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Kahan–Hirota–Kimura maps preserving original cubic Hamiltonians

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ABSTRACT

We study the class of cubic Hamiltonian vector fields whose associated Kahan–Hirota–Kimura (KHK) maps preserve the original Hamiltonian function. Our analysis focuses on these fields in \mathbb{R}^2 and \mathbb{R}^4 , extending to a family of fields in \mathbb{R}^6 . Additionally, we investigate various properties of these fields, including the existence of additional first integrals of a specific type, their role as Lie symmetries of the corresponding KHK map, and the symplecticity of these maps.

1. Introduction

The Kahan–Hirota–Kimura discretization method (KHK, from now on) is a numerical method proposed, independently, by Kahan in [1,2] and Hirota and Kimura [3,4] to integrate quadratic vector fields. It is a one-step method, which is linearly implicit, and whose inverse is also linear implicit, so it defines a birational map $\Phi_h(\mathbf{x})$, where $\mathbf{x} \in \mathbb{R}^n$, which can be written as follows (see [5], for instance): given the vector field $X = \sum_{i=1}^n X_i \partial / \partial x_i$ with associated differential system

$$\dot{\mathbf{x}} = X(\mathbf{x}),$$

its associated KHK map is

$$\Phi_h(\mathbf{x}) = \mathbf{x} + h \left(I - \frac{1}{2} h DX(\mathbf{x}) \right)^{-1} X(\mathbf{x}), \quad (1)$$

where DX is the differential matrix of the field.

This method has been shown to be especially effective for the numerical integration of integrable quadratic systems in any finite dimension. This is because, on many occasions, the resulting associated discrete system (the KHK map), in turn, admits a first integral, see [5,6] for instance. The KHK maps are also important in the context of the theory of discrete integrability because, as other families like the QRT maps introduced by Quispel, Roberts, and Thompson at the end of the 1980s [7,8], they exhibit an important display of geometric and algebraic–geometric properties related with their dynamics [5,6,9–18].

In this paper, we will consider quadratic differential systems (vector fields) in \mathbb{R}^n with $n = 2, 4, 6$ possessing a cubic Hamiltonian function. In [5] it is proved that if the vector field has a cubic Hamiltonian, then its associated KHK map has a conserved quantity or first integral:

Theorem 1 (Celledoni, McLachlan, Owren, Quispel, [5]). *For all cubic Hamiltonian systems of the form $X_H = K \nabla H$, where K is a constant anti-symmetric matrix, on symplectic vector spaces and on all Poisson vector spaces with constant Poisson structure, the KHK method has a*

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first integral given by the modified Hamiltonian

$$\tilde{H}(\mathbf{x}) = H(\mathbf{x}) + \frac{1}{3} h \nabla H(\mathbf{x})^T \left(I - \frac{1}{2} h DX(\mathbf{x}) \right)^{-1} X(\mathbf{x}). \quad (2)$$

Recall that a map $\Phi : \mathcal{U} \subset \mathbb{R}^n \rightarrow \mathbb{R}^n$ admits a *first integral* $H : \mathcal{V} \subseteq \mathcal{U} \rightarrow \mathbb{R}$ defined in an open set \mathcal{V} if $H(\Phi(\mathbf{x})) = H(\mathbf{x})$, for all $\mathbf{x} \in \mathcal{V}$.

As a consequence of the above result, for a vector field with a Hamiltonian H satisfying the hypothesis of [Theorem 1](#), H is also a first integral of its associated KHK map if and only if it holds

$$\nabla H(\mathbf{x})^T \left(I - \frac{1}{2} h DX(\mathbf{x}) \right)^{-1} X(\mathbf{x}) = 0, \quad (3)$$

in this case we say that *the KHK map preserves the original Hamiltonian*.

Our objective is to investigate which vector fields with a cubic Hamiltonian have their original first integral preserved under the KHK discretization. Our analysis will be limited to even-dimensional spaces with the canonical Poisson structure [\[5\]](#). As we will see, the set of quadratic Hamiltonian vector fields satisfying [\(3\)](#) is non-empty and, for two or more degrees of freedom, non-trivial. Our initial purpose was to examine the relation between the fact that the KHK maps preserve a given cubic Hamiltonian and the fact that the original Hamiltonian vector field is a Lie symmetry of the map (see definition in [Section 2](#)). Although all the fields that we have found with one or two degrees of freedom are, indeed, Lie symmetries, we have been able to detect several quadratic Hamiltonian fields with three degrees of freedom, whose KHK maps preserve the initial Hamiltonian but which are not Lie symmetries of these maps.

The main results are [Theorems 4](#) and [9](#), where the set of cubic Hamiltonian vector fields with one or two degrees of freedom and whose associated KHK maps preserve the original Hamiltonian are characterized, and [Proposition 10](#) which establishes that in the case of three degrees of freedom there are examples whose vector fields are not Lie symmetries of their corresponding KHK maps. These results can be found in [Sections 3–5](#) respectively. In [Section 6](#) we explore the symplecticity of the maps considered in this work. In the final section, we outline key conclusions and suggest potential directions for future research.

2. Preliminaries and some definitions

In this section we recall some definitions, as well as result in [\[5\]](#), and we obtain and a direct consequence of this result.

A map Φ preserves a measure that is absolutely continuous with respect to Lebesgue measure and has a non-vanishing density ν if $m(\Phi^{-1}(B)) = m(B)$ for any Lebesgue measurable set $B \in \mathcal{U} \subseteq \mathbb{R}^n$, where $m(B) = \int_B \nu(x, y) dx$ with $dx = dx_1 \wedge \cdots \wedge dx_n$, which implies that

$$\nu(\Phi(\mathbf{x})) |D\Phi(\mathbf{x})| = \nu(\mathbf{x}), \quad (4)$$

where $|D\Phi(\mathbf{x})|$ is the determinant of the differential matrix $D\Phi$. In [\[5\]](#) it is proved the following result:

Proposition 2 ([\[5\]](#)). *For all cubic Hamiltonian systems on symplectic vector spaces and on all Poisson vector spaces with constant Poisson structure, the KHK maps have an invariant measure with density*

$$\nu(\mathbf{x}) = \frac{1}{\left| I - \frac{1}{2} h DX(\mathbf{x}) \right|}.$$

Given a differentiable map Φ defined in an open set $\mathcal{U} \in \mathbb{R}^n$, a *Lie symmetry* of Φ is a vector field X , defined in \mathcal{U} , such that Φ maps any orbit of the differential system

$$\dot{\mathbf{x}} = X(\mathbf{x}), \quad (5)$$

into another orbit of the system. Equivalently, it is a vector field such that the differential Eq. [\(5\)](#) is invariant by the change of variables $\mathbf{u} = \Phi(\mathbf{x})$. Such a vector field is characterized by the compatibility equation

$$X_{|\Phi(\mathbf{x})} = D\Phi(\mathbf{x}) X(\mathbf{x}), \quad (6)$$

for $\mathbf{x} \in \mathcal{U}$, where $X_{|\Phi(\mathbf{x})}$ means the vector field evaluated at $\Phi(\mathbf{x})$. See [\[19\]](#), for more details.

From a dynamical viewpoint, if Φ preserves a given orbit γ of X , there exists $\tau \geq 0$ such that $\Phi(p) = \varphi(\tau, p)$, for all $p \in \gamma$, where φ is the flow of X (i.e. τ only depends on γ). As a consequence of this fact, the action of Φ over the points in γ is linear [\[20, Theorem 1\]](#).

According to [Theorem 12](#) of [\[20\]](#), we have that if Φ is a planar map with a first integral H , then the vector field $X(\mathbf{x}) = \mu(\mathbf{x}) (-H_y, H_x)$ is a Lie symmetry of Φ if and only if the map has an invariant measure with density $\nu = 1/\mu$. As a consequence of this fact and of [Proposition 2](#), we obtain that all the planar KHK maps that come from a discretization of cubic Hamiltonians have a Lie symmetry:

Proposition 3. *Let Φ_h be a KHK map associated to a planar Hamiltonian vector field X with a cubic Hamiltonian H . Then, the vector field*

$$Y(x, y) = \left| I - \frac{1}{2} h DX(x, y) \right| \left(-\tilde{H}_y, \tilde{H}_x \right),$$

where \tilde{H} is given by [\(2\)](#) is a Lie symmetry of Φ_h .

3. One-degree of freedom systems

In this section, we consider the planar (one-degree of freedom) Hamiltonian vector field

$$X = -\frac{\partial H}{\partial y} \frac{\partial}{\partial x} + \frac{\partial H}{\partial x} \frac{\partial}{\partial y},$$

whose associated system is

$$\dot{x} = -\frac{\partial H}{\partial y} = -H_y, \quad \dot{y} = \frac{\partial H}{\partial x} = H_x, \quad (7)$$

with cubic Hamiltonian function

$$H(x, y) = \sum_{0 < i+j \leq 3} a_{ij} x^i y^j. \quad (8)$$

The main result of the section is the following:

Theorem 4. *The Hamiltonian vector fields of \mathbb{R}^2 with Hamiltonian functions of degree at most three, given by (8), for which their associated KHK maps preserve the original Hamiltonian, are:*

(a) *The vector field X_1 , with associated system*

$$\dot{x} = -(a_{11}x + 2a_{02}y + a_{01}), \quad \dot{y} = \frac{a_{11}}{2a_{02}} (a_{11}x + 2a_{02}y + a_{01}),$$

and Hamiltonian $H_1(x, y) = \frac{1}{4a_{02}} (a_{11}x + 2a_{02}y) (a_{11}x + 2a_{02}y + 2a_{01})$, whose associated KHK map is

$$\Phi_1(x, y) = \left(\begin{array}{c} (-ha_{11} + 1)x - 2ha_{02}y - ha_{01} \\ \frac{ha_{11}^2 x}{2a_{02}} + (ha_{11} + 1)y + \frac{ha_{01}a_{11}}{2a_{02}} \end{array} \right).$$

The functions $(H_1)_x$ and $(H_1)_y$ are also first integrals of X_1 , but functionally dependent on H_1 .

