}{\partial p}\frac{\partial g_2}{\partial q}} \; , \tag{13}$$

$$-\frac{\partial H}{\partial q} = \frac{\frac{\partial g_1}{\partial q}\cdot f_2(g_1(q,p),g_2(q,p)) - f_1(g_1(q,p),g_2(q,p))\cdot\frac{\partial g_2}{\partial q}}{\frac{\partial g_1}{\partial q}\frac{\partial g_2}{\partial p} - \frac{\partial g_1}{\partial p}\frac{\partial g_2}{\partial q}} \; . \tag{14}$$

We can either (i) integrate one of these equation and insert the expression obtained for H into the other one, (assuming that g is of class C^2, so that h is also C^2) [6], to derive a relation between f_1, f_2, and g (or more conveniently h), or, (ii) (assuming that, in addition, the f_i's have first partial derivatives and H second partial derivatives), we can use Schwartz's theorem [6] for the same purpose. Noting $\bar{i} = 2$ if $i = 1$ and $\bar{i} = 1$ if $i = 2$, and using the inverse of Eqs.(7)-(10), we obtain, in the original coordinates, the following necessary condition for the existence of a coordinate transformation, h, and a Hamiltonian function, H, such that the Hamilton's equations (3) and (4) are satisfied:

$$\sum_{i\in\{1,2\}} \frac{\partial f_i}{\partial x_i} + f_i \cdot \frac{\frac{\partial^2 h_i}{\partial x_{\bar{i}}^2}\frac{\partial h_{\bar{i}}}{\partial x_{\bar{i}}} - \frac{\partial^2 h_i}{\partial x_1 \partial x_2}\frac{\partial h_{\bar{i}}}{\partial x_i} - \frac{\partial^2 h_{\bar{i}}}{\partial x_{\bar{i}}^2}\frac{\partial h_i}{\partial x_{\bar{i}}} + \frac{\partial^2 h_{\bar{i}}}{\partial x_1 \partial x_2}\frac{\partial h_i}{\partial x_i}}{\frac{\partial h_1}{\partial x_1}\frac{\partial h_2}{\partial x_2} - \frac{\partial h_1}{\partial x_2}\frac{\partial h_2}{\partial x_1}} = 0 \qquad . \tag{15}$$

The condition is only necessary, because Schwartz's theorem only asserts that, if a differential form is exact, then it is closed i.e. satisfies Eq.(15). The condition will be sufficient

if the open set U is simply connected according to Poincaré lemma. Then, if it is not fulfilled, one can deduce from Darboux's theorem that the system is not Hamiltonian.
We remark at this stage that, if the h_i's are linear, their second partial derivatives cancel out and we are left with the first term within the sum over i. That is to say, we retrieve the condition for the differential form to be closed in its original coordinates:

$$\frac{\partial f_1(x_1,x_2)}{\partial x_1}+\frac{\partial f_2(x_1,x_2)}{\partial x_2}=0\ . \tag{16}$$

Conversely, when this is not zero but condition (15) is fulfilled, then, necessarily, the second terms within the sum over i are not all zero. In particular, if we manage to find some h_1, h_2 such that, for each $i\in\{1,2\}$, the second term cancels the first one within the sum, the differential form will be closed.

To go further with this, we may consider the expansion of the $h_i(x_1,x_2)$'s on a set of product functions: $h_i(x_1,x_2)=\sum_{j_1,j_2}\lambda_i^{j_1,j_2}\chi_{j_1}(x_1)\chi_{j_2}(x_2)$, each factor belonging, for example, to a fixed Hilbertian basis set $(\chi_j(x))_j$. We can limit the set of coefficients $\lambda_i^{j_1,j_2}$ to deal with, by truncating this expansion. We may look for one-term expansions of the form $h_i(x_1,x_2)=\psi_i^1(x_1)\psi_i^2(x_2)$ and solve Eq.(15) for the four functions ψ_1^1, ψ_1^2, ψ_2^1, ψ_2^2. Hereafter, we make the even more drastic assumption that each coordinate is transformed independently of the others, that is to say, h_i only depends upon x_i, so that $\frac{\partial h_i}{x_{\bar{i}}}=0$. This simplifies greatly the general equations, (13) and (14), which now become,

$$\frac{\partial H}{\partial p} = \frac{f_1(g_1(q),g_2(p))}{g_1'(q)}\ , \tag{17}$$

$$-\frac{\partial H}{\partial q} = \frac{f_2(g_1(q),g_2(p))}{g_2'(p)}\ , \tag{18}$$

as well as Eq.(15),

$$\frac{\partial f_1(x_1,x_2)}{\partial x_1}+\frac{h_1''(x_1)}{h_1'(x_1)}\cdot f_1(x_1,x_2)+\frac{\partial f_2(x_1,x_2)}{\partial x_2}+\frac{h_2''(x_2)}{h_2'(x_2)}\cdot f_2(x_1,x_2)=0\ . \tag{19}$$

In the next sections, we will apply the necessary condition (19) to two different cases and show its practicality to determine the freely adjustable functions h_1 and h_2.