(b) *The vector field X_2 , with associated system*

$$\dot{x} = 0, \quad \dot{y} = 3a_{30}x^2 + 2a_{20}x + a_{10},$$

and Hamiltonian $H_2(x, y) = x(x^2a_{30} + a_{20}x + a_{10})$ whose associated KHK map is

$$\Phi_2(x, y) = \left(\begin{array}{c} x \\ 3hx^2a_{30} + 2ha_{20}x + ha_{10} + y \end{array} \right).$$

The function $(H_2)_x$ is also a first integral of X_2 , but functionally dependent on H_2 .

(c) *The vector field X_3 , with associated system*

$$\dot{x} = -a_{01}, \quad \dot{y} = a_{10},$$

and Hamiltonian $H_3(x, y) = a_{10}x + a_{01}y$ whose associated KHK map is $\Phi_3(x, y) = \left(\begin{array}{c} x - ha_{01} \\ y + ha_{10} \end{array} \right)$.

(d) *The vector field X_4 , with associated system*

$$\dot{x} = -3a_{03}y^2 - 2a_{02}y - a_{01}, \quad \dot{y} = 0,$$

and Hamiltonian $H_4(x, y) = y(a_{03}y^2 + a_{02}y + a_{01})$ whose associated KHK map is

$$\Phi_4(x, y) = \left(\begin{array}{c} -3ha_{03}y^2 - 2ha_{02}y - ha_{01} + x \\ y \end{array} \right).$$

The function $(H_4)_y$ is also a first integral of X_4 , but functionally dependent on H_4 .

(e) *The vector field X_5 , with associated system*

$$\dot{x} = -\frac{1}{3a_{03}a_{12}}P(x, y), \quad \dot{y} = \frac{1}{9a_{03}^2}P(x, y),$$

where $P(x, y) = a_{12}^3x^2 + 6a_{03}a_{12}^2xy + 9a_{03}a_{12}y^2 + 3a_{03}a_{11}a_{12}x + 9a_{03}^2a_{11}y + 9a_{03}^2a_{10}$, and Hamiltonian

$$H_5(x, y) = \frac{1}{54a_{03}^2a_{12}} (a_{12}x + 3a_{03}y) (2a_{12}^3x^2 + 12a_{03}a_{12}^2xy + 18a_{03}a_{12}y^2 + 9a_{03}a_{11}a_{12}x + 27a_{03}^2a_{11}y + 54a_{03}^2a_{10})$$

whose associated KHK map is

$$\Phi_5(x, y) = \left(\begin{array}{c} -\frac{ha_{12}^2x^2}{3a_{03}} + (-2ha_{12}y - ha_{11} + 1)x - 3ha_{03}y^2 - \frac{3ha_{11}a_{03}y}{a_{12}} - \frac{3ha_{10}a_{03}}{a_{12}} \\ \frac{ha_{12}^3x^2}{9a_{03}^2} + \left(\frac{2ha_{12}^2y}{3a_{03}} + \frac{ha_{11}a_{12}}{3a_{03}} \right)x + ha_{12}y^2 + (ha_{11} + 1)y + ha_{10} \end{array} \right).$$

The functions $(H_5)_x$ and $(H_5)_y$ are also first integrals of X_5 but functionally dependent on H_5 .

Furthermore, each vector field X_i , $i = 1, \dots, 5$ is a Lie symmetry of the corresponding map Φ_i .

We emphasize that, according to [Corollary 15](#) in Section 6, all the aforementioned maps Φ_i , $i = 1, \dots, 5$, are symplectic.

Remark 5. Additionally, we point out the following:

- (a) For all the families of vector fields $X = (P, Q)$ of [Theorem 4](#) we have $\Phi_h = (x + hP, y + hQ)$.
- (b) Under the change of coordinates $X = y, Y = x$ and $T = -t$ and renaming the constants $a_{30} \rightarrow a_{03}, a_{20} \rightarrow a_{02}, a_{10} \rightarrow a_{01}$ families X_2 and X_4 are the same.
- (c) For each specific case outlined in [Theorem 4](#), it is possible to apply particular rescalings to eliminate some of the parameters a_{ij} , thereby simplifying the expressions. However, in this article, we have chosen not to perform these specific rescalings in order to facilitate comparisons between the different families by maintaining a consistent set of common parameters.

To prove [Theorem 4](#), we first establish the following characterization of the conditions under which a system of the form (7) has an associated KHK map that preserves the original Hamiltonian.

Lemma 6. The KHK map (1) associated to a planar Hamiltonian system (7) preserves the original Hamiltonian function (8) if and only if

$$2H_x H_y H_{xy} - H_{xx} H_y^2 - H_{yy} H_x^2 = 0. \quad (9)$$

Observe that, by using the notation $\dot{g} = \{H, g\}$, where $\{ \}$ is the usual Poisson bracket and $\dot{} = d/dt$, see [21], Eq. (9) also writes as $\dot{H}_x H_y - \dot{H}_y H_x = 0$.

Proof of Lemma 6. Set $\mathbf{x} = (x, y)$ and $X(\mathbf{x}) = (-H_y, H_x)^T$, then we have

$$I - \frac{1}{2} h D X(\mathbf{x}) = \begin{pmatrix} 1 + \frac{1}{2} h H_{xy} & \frac{1}{2} h H_{yy} \\ -\frac{1}{2} h H_{xx} & 1 - \frac{1}{2} h H_{xy} \end{pmatrix}.$$

Relation (3) is

$$\begin{aligned} 0 &= \nabla H(\mathbf{x})^T \left(I - \frac{1}{2} h D X(\mathbf{x}) \right)^{-1} X(\mathbf{x}) \\ &= \frac{1}{A(x, y)} (H_x, H_y) \begin{pmatrix} 1 - \frac{1}{2} h H_{xy} & -\frac{1}{2} h H_{xx} \\ -\frac{1}{2} h H_{yy} & 1 + \frac{1}{2} h H_{xy} \end{pmatrix} \begin{pmatrix} -H_y \\ H_x \end{pmatrix} = 0, \end{aligned}$$

where $A(x, y) = 1 + \frac{1}{4} h^2 (H_{xx} H_{yy} - H_{xy}^2)$, which yields to

$$2H_x H_y H_{xy} - H_{xx} H_y^2 - H_{yy} H_x^2 = \{H, H_x\} H_y - \{H, H_y\} H_x = \dot{H}_x H_y - \dot{H}_y H_x = 0. \quad \blacksquare$$

Proof of Theorem 4. By imposing the relation (9) on a Hamiltonian of the form (7), and equating the coefficients with the aid of a computer algebra system, we obtain the following system of 21 equations given by:

$$\begin{aligned} a_{01}^2 a_{20} - a_{01} a_{10} a_{11} + a_{02} a_{10}^2 &= 0, \\ 2a_{02} a_{12} a_{30} + 3a_{03} a_{11} a_{30} + 2a_{03} a_{20} a_{21} - a_{11} a_{12} a_{21} &= 0, \\ 12a_{01} a_{02} a_{30} - 2a_{01} a_{11} a_{21} + 4a_{02} a_{11} a_{20} + 12a_{03} a_{10} a_{20} - 2a_{10} a_{11} a_{12} - a_{11}^3 &= 0, \\ 3a_{01}^2 a_{30} - 2a_{01} a_{10} a_{21} + 4a_{02} a_{10} a_{20} + a_{10}^2 a_{12} - a_{10} a_{11}^2 &= 0, \\ a_{30} (3a_{12} a_{30} - a_{21}^2) &= 0, \\ 4a_{02} a_{03} a_{21} - a_{02} a_{12}^2 + 3a_{03}^2 a_{20} - a_{03} a_{11} a_{12} &= 0, \\ 3a_{01} a_{11} a_{30} - 2a_{01} a_{20} a_{21} + 6a_{02} a_{10} a_{30} + 4a_{02} a_{20}^2 - 3a_{10} a_{11} a_{21} + 4a_{10} a_{12} a_{20} - a_{11}^2 a_{20} &= 0, \\ 6a_{02} a_{20} a_{30} + 3a_{10} a_{12} a_{30} - a_{10} a_{21}^2 - 2a_{11} a_{20} a_{21} + 2a_{12} a_{20}^2 &= 0, \\ 9a_{03} a_{30}^2 + 2a_{12} a_{21} a_{30} - a_{21}^3 &= 0, \\ 6a_{03} a_{21} a_{30} + a_{12}^2 a_{30} - a_{12} a_{21}^2 &= 0, \\ 6a_{02} a_{03} a_{30} + a_{03} a_{11} a_{21} + 2a_{03} a_{12} a_{20} - a_{11} a_{12}^2 &= 0, \\ 3a_{01} a_{12} a_{30} - a_{01} a_{21}^2 + 6a_{02} a_{11} a_{30} + 2a_{02} a_{20} a_{21} + 9a_{03} a_{10} a_{30} + 6a_{03} a_{20}^2 - a_{10} a_{12} a_{21} \\ - 2a_{11}^2 a_{21} &= 0, \end{aligned}$$

along with the equations derived from the above ones and the symmetry of the coefficients $a_{ij} \leftrightarrow a_{ji}$. The complete set of equations can be found in the extended version of this work, available on arXiv [22].

Using again the assistance of a symbolic computing software, we obtain the solutions of this system, obtaining that the only solutions are those that give rise to the Hamiltonians H_i , $i = 1, \dots, 5$, and its associated vector fields X_i and differential systems in the statement.

We can find the KHK maps associated with the corresponding Hamiltonian vector fields by using (1). Finally, by using the compatibility Eq. (6), we find that $X_{i|\Phi_i(x)} = D\Phi_i(x)X_i(x)$ for $i = 1, \dots, 5$, so each vector field X_i is a Lie symmetry of the maps Φ_i . ■

The dynamical and the algebraic–geometric properties of the KHK maps associated with *generic* planar Hamiltonian vector fields with cubic Hamiltonians have been studied in [14,16]. Remember that the space \mathcal{H}_3 of planar vector fields with cubic Hamiltonians is homeomorphic to \mathbb{R}^9 in the topology of the coefficients [23, p. 202]. A subset of this space is *generic* if it is open and dense. As a consequence of Theorem 1, the KHK maps associated with Hamiltonian vector fields preserve the cubic first integral \tilde{H} defined in (2). For the generic cases, the energy levels of this Hamiltonian \tilde{H} are, except perhaps for a finite set of levels, elliptic curves. Thus, the KHK maps associated with cubic Hamiltonians are, generically, birational integrable maps preserving genus-1 fibrations, and therefore can be described in terms of the linear action on the group structure of the preserved elliptic curves [24,25]. We notice, however, that the cases presented in Theorem 4 are, obviously, non-generic within the topological space of vector fields with cubic Hamiltonians, since Eq. (3) must be satisfied. More specifically:

Remark 7. The cases obtained in Theorem 4 correspond to instances where the pencil of elliptic curves associated with the Hamiltonian is always factorizable. The structure of the singular fibers of the elliptic fibrations associated with the modified Hamiltonians has been studied in [26, Corollary 2.12]. The families described in Theorem 5 are singular cases of those characterized in that reference.

As noticed in the above Remark there is no planar quadratic Hamiltonian system satisfying condition (3) (or equivalently, (9)) with cubic irreducible Hamiltonian function. Also, no one of the associated vector fields have coprime components. A straightforward analysis indicates that in all the cases in Theorem 4, the energy level sets are given by parallel straight lines, some of them (at most two) full of singular points of the associated differential systems. From a qualitative point of view, the dynamics of these fields is trivial, because either they are linear or, by reparameterizing the time, they give rise to systems with constant components. The dynamics of the associated KHK maps is, therefore, not so rich as the ones that are displayed in the general case studied, for instance in [6,12,14,16]. By construction, the obtained KHK maps will preserve the above mentioned invariant straight lines. This is also a consequence of the fact that, in general, the KHK maps preserve the affine Darboux polynomials of any quadratic ODE [27, Theorem 1] as well as, notably, the Runge–Kutta methods do [28, Theorem 3.1] (see also [29] for more information on using Darboux polynomials for the study of KHK maps). Let us give an example:

Example A. Consider the following Hamiltonian that belongs to the class of systems considered in statement (e) of Theorem 4:

$$\begin{aligned} H_5(x, y) &= \frac{1}{27}x^3 + \frac{1}{3}x^2y + xy^2 + y^3 - \frac{1}{6}x^2 - xy - \frac{3}{2}y^2 - x - 3y \\ &= \frac{1}{27}(x+3y)\left(x+3y-\frac{9}{4}+\frac{3\sqrt{57}}{4}\right)\left(x+3y-\frac{9}{4}-\frac{3\sqrt{57}}{4}\right). \end{aligned} \quad (10)$$

The Hamiltonian vector field has associated differential system $\{\dot{x} = -\frac{1}{3}P(x, y), \dot{y} = \frac{1}{9}P(x, y)\}$, with $P(x, y) = x^2 + 6xy + 9y^2 - 3x - 9y - 9$. The phase portrait of the system is, therefore, very simple: all the orbits lie in straight lines of the form $y = -x/3 + c$. The lines $y = -x/3 + (1 \pm \sqrt{5})/2$ are filled by singular points. Any orbit with initial condition (x_0, y_0) such that $-x_0/3 + (1 - \sqrt{5})/2 < y_0 < -x_0/3 + (1 + \sqrt{5})/2$ evolves to the right and down through a line of the form $y = -x/3 + c$. The rest of orbits, not in the singular lines, evolve to the left and up, see Fig. 1. The associated KHK map

$$\begin{aligned} \Phi(x, y) &= \left(-\frac{hx^2}{3} - 2hxy + (h+1)x - 3hy^2 + 3hy + 3h, \right. \\ &\quad \left. \frac{hx^2}{9} + \frac{2hxy}{3} - \frac{hx}{3} + hy^2 + (-h+1)y - h \right), \end{aligned}$$

captures these behaviors.

4. Two-degrees of freedom Hamiltonian systems

We consider Hamiltonian vector fields with two degrees of freedom

$$X = -\frac{\partial H}{\partial y} \frac{\partial}{\partial x} + \frac{\partial H}{\partial x} \frac{\partial}{\partial y} - \frac{\partial H}{\partial w} \frac{\partial}{\partial z} + \frac{\partial H}{\partial z} \frac{\partial}{\partial w},$$

with cubic Hamiltonian function

$$H(x, y, z, w) = \sum_{0 < i+j+k+l \leq 3} a_{ijkl} x^i y^j z^k w^l, \quad (11)$$

The associated two degrees of freedom Hamiltonian system is

$$\dot{x} = -\frac{\partial H}{\partial y} = -H_y, \quad \dot{y} = \frac{\partial H}{\partial x} = H_x, \quad \dot{z} = -\frac{\partial H}{\partial w} = -H_w, \quad \dot{w} = \frac{\partial H}{\partial z} = H_z. \quad (12)$$

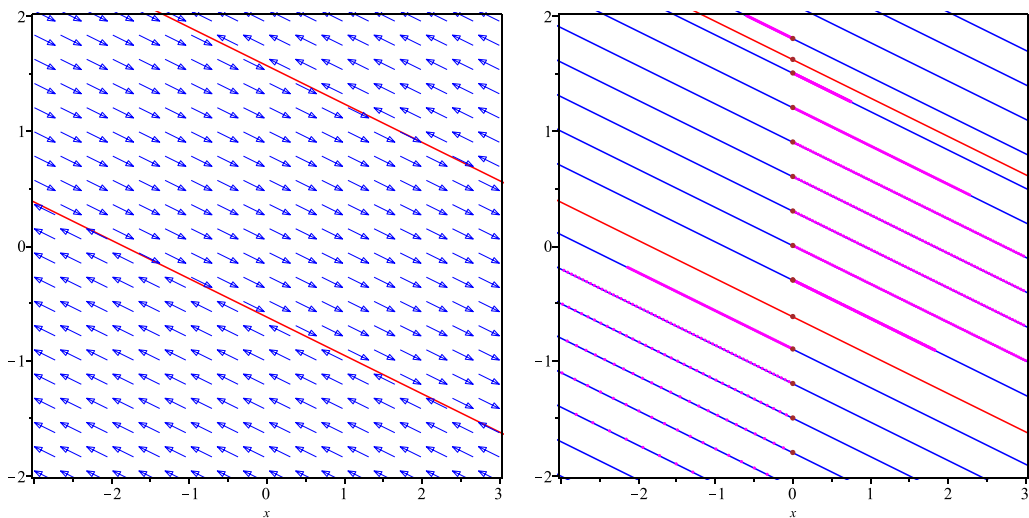


Fig. 1. (Left) Vector field associated to the Hamiltonian (10). The lines $y = -x/3 + (1 \pm \sqrt{5})/2$ are full of singular points, in red. (Right) Orbits of the Hamiltonian system (in blue). There are also shown 100 iterates of some orbits of the map Φ_h with $h = 0.01$ (in magenta), with initial conditions in brown. The lines filled by singular points of the vector field are also filled by fixed points of the map.

These fields can also be written in the form $q_i = \partial H / \partial p_i$, $p_i = -\partial H / \partial q_i$, with $q_1 = x, q_2 = z$ and $p_1 = y, p_2 = w$. The relation between the associated KHK maps Ψ_h of these vector fields and Φ_h , the ones associated with the fields in Eq. (12), is given by $\Psi_h(q_1, q_2, p_1, p_2) = (\Phi_{1,-h}, \Phi_{3,-h}, \Phi_{2,-h}, \Phi_{4,-h})(q_1, p_1, q_2, p_2)$. See Lemma 19 in Appendix.

The following result gives a characterization the conditions for which a system of the form (12) has an associated KHK map that preserves the original Hamiltonian.