2.2 Volterra's model as a test example

The first example appearing in Ref. [13], of a dynamical system that is non-canonical in its original coordinates, is Volterra's model of sharks and sardines [11]:

$$\dot{x}_1 = a\ x_1 - b\ x_1x_2\ , \tag{20}$$

$$\dot{x}_2 = -c\ x_2 + d\ x_1x_2, \tag{21}$$

with $a,b,c,d\in\mathbb{R}^{+*}$. In these variables, assuming that $\dot{x}_1=\pm\frac{\partial H}{\partial x_2}$ and $\dot{x}_2=\mp\frac{\partial H}{\partial x_1}$, Schwartz's theorem applied to H, would not be satisfied since $(a-bx_2)\neq\pm(c-dx_1)$.

Eq.(19) gives the condition:

$$(a-b\ x_2)\left(1+\frac{h_1''(x_1)}{h_1'(x_1)}\cdot x_1\right)+(-c\ +d\ x_1)\left(1+\frac{h_2''(x_2)}{h_2'(x_2)}\cdot x_2\right)=0\ . \tag{22}$$

The condition will be clearly fulfilled if,

$$\begin{aligned} \frac{h_1''(x_1)}{h_1'(x_1)} &= -\frac{1}{x_1} \ , \\ \frac{h_2''(x_2)}{h_2'(x_2)} &= -\frac{1}{x_2} \ . \end{aligned}$$

These are easy to integrate, recognizing logarithmic derivatives on both sides,

$$\begin{aligned} \ln(h_1'(x_1)) &= \ln(\frac{1}{x_1}) + c_1 \ , \\ \ln(h_2'(x_2)) &= \ln(\frac{1}{x_2}) + c_2 \ . \end{aligned}$$

Choosing $c_1 = c_2 = 0$, and integrating a second time with zero as integration constants, we finally define the new variables in the following way:

$$q = h_1(x_1) = \ln(x_1) \ , \tag{23}$$

$$p = h_2(x_2) = \ln(x_2) \ , \tag{24}$$

that is to say,

$$x_1 = \exp(q) \ , \tag{25}$$

$$x_2 = \exp(p) \ . \tag{26}$$

The canonical Hamiltonian is obtained from Hamilton's equations (17) and (18),

$$H_{Volterra} = a \cdot p - b \cdot \exp(p) + c \cdot q - d \cdot \exp(q) \ . \tag{27}$$

Not surprisingly for such a popular model, Hamiltonian's forms are already known [9, 12, 14, 7, 8, 15, 16, 17, 18]. However, the derivation of Eq.(27) is particularly straightforward with our approach. The number of coordinates is still two, unlike in Volterra's work [12, 18]. These coordinates are conjugate for the canonical Poisson bracket, unlike in [9, 15, 10] where a generalized Poisson bracket is used or appear from a time coordinate rescaling. The new coordinates are physically relevant: the original ones would evolve exponentially, if they were not coupled, so, it makes sense to describe the system on a logarithmic scale. This is what is achieved thanks to the new coordinates.

2.3 A classical system derived from a forced, two-level, quantum model

Consider the following dynamical system derived from a forced, two-level, quantum model [19]:

$$\dot{x}_1 = -\sin(x_2) \ , \tag{28}$$

$$\dot{x}_2 = B - \cot(x_1)\cos(x_2), \tag{29}$$

where x_1 and x_2 are two real dynamical coordinates, and B a constant. This system is not canonical, for, suppose there exists H such that $\dot{x}_1 = \pm\frac{\partial H}{\partial x_2}$ and $\dot{x}_2 = \mp\frac{\partial H}{\partial x_1}$, the right hand sides of Eqs. (28) and (29) being differentiable, we can search for an H that is derivable twice. Then, Schwartz's theorem permits to conclude at the non-existence of such H, since $\frac{\partial \sin(x_2)}{\partial x_1} = 0$ and $\frac{\partial B - \cot(x_1)\cos(x_2)}{\partial x_2} = \cot(x_1)\sin(x_2) \neq 0$.