Lemma 8. *The KHK map (1) associated with a Hamiltonian system (12) preserves the original Hamiltonian function (11) if and only if*

$$H_x \{H, H_y\} - H_y \{H, H_x\} + \{H, H_w\} H_z - \{H, H_z\} H_w = 0 \text{ and}$$

$$\begin{aligned} & H_x (\{H, H_y\} \{H_z, H_w\} - \{H, H_z\} \{H_y, H_w\} + \{H, H_w\} \{H_y, H_z\}) \\ & - H_y (\{H, H_x\} \{H_z, H_w\} - \{H, H_z\} \{H_x, H_w\} + \{H, H_w\} \{H_x, H_z\}) \\ & + H_z (\{H, H_x\} \{H_y, H_w\} - \{H, H_y\} \{H_x, H_w\} + \{H, H_w\} \{H_x, H_y\}) \\ & - H_w (\{H, H_x\} \{H_y, H_z\} - \{H, H_y\} \{H_x, H_z\} + \{H, H_z\} \{H_x, H_y\}) = 0. \end{aligned} \quad (13)$$

The first equation in (13) also writes as $\dot{H}_x H_y - \dot{H}_y H_x + \dot{H}_z H_w - \dot{H}_w H_z = 0$, where $\dot{g} = \{H, g\}$.

Proof of Lemma 8. In this case, the relation (3) gives

$$\nabla H(\mathbf{x})^T \left(I - \frac{1}{2} h D^2 X(\mathbf{x}) \right)^{-1} X(\mathbf{x}) = \frac{h(\Lambda_0 + \Lambda_2 h^2)}{\left| I - \frac{1}{2} h D^2 X(\mathbf{x}) \right|} = 0, \quad (14)$$

with

$$\begin{aligned} \Lambda_0 = & 8 (H_w^2 H_{zz} - 2H_w H_x H_{yz} + 2H_w H_{xz} H_y - 2H_w H_z H_{zw} + H_{ww} H_z^2 + H_x^2 H_{yy} \\ & - 2H_x H_{xy} H_y + 2H_x H_{yw} H_z - 2H_{xw} H_y H_z + H_{xx} H_y^2), \end{aligned}$$

and

$$\begin{aligned} \Lambda_2 = & 2 \left(H_x^2 H_{yy} H_{zz} H_{ww} - H_x^2 H_{yy} H_{zw}^2 - H_x^2 H_{yz}^2 H_{ww} + 2H_x^2 H_{yz} H_{yw} H_{zw} - H_x^2 H_{yz}^2 H_{zz} \right. \\ & - 2H_x H_y H_{xy} H_{zz} H_{ww} + 2H_x H_y H_{xy} H_{zw}^2 + 2H_x H_y H_{xz} H_{yz} H_{ww} - 2H_x H_y H_{xz} H_{yw} H_{zw} \\ & - 2H_{xw} H_x H_y H_{yz} H_{zw} + 2H_{xw} H_x H_y H_{yw} H_{zz} + 2H_x H_z H_{xy} H_{yz} H_{ww} \\ & - 2H_x H_z H_{xy} H_{yw} H_{zw} - 2H_x H_z H_{xz} H_{yy} H_{ww} + 2H_x H_z H_{xz} H_{yw}^2 + 2H_{xw} H_x H_z H_{yy} H_{zw} \\ & - 2H_{xw} H_x H_z H_{yz} H_{yw} - 2H_x H_w H_{xy} H_{yz} H_{zw} + 2H_x H_w H_{xy} H_{yw} H_{zz} \\ & + 2H_x H_w H_{xz} H_{yy} H_{zw} - 2H_x H_w H_{xz} H_{yz} H_{yw} - 2H_{xw} H_x H_w H_{yy} H_{zz} + 2H_{xw} H_x H_w H_{yz}^2 \\ & + H_y^2 H_{xx} H_{zz} H_{ww} - H_y^2 H_{xx} H_{zw}^2 - H_y^2 H_{xz}^2 H_{ww} + 2H_{xw} H_y^2 H_{xz} H_{zw} - H_{xw}^2 H_y^2 H_{zz} \\ & \left. - 2H_y H_z H_{xx} H_{yz} H_{ww} + 2H_y H_z H_{xx} H_{yw} H_{zw} + 2H_y H_z H_{xy} H_{xz} H_{ww} \right) \end{aligned}$$

$$\begin{aligned}
& -2H_{xw}H_yH_zH_{xy}H_{zw} - 2H_{xw}H_yH_zH_{xz}H_{yw} + 2H_{xw}^2H_yH_zH_{yz} + 2H_yH_wH_{xx}H_{yz}H_{zw} \\
& - 2H_yH_wH_{xx}H_{yw}H_{zz} - 2H_yH_wH_{xy}H_{xz}H_{zw} + 2H_{xw}H_yH_wH_{xy}H_{zz} + 2H_yH_wH_{xz}^2H_{yw} \\
& - 2H_{xw}H_yH_wH_{xz}H_{yz} + H_z^2H_{xx}H_{yy}H_{ww} - H_z^2H_{xx}H_{yw}^2 - H_z^2H_{xy}^2H_{ww} \\
& + 2H_{xw}H_z^2H_{xy}H_{yw} - H_{xw}^2H_z^2H_{yy} - 2H_zH_wH_{xx}H_{yy}H_{zw} + 2H_zH_wH_{xx}H_{yz}H_{yw} \\
& + 2H_zH_wH_{xy}^2H_{zw} - 2H_zH_wH_{xy}H_{xz}H_{yw} - 2H_{xw}H_zH_wH_{xy}H_{yz} + 2H_{xw}H_zH_wH_{xz}H_{yy} \\
& + H_w^2H_{xx}H_{yy}H_{zz} - H_w^2H_{xx}H_{yz}^2 - H_w^2H_{xy}^2H_{zz} + 2H_w^2H_{xy}H_{xz}H_{yz} - H_w^2H_{xz}^2H_{yy} \Big).
\end{aligned}$$

A computation shows that

$$\begin{aligned}
\frac{A_0}{8} &= \{H, H_x\}H_y - \{H, H_y\}H_x + \{H, H_z\}H_w - \{H, H_w\}H_z \\
&= \dot{H}_xH_y - \dot{H}_yH_x + \dot{H}_zH_w - \dot{H}_wH_z,
\end{aligned}$$

where $\dot{} = d/dt$, so we obtain the first equation in (13). Analogously, an involved but straightforward computation shows that $A_2/2$ is the left hand side of the second equation. ■

The following result summarizes the information we have obtained by solving Eq. (13) for a Hamiltonian of the form (11). Our calculations rely on the use of computer algebra software (Maple, in our case). In the expanded version of this work [22], we present 54 non-trivial families of Hamiltonians preserved by the associated KHK maps. Unfortunately, we cannot guarantee that these solutions are the only ones. Given the length and complexity of the formulas, we believe it is not practical to explicitly list these families in this paper. Instead, we refer the reader to the aforementioned extended version of this article.

Theorem 9. *The following statements hold:*

- (a) *There are 54 families of Hamiltonian vector fields X_i for $i = 1, \dots, 54$ in \mathbb{R}^4 , with Hamiltonian functions of degree at most three, as given by (11), for which their associated KHK maps $\Phi_{i,h}$ preserve the original Hamiltonian. The corresponding Hamiltonians H_i are listed in Appendix B of [22].*
- (b) *All vector fields corresponding to these Hamiltonians are Lie symmetries of the associated KHK maps.*
- (c) *Some of the vector fields in the list, with Hamiltonian H , admit at least one additional first integral from the set $\{H_x, H_y, H_z, H_w\}$, with only one being functionally independent of H . These vector fields are presented in Tables 1 and 2 below. In all cases, the corresponding KHK maps also preserve the same additional first integrals.*
- (d) *All Hamiltonian vector fields in the list, with Hamiltonian H , that possess another first integral from the set $\{H_x, H_y, H_z, H_w\}$, which is functionally independent of H , commute with the Hamiltonian vector field associated with the additional first integral.*

All the KHK maps associated with the vector fields referred to in the previous result are symplectic in the sense that they satisfy Eq. (25) from Section 6. See Proposition 16 for further details.

Proof (a). By imposing that a Hamiltonian of the form (11) satisfies the condition (13), we find that the expressions A_0 and A_2 , which appear in Eq. (14), are polynomials that must be identically zero. These polynomials have degrees 5 and 7 in the variables x, y, z, w , and contain 126 and 330 coefficients, respectively. Setting them to zero, we obtain a system of 456 equations in the coefficients. By solving this system using the computer algebra software Maple on a laptop, we find 54 solutions, which correspond to 54 Hamiltonians presented in Appendix B of [22].

By directly inspecting the vector fields X_i associated with the corresponding Hamiltonians H_i $i = 1, \dots, 54$, we compile the information presented in the first four columns of Table 1. Statements (b), (c), and (d) are derived through straightforward computations, which can be carried out using a computer algebra system. ■

We present two examples.

Example B. We consider the following Hamiltonian function, which corresponds to a particular case of the family H_3 in [22, Appendix B], given by

$$\begin{aligned}
H(x, y, z, w) &= x^3 - 2x^2z - 2x^2w + xz^2 + 2xzw + xw^2 - 2x^2 - xy + 2xz \\
&\quad + xw + yz + yw + zw + w^2 + x + y + w \\
&= (-x + z + w + 1)(-x^2 + xz + xw + x + y + w).
\end{aligned}$$

The Hamiltonian vector field X is given by the differential system:

$$\begin{aligned}
\dot{x} &= x - z - w - 1, \\
\dot{y} &= 3x^2 - 4xz - 4xw + z^2 + 2zw + w^2 - 4x - y + 2z + w + 1, \\
\dot{z} &= 2x^2 - 2xz - 2xw - x - y - z - 2w - 1, \\
\dot{w} &= -2x^2 + 2xz + 2xw + 2x + y + w.
\end{aligned} \tag{15}$$

The associated KHK map of the vector field (15) is: $\Phi_h(x, y, z, w) = (\Phi_1, \Phi_2, \Phi_3, \Phi_4)$, where

$$\Phi_1 = (h+1)x - wh - zh - h,$$

Table 1Collected information about the vector fields X_i associated to the Hamiltonians H_i in [22, Appendix B].

\exists null components	\exists common factors	Linear systems	True quadratic
$X_1, X_6, X_8, X_9,$ $X_{10}, X_{11}, X_{12}, X_{13},$ $X_{14}, X_{15}, X_{20}, X_{37},$ X_{42}, X_{51}	$X_1, X_8, X_9, X_{12},$ $X_{13}, X_{14}, X_{20}, X_{22},$ $X_{28}, X_{32}, X_{38}, X_{39},$ $X_{42}, X_{44}, X_{45}, X_{46},$ $X_{47}, X_{49}, X_{50}, X_{51},$ X_{53}	$X_4, X_5, X_7, X_{17},$ $X_{21}, X_{23}, X_{24}, X_{25},$ $X_{26}, X_{27}, X_{29}, X_{32},$ $X_{33}, X_{34}, X_{35}, X_{36},$ $X_{40}, X_{41}, X_{42}, X_{43},$ $X_{44}, X_{48}, X_{49}, X_{52},$ X_{54}	$X_1, X_2, X_3, X_6,$ $X_8, X_9, X_{10}, X_{11},$ $X_{12}, X_{13}, X_{14}, X_{15},$ $X_{16}, X_{18}, X_{19}, X_{20},$ $X_{22}, X_{28}, X_{30}, X_{31},$ $X_{37}, X_{38}, X_{39}, X_{45},$ $X_{46}, X_{47}, X_{50}, X_{53}$
First integral H_x	First integral H_y	First integral H_z	First integral H_w
$X_1, X_6, X_8, X_9, X_{10},$ $X_{11}, X_{12}, X_{13}, X_{14},$ $X_{20}, X_{25}, X_{38}, X_{39},$ $X_{42}, X_{44}, X_{45}, X_{46},$ $X_{47}, X_{49}, X_{50}, X_{53}$	$X_3, X_8, X_9, X_{10}, X_{12},$ $X_{13}, X_{14}, X_{22}, X_{25},$ $X_{28}, X_{32}, X_{34}, X_{37},$ $X_{38}, X_{39}, X_{42}, X_{44},$ $X_{45}, X_{46}, X_{47}, X_{49},$ X_{50}, X_{51}, X_{53}	$X_1, X_8, X_9, X_{11}, X_{12},$ $X_{13}, X_{14}, X_{15}, X_{20},$ $X_{25}, X_{32}, X_{38}, X_{39},$ $X_{44}, X_{45}, X_{46}, X_{47},$ $X_{49}, X_{50}, X_{51}, X_{53}$	$X_1, X_6, X_{15}, X_{20}, X_{22},$ $X_{25}, X_{28}, X_{30}, X_{31},$ $X_{37}, X_{38}, X_{39}, X_{42},$ $X_{44}, X_{45}, X_{46}, X_{47},$ $X_{49}, X_{50}, X_{51}, X_{53}$

Table 2Additional first integrals for the systems X_i associated to the Hamiltonians H_i in [22, Appendix B].

X	First integrals	Rank	c	X	First integrals	Rank	c
X_1	$H, H_x, H_z = cH_w$	2	$c = \frac{a_{1001}}{2a_{1002}}$	X_2	H	1	
X_3	H, H_y	2		X_4	H	1	
X_5	H	1		X_6	H, H_x, H_w	2	
X_7	H	1		X_8	$H, H_x = cH_y, H_z$	2	$c = \frac{a_{1100}}{2a_{0200}}$
X_9	$H, H_x = cH_y, H_z$	2	$c = \frac{a_{1110}}{2a_{0210}}$	X_{10}	H, H_x, H_y	2	
X_{11}	H, H_x, H_z	2		X_{12}	$H, H_x = cH_y, H_z$	2	$c = \frac{a_{1110}}{2a_{0210}}$
X_{13}	$H, H_x = cH_y, H_z$	2	$c = \frac{a_{1100}}{2a_{0200}}$	X_{14}	$H, H_x = cH_y, H_z$	2	$c = \frac{a_{1110}}{2a_{0210}}$
X_{15}	H, H_z, H_w	2		X_{16}	H	1	
X_{17}	H	1		X_{18}	H	1	
X_{19}	H	1		X_{20}	$H, H_x, H_z = cH_w$	2	$c = \frac{a_{0011}}{2a_{0002}}$
X_{21}	H	1		X_{22}	$H, H_y = cH_w$	2	$c = \frac{a_{0110}}{a_{0011}}$
X_{23}	H	1		X_{24}	H	1	
X_{25}	H, H_x, H_y, H_z, H_w	2		X_{26}	H	1	
X_{27}	H	1		X_{28}	$H, H_y = cH_w$	2	$c = \frac{a_{0100}}{a_{0001}}$
X_{29}	H	1		X_{30}	H, H_w	2	
X_{31}	H, H_w	2		X_{32}	$H, H_y = cH_z,$	2	$c = \frac{a_{0101}}{a_{1100}}$
X_{33}	H	1		X_{34}	H, H_y	2	
X_{35}	H	1		X_{36}	$H,$	1	
X_{37}	H, H_y, H_w	2		X_{38}	$H, H_x = c_1 H_z, H_y = c_2 H_w$	2	$c_1 = -\frac{a_{0101}}{2a_{0200}}, c_2 = \frac{2a_{0200}}{a_{0101}}$
X_{39}	$H, H_x = c_1 H_z, H_y = c_2 H_w$	2	$c_1 = -\frac{a_{0101}}{2a_{0200}}, c_2 = \frac{2a_{0200}}{a_{0101}}$	X_{40}	H	1	
X_{41}	H	1		X_{42}	$H, H_x = H_y, H_w$	2	
X_{43}	H	1		X_{44}	$H, H_x, H_y = cH_w, H_z$	2	$c = \frac{2a_{0200}}{a_{0101}}$
X_{45}	$H, H_x, H_y = cH_w, H_z$	2	$c = -\frac{a_{1000}}{a_{2010}}$	X_{46}	$H, H_x, H_y = cH_w, H_z$	2	$= -\frac{a_{1020}}{a_{2010}}$
X_{47}	$H, H_x, H_y = cH_w, H_z$	2	$c = \frac{2a_{0200}}{a_{0101}}$	X_{48}	H	1	
X_{49}	$H, H_x, H_y = cH_w, H_z$	2	$c = -\frac{a_{1010}}{2a_{0200}}$	X_{50}	$H, H_x, H_y = cH_w, H_z$	2	$c = -\frac{a_{1010}}{2a_{0200}}$
X_{51}	$H, H_y, H_z = cH_w$	2	$c = \frac{a_{0110}}{a_{0101}}$	X_{52}	$H,$	1	
X_{53}	$H, H_x, H_y = cH_w, H_z$	2	$c = \frac{2a_{0200}}{a_{0101}}$	X_{54}	H	1	

$$\begin{aligned}
\Phi_2 &= \frac{h(h+6)x^2}{2} - h(h+4)xz - h(h+4)xw - h(h+4)x + (1-h)y + \frac{h(h+2)z^2}{2} \\
&\quad + h(h+2)zw + h(h+2)z + \frac{h(h+2)w^2}{2} + h(h+1)w + \frac{h(h+2)}{2}, \\
\Phi_3 &= \frac{h(h+4)x^2}{2} - h(h+2)xz - h(h+2)xw - h(h+1)x - hy + \frac{h^2z^2}{2} + h^2wz \\
&\quad + (h^2 - h + 1)z + \frac{h^2w^2}{2} + h(h-2)w + \frac{h(h-2)}{2}, \\
\Phi_4 &= -\frac{h(h+4)x^2}{2} + h(h+2)xz + h(h+2)xw + h(h+2)x + hy - \frac{h^2z^2}{2} - h^2wz - h^2z \\
&\quad - \frac{h^2w^2}{2} + (-h^2 + h + 1)w - \frac{h^2}{2}.
\end{aligned}$$

An interesting issue is that the vector field X commute with the constant vector field Y associated to the Hamiltonian function H_y , whose differential system is $\{\dot{x} = 0, \dot{y} = -1, \dot{z} = -1, \dot{w} = 1\}$, that is: $[X, Y] = 0$. This fact has led us to verify, using a computer algebra software, that this happens for each of the families of vector fields in [Theorem 9](#), as reads its statement (d). Furthermore, in the above example, the maps Φ_h commute with the KHK maps associated with Y , given by $\Psi_k(x, y, z, w) = (x, y - k, z - k, w + k)$. That is, $\Phi_h \circ \Psi_k = \Psi_k \circ \Phi_h$ for all h and $k \in \mathbb{R}$.