Equation (15) applied to this system gives,

$$\left(\cot(x_1) - \frac{h_1''(x_1)}{h_1'(x_1)}\right)\sin(x_2) + (B - \cot(x_1)\cos(x_2))\,\frac{h_2''(x_2)}{h_2'(x_2)} = 0\ . \tag{30}$$

This can be satisfied by taking h_2 linear, and $\frac{h_1''(x_1)}{h_1'(x_1)} = \cot(x_1)$. We recognize again logarithmic derivatives and integrate, this gives $\ln(h_1'(x_1)) = \ln(\sin(x_1)) + c$. The simplest choice of integration constants leads to $h_2(x_2) = x_2$ and $h_1(x_1) = \cos(x_1)$. Therefore, we define the new coordinates as

$$q = cos(x_1) \tag{31}$$

$$p = x_2,, \tag{32}$$

and the dynamical system becomes:

$$\dot{q} = \sqrt{1-q^2}\,\sin(p) \tag{33}$$

$$\dot{p} = B - \frac{q}{\sqrt{1-q^2}}\cos(p). \tag{34}$$

We easily verify that Eqs. (33) and (34) are the Hamilton-jacobi equations for the Hamiltonian,

$$H = -Bq - \sqrt{1-q^2}\ \cos(p)\ . \tag{35}$$

3 Generalization to a dynamical system in $\mathbb{R}^N$

3.1 Theory

We now consider a dynamical system in N real coordinates:

$$\forall i \in \{1, \cdots, N\} \quad \dot{x}_i = f_i(x_1, \cdots, x_N)\ . \tag{36}$$

If N is odd, one can always add an extra dummy coordinate, which is constant and whose initial value is zero. So, without loss of generality, we can assume N even: $N = 2n$, and search for a canonical Hamiltonian H, and a transformation of the initial variables, $x_1, \ldots, x_{2n}$ into two sets $\{q_1, \cdots, q_n\}$, $\{p_1, \cdots, p_n\}$, such that:

$$\forall i \in \{1, \cdots, n\}, \quad \dot{q}_i = \frac{\partial H}{\partial p_i} \tag{37}$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}\ . \tag{38}$$

The general equations (13), (14) and (15) can easily be generalized to a diffeomorphism $h(x_1, \cdots, x_{2n})$, if the $2n$ coordinates are partitionned into pairs $\{x_{i_1}, x_{i_2}\}$, and if h acts on each pair independently of the others, that is to say, if for each pair (i_1, i_2), it has a corresponding pair of components h_{j_1} and h_{j_2}, which only depend upon the two coordinates x_{i_1} and x_{i_2}. Then, without loss of generality, the coordinates and the components can be reordered, so that

$$\forall i \in \{1, \cdots, n\}, \quad q_i = h_{2i-1}(x_{2i-1}, x_{2i}) \tag{39}$$

$$p_i = h_{2i}(x_{2i-1}, x_{2i})\ . \tag{40}$$

A fortiori, if each h_i only depends upon x_i, Eqs. (17), (18) and (19) can be generalized. This will give as many necessary conditions of the form (19) to be satisfied simultaneously, as the number of canonically conjugate disjoint pairs to be found. An example is given in the next section.

3.2 Kermack-McKendrick's model

The Kermack-McKendrick's model is a dynamical system for 3 real coordinates of the form,

$$\begin{aligned} \dot{x}_1 &= -rx_1x_2 && (41)\\ \dot{x}_2 &= +rx_1x_2 - ax_2 && (42)\\ \dot{x}_3 &= +ax_2\ , && (43) \end{aligned}$$

with $a, r \in \mathbb{R}^{+*}$, to which we add a dummy one:

$$\dot{x}_4 = 0 \quad \text{with} \quad x_4(0) = 0\ . \qquad (44)$$

We easily calculate:

$$\begin{aligned} \frac{\partial f_1(x_1,\cdots,x_4)}{\partial x_1} + \frac{d\ln(h_1'(x_1))}{dx_1}\cdot f_1(x_1,\cdots,x_4) &= -rx_2\left(1+\frac{d\ln(h_1'(x_1)}{dx_1}\cdot x_1\right)\\ \frac{\partial f_2(x_1,\cdots,x_4)}{\partial x_2} + \frac{d\ln(h_2'(x_2))}{dx_2}\cdot f_2(x_1,\cdots,x_4) &= (rx_1-a)\left(1+\frac{d\ln(h_2'(x_2)}{dx_2}\cdot x_2\right)\\ \frac{\partial f_3(x_1,\cdots,x_4)}{\partial x_3} + \frac{d\ln(h_3'(x_3))}{dx_3}\cdot f_3(x_1,\cdots,x_4) &= ax_2\frac{d\ln(h_3'(x_3)}{dx_3}\\ \frac{\partial f_4(x_1,\cdots,x_4)}{\partial x_4} + \frac{d\ln(h_4'(x_4))}{dx_4}\cdot f_4(x_1,\cdots,x_4) &= 0. \end{aligned}$$