Finally, from [Theorem 9\(b\)](#), the vector field X is a Lie symmetry of Φ_h , since an easy computation shows that $X|_{\Phi_h} = D\Phi_h X$. Interestingly, a computation also shows that $Y|_{\Phi_h} = D\Phi_h Y$ so the vector field Y is also a Lie symmetry of Φ_h .

As a final remark, we notice that, of course, using the extra first integral H_y , we can do a dimension reduction, so that the vector field X is reduced to linear vector field in \mathbb{R}^3 . This reduced vector field has a linear first integral that allows a new dimension reduction.

Example C. We consider the following Hamiltonian function, which corresponds to a particular case of the family H_1 in [\[22\]](#), given by

$$H(x, y, z, w) = -2x^3 - 4x^2z - 4x^2w + \frac{1}{2}xz^2 + xzw + \frac{1}{2}xw^2 + x^2 + 3xz + 3xw + \frac{1}{2}z^2 + zw + \frac{1}{2}w^2.$$

The associated vector field X is given by

$$\begin{aligned}\dot{x} &= 0, \\ \dot{y} &= -6x^2 - 8xz - 8xw + \frac{1}{2}z^2 + zw + \frac{1}{2}w^2 + 2x + 3z + 3w, \\ \dot{z} &= 4x^2 - xz - xw - 3x - z - w, \\ \dot{w} &= -4x^2 + xz + xw + 3x + z + w,\end{aligned}$$

and it has an associated KHK map is $\Phi_h(x, y, z, w) = (\Phi_1, \Phi_2, \Phi_3, \Phi_4)$, with

$$\begin{aligned}\Phi_1 &= x, \\ \Phi_2 &= -6hx^2 - 8hxz - 8hxw + \frac{1}{2}hz^2 + hzw + \frac{1}{2}hw^2 + 2hx + y + 3hz + 3hw, \\ \Phi_3 &= 4hx^2 - hxz - hxw - 3hx + (1-h)z - hw, \\ \Phi_4 &= -4hx^2 + hxz + hxw + 3hx + hz + hw + w.\end{aligned}$$

The vector field X has another first integral

$$H_x(x, y, z, w) = -6x^2 - 8xz - 8xw + \frac{1}{2}z^2 + zw + \frac{1}{2}w^2 + 2x + 3z + 3w,$$

which is functionally independent on H . The linear Hamiltonian vector field Y associated with H_x is given by

$$\begin{aligned}\dot{x} &= 0, \\ \dot{y} &= -12x - 8z - 8w + 2, \\ \dot{z} &= 8x - z - w - 3, \\ \dot{w} &= -8x + z + w + 3,\end{aligned}$$

and it has the associated KHK map

$$\Psi_k(x, y, z, w) = (x, y + k(-12x - 8z - 8w + 2), z + k(8x - z - w - 3), w + k(8x - z - w - 3)).$$

As in the Example B, a straightforward computation shows that $[X, Y] = 0$ and, therefore, the vector fields commute; also for all $k, h \in \mathbb{R}$, it holds that $\Phi_h \circ \Psi_k = \Psi_k \circ \Phi_h$.

Of course, since one of the components of the vector field X is null and there exists another first integral which is functionally independent on H , the vector field X admits suitable dimension reductions.

5. Three-degrees of freedom Hamiltonian systems

We consider the planar three-degrees of freedom Hamiltonian vector field

$$X = -\frac{\partial H}{\partial y} \frac{\partial}{\partial x} + \frac{\partial H}{\partial x} \frac{\partial}{\partial y} - \frac{\partial H}{\partial w} \frac{\partial}{\partial z} + \frac{\partial H}{\partial z} \frac{\partial}{\partial w} - \frac{\partial H}{\partial s} \frac{\partial}{\partial r} + \frac{\partial H}{\partial r} \frac{\partial}{\partial s},$$

with cubic Hamiltonian function

$$H(x, y, z, w, r, s) = \sum_{0 \leq i+j+k+l+m+n \leq 3} a_{ijklmn} x^i y^j z^k w^l r^m s^n. \quad (16)$$

The associated two degrees of freedom Hamiltonian system is

$$\dot{x} = -H_y, \quad \dot{y} = H_x, \quad \dot{z} = -H_w, \quad \dot{w} = H_z, \quad \dot{r} = -H_s, \quad \dot{s} = H_r, \quad (17)$$

which also can be re-written as $q_i = \partial H / \partial p_i$, $p_i = -\partial H / \partial q_i$, with $q_1 = x, q_2 = z, q_3 = r$ and $p_1 = y, p_2 = w, p_3 = s$. The relationship between the fields in both notations and their associate KHK maps is explained in Lemma 19 in Appendix.

By imposing condition (3) on a Hamiltonian function (16) with the aid of a computer algebra system, we obtain that the KHK map (1) associated to a Hamiltonian system (17) preserves the original Hamiltonian function (16) if and only if

$$\nabla H(\mathbf{x})^T \left(I - \frac{1}{2} h D X(\mathbf{x}) \right)^{-1} X(\mathbf{x}) = \frac{h(A_0 + A_2 h^2 + A_4 h^4)}{\left| I - \frac{1}{2} h D X(\mathbf{x}) \right|} = 0, \quad (18)$$

where A_0, A_2, A_4 are polynomials in the partial derivatives of first and second order of H with respect x, y, z, w, r , and s , of degrees 3, 5 and 7, respectively, in these partial derivatives (see Remark 12, below). For instance, the polynomial A_0 is given by

$$\begin{aligned} A_0 = & 32 \left(-H_x^2 H_{yy} + 32 H_x H_y H_{xy} - 32 H_x H_z H_{yw} + 32 H_x H_w H_{yz} + 32 H_x H_s H_{yr} \right. \\ & - 32 H_x H_r H_{ys} - H_y^2 H_{xx} + 32 H_y H_z H_{xw} - 32 H_y H_w H_{xz} - 32 H_y H_s H_{xr} \\ & + 32 H_y H_r H_{xs} - H_z^2 H_{ww} + 32 H_z H_w H_{zw} + 32 H_z H_s H_{wr} - 32 H_z H_r H_{ws} \\ & \left. - H_w^2 H_{zz} - 32 H_w H_s H_{zr} + 32 H_w H_r H_{zs} - H_s^2 H_{rr} + 32 H_s H_r H_{rs} - H_r^2 H_{ss} \right). \end{aligned} \quad (19)$$

We do not reproduce A_2 and A_4 here because they have 450 and 2073 coefficients, respectively, as polynomials in the partial derivatives.

The polynomials A_0, A_2, A_4 have degree 5, 7 and 9 in the variables x, y, z, w, r and s , respectively, so they have 462,1716 and 5005 coefficients respectively. Equaling them to zero we obtain that the Hamiltonians in \mathbb{R}^6 satisfying condition (3), must satisfy a system of 7183 equations in their coefficients. We have tried to solve the system using Maple in a parallel computer server formed by 9 nodes with 512 GB RAM memory, in a Beowulf configuration, but we have not succeeded.

By imposing some additional restrictions on the equations we have been able to find several dozens of non-trivial solutions. However, we are far from being able to claim that we have achieved all the solutions. In any case, as we will see below, the most interesting thing is that we have obtained cases for which the associated vector field (17) is not a Lie symmetry of the associated KHK map:

Proposition 10. *There exist Hamiltonian vector fields of \mathbb{R}^6 with Hamiltonian functions (16) of degree at most three, for which their associated KHK maps preserve the original Hamiltonian function. Furthermore, not all of them give rise to Hamiltonian vector fields of the form (17) which are Lie symmetries of the corresponding KHK maps.*

Proof. Imposing, for example, $H_x = H_y$ (the choice of the pair x and y is not relevant, analogous results would be obtained by imposing $H_z = H_w$ or $H_r = H_s$) and solving with Maple the equation $A_0 = 0$ we obtain a list of non-trivial solutions which also satisfy Eq. (18). Among them, the one that corresponds to the 10-parameter family of Hamiltonian systems given in Proposition 22 of the extended version of this work [22, Appendix C]. A simple example in this family is:

$$H = (x + y)(azr + w) + bzs. \quad (20)$$

with associated vector field

$$X = (-azr - w, azr + w, -x - y, ar(x + y) + bs, -bz, az(x + y)),$$

whose KHK map is $\Phi_h = (\Phi_{1,h}, \Phi_{2,h}, \Phi_{3,h}, \Phi_{4,h}, \Phi_{5,h}, \Phi_{6,h})$ with

$$\begin{aligned} \Phi_{1,h} &= (-haz(h^2b(x+y) - 2hbz + 4r) + 4x - 4hw - 2bh^2s) / 4, \\ \Phi_{2,h} &= (haz(h^2b(x+y) - 2hbz + 4r) + 4y + 4hw + 2bh^2s) / 4, \\ \Phi_{3,h} &= -h(x + y) + z, \\ \Phi_{4,h} &= ha(x + y)r + w + bhs, \\ \Phi_{5,h} &= (h^2b(x + y) - 2hbz + 2r) / 2, \\ \Phi_{6,h} &= (-ah(x + y)(h(x + y) - 2z) + 2s) / 2. \end{aligned} \quad (21)$$

A straightforward computation shows that

$$X|_{\Phi_h} - D\Phi_h X = \left(\frac{ab(x+y)^2 h^3}{4}, -\frac{ab(x+y)^2 h^3}{4}, 0, 0, 0, 0 \right)^T.$$

Hence, if $ab \neq 0$, then the vector field X is not a Lie symmetry of Φ_h . ■

The following observations are due to a reviewer of a previous version. We have not delved into these questions in this work.

Remark 11. *The direct inspection of the components of the first iterates of the KHK map Φ_h in Eq. (21), indicates that the (algebraic) degree of the first iterates remains constant, which, if confirmed, would imply that the algebraic entropy of this map is 0, as well as the possible existence of a linearization and additional first integrals, [30,31].*

Remark 12. Based on the formulas in the proof of Lemma 6 as well as Eqs. (14) and (18), it appears that a pattern may emerge regarding the conditions for exact preservation of the Hamiltonian. It seems that for a general system with d -degrees of freedom, the condition (3) can be expressed as:

$$\nabla H(\mathbf{x})^T \left(I - \frac{1}{2} h DX(\mathbf{x}) \right)^{-1} X(\mathbf{x}) = \frac{h}{\left| I - \frac{1}{2} h DX(\mathbf{x}) \right|} \sum_{\ell=0}^{d-1} h^{2\ell} \Lambda_{2\ell} = 0$$

for some suitable polynomials $\Lambda_{2\ell}$ of degree $2(\ell + 1) + 1$ in the derivatives of H .

6. Some considerations on the symplecticity of the maps

As we have indicated in the introduction, our initial purpose was to examine analytically whether the Hamiltonian fields X_H in \mathbb{R}^n for which their associated KHK maps preserve the same cubic Hamiltonian H were also Lie symmetries of these maps. From Proposition 10, we now know that this is not true in general, although it is true in all the cases found in \mathbb{R}^2 and \mathbb{R}^4 .

Once this point was clarified, a second objective was to explore if under the initial hypothesis of the preservation of the original Hamiltonian H , the fact that the field X_H is a Lie symmetry of the KHK map Φ_h is related with the symplecticity of the map. In this section, we will see that if a symplectic map Φ (not necessarily KHK) preserves a C^1 first integral, then the Hamiltonian vector field X_H is a Lie symmetry of Φ . The converse is true for planar maps (Proposition 14).

Set $\mathbf{x} \in \mathbb{R}^{2n}$. A map $\Phi(\mathbf{x})$ is symplectic if and only if $D\Phi(\mathbf{x})^t \Omega D\Phi(\mathbf{x}) = \Omega$, where

$$\Omega = \begin{pmatrix} \mathbf{0} & I_n \\ -I_n & \mathbf{0} \end{pmatrix},$$

see [21]. By using that a matrix M is symplectic if and only if M^t is symplectic, we will use the following equivalent condition of symplecticity:

$$D\Phi(\mathbf{x}) \Omega D\Phi(\mathbf{x})^t = \Omega. \quad (22)$$

For general C^1 maps, we have the following result:

Proposition 13. Let Φ be a symplectic C^1 map defined in an open set $\mathcal{U} \subseteq \mathbb{R}^{2n}$. Let H be a C^1 first integral of Φ in \mathcal{U} . Then, the Hamiltonian vector field $X_H = \Omega \nabla H$ is a Lie symmetry of Φ .

Proof. Observe that if H is a first integral of Φ , then $\nabla H(\Phi(\mathbf{x}))^t D\Phi(\mathbf{x}) = \nabla H(\mathbf{x})^t$, hence

$$\nabla H(\mathbf{x}) = D\Phi(\mathbf{x})^t \nabla H(\Phi(\mathbf{x})). \quad (23)$$

We have to prove that the compatibility relation (6) holds. By using the symplecticity condition (22) and Eq. (23) we have,

$$X_H|_{\Phi(\mathbf{x})} = \Omega \nabla H(\Phi(\mathbf{x})) = D\Phi(\mathbf{x}) \Omega D\Phi(\mathbf{x})^t \nabla H(\Phi(\mathbf{x})) = D\Phi(\mathbf{x}) \Omega \nabla H(\mathbf{x}) = D\Phi(\mathbf{x}) X_H(\mathbf{x}). \quad \blacksquare$$

Proposition 13 agrees with the result of Ge (that can be found in the work of Ge and Marsden [32, p. 135]), that states that if a discretization method for a Hamiltonian vector field with no other first integral, preserves the Hamiltonian function and it is symplectic, then it is the time advance map up to a reparametrization of time. This time advance property happens when a field X is a Lie symmetry of a C^1 map Φ which preserves the orbits of X , see [20, Proposition 6], and also Section 2.

The converse of Proposition 13 is true for fields in \mathbb{R}^2 :

Proposition 14. Let Φ be a C^1 map defined in an open set $\mathcal{U} \subseteq \mathbb{R}^2$, and let H be a C^1 first integral of Φ in \mathcal{U} . Then, the planar Hamiltonian vector field $X_H = \Omega \nabla H$ is a Lie symmetry of Φ if and only if the map is symplectic.

Proof. Taking into account Proposition 13, we only have to prove the converse relation, that is, that if X_H is a Lie symmetry of the map Φ , then the map is symplectic. A straightforward computation shows that for $\mathbf{x} \in \mathbb{R}^2$,

$$D\Phi(\mathbf{x}) \Omega D\Phi(\mathbf{x})^t - \Omega = (|D\Phi(\mathbf{x})| - 1) \Omega.$$

Hence, a planar C^1 map Φ defined in an open set $\mathcal{U} \subseteq \mathbb{R}^2$ is symplectic if and only if $|D\Phi(\mathbf{x})| = 1$ for $\mathbf{x} \in \mathcal{U}$. On the other hand, as mentioned in Section 2, a vector field

$$X(\mathbf{x}) = \frac{1}{v(\mathbf{x})} (-H_y, H_x) = -\frac{1}{v(\mathbf{x})} \Omega \nabla H,$$

is a Lie symmetry of a map Φ , with first integral H , if and only if v is an invariant measure. As a consequence, the Hamiltonian field $X = (-H_y, H_x) = -\Omega \nabla H = -X_H$ is a Lie symmetry of a map Φ in \mathcal{U} if and only if the map preserves the measure with density $v(\mathbf{x}) = 1$ for $\mathbf{x} \in \mathcal{U}$, but in this case, from Eq. (4), we get that $|D\Phi(\mathbf{x})| = 1$. Of course, if X is a Lie symmetry so is $X_H = -X$, and the result follows. \blacksquare

Corollary 15. The planar KHK maps associated with the Hamiltonian fields in Theorem 4 are symplectic.

Note that, the Hamiltonian vector fields in Sections 4 and 5 have the form $X(\mathbf{x}) = B\nabla H(\mathbf{x})$, where B is the $(2n) \times (2n)$ matrix given by the anti-symmetric matrix

$$B = \begin{pmatrix} 0 & -1 & & 0 & 0 \\ 1 & 0 & & 0 & 0 \\ & & \ddots & & \\ 0 & 0 & & 0 & -1 \\ 0 & 0 & & 1 & 0 \end{pmatrix}. \quad (24)$$

The Lemma 19 in Appendix relates this kind of Hamiltonian vector fields and their associated KHK maps with the Hamiltonian fields written in canonical form and their associated KHK map. In summary, a field of the form $X(\mathbf{x}) = B\nabla H(\mathbf{x})$ with associated KHK map $\Phi_h(\mathbf{x})$, where $\mathbf{x} = (x_1, \dots, x_{2n}) \in \mathbb{R}^{2n}$, conjugates through the change of variables $x_1 = q_1, x_2 = p_1, x_3 = q_2, x_4 = p_2, \dots, x_{2n-1} = q_n, x_{2n} = p_n$, and a time parametrization $t \rightarrow -t$, with the field

$$Y_{\tilde{H}}(\mathbf{y}) = \Omega \nabla \tilde{H}(\mathbf{y}),$$

where $\mathbf{y} = (q_1, \dots, q_n, p_1, \dots, p_n) \in \mathbb{R}^{2n}$, and $\tilde{H}(\mathbf{y}) = H(P\mathbf{y})$, being P the permutation matrix such that $\mathbf{x} = P\mathbf{y}$. Furthermore, the KHK map associated with $Y_{\tilde{H}}(\mathbf{y})$ is given by

$$\Psi_h(\mathbf{y}) = P^t \Phi_{-h}(P\mathbf{y}).$$

Using Lemma 19 and by a verification carried out by using Maple, we obtain the statement of the following result concerning the KHK maps associated with the vector fields in Theorem 9 for vector fields in \mathbb{R}^4 .

Proposition 16. *Let $\Phi_h = (\Phi_{1,h}, \Phi_{2,h}, \Phi_{3,h}, \Phi_{4,h})$ be any of the KHK maps associated with the Hamiltonian fields X in Theorem 9. Then, the map*

$$\Psi_h(q_1, q_2, p_1, p_2) = (\Phi_{1,-h}, \Phi_{3,-h}, \Phi_{2,-h}, \Phi_{4,-h})(q_1, p_1, q_2, p_2)$$

is symplectic.