These four quantities cancel out independently, if one takes: $h_1(x_1) = ln(x_1)$, $h_2(x_2) = ln(x_2)$, $h_3(x_3) = x_3$, $h_4(x_4) = x_4$, then, any two pairs can be canonically conjugate for a Hamiltonian system. Choosing $q_1 = h_1(x_1)$, $p_1 = h_2(x_2)$, $q_2 = h_3(x_3)$, $p_2 = h_4(x_4)$ and integrating the Hamilton equations we obtain the Hamiltonian, $H_{Kermack-McKendrick} = -r\exp q_1 + aq_1 + (ap_2 - r)\exp p_1$, which gives the correct equations, given that, solving the Hamilton's equations, $p_2 = x_4 = x_4(0) = 0$.

4 Concluding remarks

Since, it is possible that not all but only a subset of coordinates fulfills the necessary conditions imposed by the Schwartz equalities, we propose the following method to detect one or more pairs of variables amenable to be transformed into conjugate canonical variables following a canonical Hamiltonian dynamics.
(i) Calculate $\forall i \in \{1,\cdots,N\}$ the f_i-dependent part of $\frac{\partial f_i(x_1,\cdots,x_N)}{\partial x_i} + \frac{d\ln(h_i'(x_i))}{dx_i}\cdot f_i(x_1,\cdots,x_N)$
(ii) For all $i < N$, and $j > i$, try to find h_i and h_j such that Eq. (19) is satisfied for the pair (i,j). In case of success, add pair (i,j) to a set, $\mathcal{C}$, of potentially conjugate pairs.
(iii) Choose a maximal subset of disjoint pairs of $\mathcal{C}$, and transform the associated variables using the corresponding h functions.

Following such a path, it is possible to transform the three non-canonical systems considered in this work, namely a classical system derived from a forced two-level quantum model, Volterra's model and Kermack-McKendrick's model into canonical ones, in a very simple and straightforward fashion.

There is a lot of freedom in the choice of the two one-variable functions, h_1 and h_2, to fulfill constraint (19). So, we can expect that a large class of dynamical systems should be convertible into canonical ones, even within the severe restriction that the variables be transformed independently of each others.

Of course, not all dynamical systems are supposed to be amenable to our treatment. In particular, one could think of non-conservative systems, such as the damped pendulum,

$$\dot{x}_1 = x_2 \ , \tag{45}$$
$$\dot{x}_2 = -\omega^2 \ sin(x_1) - \mu \ x_2. \tag{46}$$

or the harmonic oscillator with friction (which is just its linearized version obtained by substituting x_1 to $sin(x_1)$). However, in these particular cases, and in fact, for any system with a force deriving from a potential $f(x_1) = -\frac{dV(x_1)}{dx_1}$ with a damping term of the form $-\mu(t)\dot{x}_1$,

$$\dot{x}_1 = x_2 \ , \tag{47}$$
$$\dot{x}_2 = -\frac{dV(x_1)}{dx_1} - \mu(t) \ x_2, \tag{48}$$

one can easily extend our method by using time-dependent transformations.
More explicitly, one retrieves the original, non-autonomous, non conservative, dynamical system by applying canonical Eqs. (3) and (4) to the conjugate coordinates q, p and the Hamiltonian H defined by the following equations:

$$q = h_1(x_1) = x_1 \ , \tag{49}$$
$$p = h_2(x_2) = exp\left(\int_0^t \mu(t')dt'\right) \ x_2, \tag{50}$$
$$H = \frac{exp\left(-\int_0^t \mu(t')dt'\right)}{2} p^2 + exp\left(\int_0^t \mu(t')dt'\right) V(q). \tag{51}$$

So, in fact, the applicability of our proposed method goes beyond what common belief would assume.

Acknowledgements

The Hamiltonian of the forced, two-level, quantum system was brought to our attention by Prof. Gilbert Reinisch. We acknowledge fruitful discussions with Profs. Zhiyan Zhao and Didier Clamond from Université Côte d'Azur. We are grateful to the referee for suggesting many improvements to our manuscript.

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