Notice that, from Lemma 19(c), to prove the above result it is only necessary to check that the KHK maps Φ_h associate with the Hamiltonian vector field in Theorem 9 satisfy

$$D\Phi_h(\mathbf{x}) B D\Phi_h(\mathbf{x})^t = B. \quad (25)$$

As a consequence of Propositions 10 and 13, and Lemma 19(d), for vector fields in \mathbb{R}^6 , we obtain

Corollary 17. *The map*

$$\Psi_h(q_1, q_2, q_3, p_1, p_2, p_3) = (\Phi_{1,-h}, \Phi_{3,-h}, \Phi_{5,-h}, \Phi_{2,-h}, \Phi_{4,-h}, \Phi_{6,-h})(q_1, p_1, q_2, p_2, q_3, p_3),$$

where $\Phi_h = (\Phi_{1,h}, \Phi_{2,h}, \Phi_{3,h}, \Phi_{4,h}, \Phi_{5,h}, \Phi_{6,h})$ is any of the KHK maps associated with the Hamiltonians of \mathbb{R}^6 for which the field X is not a Lie symmetry of Φ_h , is not symplectic.

The following remark was suggested by a reviewer of a prior version of this paper.

Remark 18. *The preceding result demonstrates that the KHK map Φ_h in the counterexample given in the proof of Proposition 10, with associate Hamiltonian (20), is not symplectic. However, it is worth noticing that it still preserves the deformation of the symplectic structure (25) given by $B_h = B + h^2 B_2$, where*

$$B_2 = \begin{pmatrix} 0 & 0 & 0 & -\alpha & b/4 & 0 \\ 0 & 0 & 0 & \alpha & -b/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \alpha & -\alpha & 0 & 0 & 0 & 0 \\ -b/4 & b/4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

being α any arbitrary constant.

7. Conclusions

We have investigated the set of cubic Hamiltonian vector fields for which their associated Kahan–Hirota–Kimura maps preserve the original Hamiltonian function. For fields in \mathbb{R}^2 and \mathbb{R}^4 , we have identified nontrivial examples and in all the cases we found, the associated fields are Lie symmetries of the corresponding KHK maps, which preserve a symplectic structure. In the planar case, all the fields we identified correspond to factorizable Hamiltonians, representing singular cases of those characterized in [26], with associated trivial dynamics. In contrast, for \mathbb{R}^6 , we have discovered nontrivial cases where the field is not a Lie symmetry of the KHK map.

Our study has been limited to even-dimensional cases where a Poisson structure is present. Additional work could potentially be conducted in odd dimensions, particularly in the three-dimensional case, where the KHK method and its extensions have proven to be fruitful [9,15,33].

Similarly, it is natural to explore what happens to the KHK maps when considering vector fields with an integrating factor, a Jacobi multiplier [34], or those of the form $X(\mathbf{x}) = B(\mathbf{x})\nabla H(\mathbf{x})$, that is, when the anti-symmetric matrix $B(\mathbf{x})$ is no longer constant. For some of these systems, many interesting results have been obtained, which could be analyzed within the framework of exact preservation; see, for instance, [11,12,18,35].

CRedit authorship contribution statement

Víctor Mañosa: Conceptualization, Formal analysis, Funding acquisition, Investigation, Methodology, Software, Writing – original draft, Writing – review & editing. **Chara Pantazi:** Conceptualization, Formal analysis, Funding acquisition, Investigation, Methodology, Software, Writing – original draft, Writing – review & editing.

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Appendix

We consider the real vectors $\mathbf{x} = (x_1, \dots, x_{2n})$ and $\mathbf{y} = (q_1, \dots, q_n, p_1, \dots, p_n)$ related through the change of variables $x_1 = q_1$, $x_2 = p_1$, $x_3 = q_2$, $x_4 = p_2, \dots, x_{2n-1} = q_n$, $x_{2n} = p_n$ or, in other words, via $\mathbf{x} = P\mathbf{y}$ where P is a permutation matrix. The permutation matrices in \mathbb{R}^4 and \mathbb{R}^6 are given by

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \text{ and } P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

respectively.

The following result relates the fields of the form $X(\mathbf{x}) = B\nabla H(\mathbf{x})$, where B is given by expression (24), and their associated KHK maps with the Hamiltonian fields written in canonical form and their associated KHK maps.

Lemma 19. *Let H be a C^1 function in an open set of \mathbb{R}^{2n} . The following statements hold:*

- (a) *Through the change of variables $\mathbf{x} = P\mathbf{y}$ and the time reparametrization $t \rightarrow -t$, the Hamiltonian vector field $X(\mathbf{x}) = B\nabla H(\mathbf{x})$ is conjugate with $Y_{\tilde{H}}(\mathbf{y}) = \Omega\nabla\tilde{H}(\mathbf{y})$, with $\tilde{H}(\mathbf{y}) = H(P\mathbf{y})$.*
- (b) *Let Ψ_h and ϕ_h the KHK maps associated with the vector fields $Y_{\tilde{H}}$ and X_H , respectively, then*

$$\Psi_h(\mathbf{y}) = P^t \Phi_{-h}(P\mathbf{y}).$$

- (c) *The map Ψ_h is symplectic if and only if*

$$D\Phi_h(\mathbf{x}) B D\Phi_h(\mathbf{x})^t = B.$$

- (d) *The vector field X is a Lie symmetry of Φ_h if and only if the vector field $Y_{\tilde{H}}$ is a Lie symmetry of Ψ_h .*

To prove the above result, we need the following technical Lemma, that uses the matrix identity

$$(I + UV)^{-1}U = U(I + VU)^{-1}, \quad (26)$$

where U and V are conformable matrices, which is obtained directly from the identity $U(I + VU) = (I + UV)U$. We also recall that since P is a permutation matrix, then $P^{-1} = P^t$.

Lemma 20. *Let $\Phi_h(\mathbf{x})$ be the KHK map associated with a vector field $X(\mathbf{x})$. Let $\mathbf{x} = P\mathbf{y}$ and $\Psi_h(\mathbf{y})$ be the KHK map associated with the vector field $Y(\mathbf{y}) = P^t X(P\mathbf{y})$. Then*

$$\Psi_h(\mathbf{y}) = P^t \Phi_h(P\mathbf{y}).$$

Proof. Setting $U = P^t$, $V = -\frac{1}{2}hDX(Py)P$, using the identity (26) and $P^{-1} = P^t$, we have that the KHK map associated with $Y(y)$ satisfies

$$\begin{aligned}\Psi_h(y) &= y + h \left(I - \frac{1}{2}hDY(y) \right)^{-1} Y(y) \\ &= y + h \left(I - \frac{1}{2}hP^tDX(Py)P \right)^{-1} P^tX(Py) \\ &= P^tx + hP^t \left(I - \frac{1}{2}hDX(Py)PP^t \right)^{-1} X(Py) \\ &= P^t \left(x + h \left(I - \frac{1}{2}hDX(x) \right)^{-1} X(x) \right) \\ &= P^t\phi_h(x) = P^t\phi_h(Py). \quad \blacksquare\end{aligned}$$

Lemma 21. Set $x, y \in \mathbb{R}^m$, and let $x = Py$ where P is a permutation matrix. Then, the vector field $X(x)$ is a Lie symmetry of a C^1 map $\Phi(x)$ if and only if the vector field $Y(y) = P^tX(Py)$ is a Lie symmetry of the map $\Psi(y) = P^t\Phi_h(Py)$.

Proof. Using the compatibility Eq. (6), $X|_{\Phi(x)} = D\Phi(x)X(x)$, and the fact that $P^{-1} = P^t$ we obtain

$$\begin{aligned}X|_{\Phi(Py)} &= D\Phi(Py)X(Py) \Leftrightarrow X|_{\Phi(Py)} = P D\Psi(y)P^tX(Py) \Leftrightarrow \\ X|_{P\Psi(y)} &= P D\Psi(y)P^tX(Py) \Leftrightarrow P^tX|_{P\Psi(y)} = D\Psi(y)P^tPY(y) \Leftrightarrow \\ Y|_{\Psi(y)} &= D\Psi(y)Y(y). \quad \blacksquare\end{aligned}$$

Proof of Lemma 19. (a) If $\tilde{H}(y) = H(Py)$, then $\nabla\tilde{H}(y) = P^t\nabla H(Py)$. A computation shows that

$$P^tBP = -\Omega. \quad (27)$$

Using this equation and that $P^{-1} = P^t$, we have

$$\dot{y} = P^t\dot{x} = P^tB\nabla H(x) = P^tB\nabla H(Py) = P^tBP\nabla\tilde{H}(y) = -\Omega\nabla\tilde{H}(y).$$

By using the time reparametrization $t \rightarrow -t$ we obtain the result.

Statement (b) is a direct consequence of Lemma 20 and the well know fact that time reparametrization $t \rightarrow -t$ affects KHK maps only in the fact that the discretization step must be changed so that $h \rightarrow -h$.

(c) Assume that Ψ_h is symplectic. From equation

$$D\Psi_h(y)\Omega D\Psi_h(y)^t = \Omega,$$

and by using that $\Psi_h(y) = P^t\Phi_{-h}(Py)$, we get

$$P^tD\Phi_{-h}(x)P\Omega P^tD\Phi_{-h}(x)^tP = -P^tBP.$$

By Eq. (27), we have $P\Omega P^t = -B$, so we finally obtain

$$D\Phi_h(x)BD\Phi_h(x)^t = B.$$

The converse statement is obtained, by reversing the computations.

Statement (d) is a direct consequence of Lemma 21. \blacksquare

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