An introduction to Contact Hamiltonian Systems

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Outline of the seminar

1. Motivation
2. Contact Manifolds
3. Contact Hamiltonian Dynamics
4. Applications
5. Conclusions & Further subjects

Motivation

Motivation 1: Geometry

Quote (Arnold,1990)

"Every mathematician knows it is impossible to understand an elementary course in thermodynamics. The reason is that thermodynamics is based–as Gibbs has explicitly proclaimed–on a rather complicated mathematical theory, on the contact geometry. Contact geometry is one of the few simple geometries of the so-called Cartan's list, but it is still mostly unknown to the physicist–unlike the Riemannian geometry and the symplectic or Poisson geometries, whose fundamental role in physics is today generally accepted"

[Mrugala, Nulton, Schön, & Salamon, Contact structure in thermodynamic theory. RepsMathPhys, 29(1), 109-121, (1991)]

[Grmela, & Öttinger, Dynamics and thdyn of complex fluids. I., PRE, 56(6), 6620, (1997)]

[Eberard, Maschke, & Van Der Schaft, An extension of Ham. sys. to the thdyn phase space: Towards a geometry of nonreversible processes, Reps Math Phys, 60(2), 175-198, (2007)]

[Bravetti, Contact geometry and thdyn. IJGMMP, 16(supp01), 1940003, (2019)]

[Simoes, De León, Valcázar, & De Diego, Contact geometry for simple thdyn systems with friction. PRSA, 476(2241), 20200244, (2020)]

[Entov & Polterovich, Contact topology and non-equilibrium thdyn, Nonlinearity, 36(6), 3349, (2023)]

Motivation 2: Dyn. Sys.

Damped sys.

$$\ddot{q} = -\frac{\partial V}{\partial q} - \gamma\,\dot{q}$$

Damped-driven sys.

$$\ddot{q} = -\frac{\partial V(q,t)}{\partial q} - f(t)\,\dot{q}$$

Controlled sys.

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -\frac{\partial V}{\partial q} - p\,w \\ \dot{w} &= p\frac{\partial H}{\partial p} - c \end{aligned}$$

Do they have some underlying geometric structure?

Can we use it to understand the dynamics?

Motivation 3: Physics

Damped sys.

$$\ddot{q} = -\frac{\partial V}{\partial q} - \gamma\,\dot{q}$$

Damped-driven sys.

$$\ddot{q} = -\frac{\partial V(q,t)}{\partial q} - f(t)\,\dot{q}$$

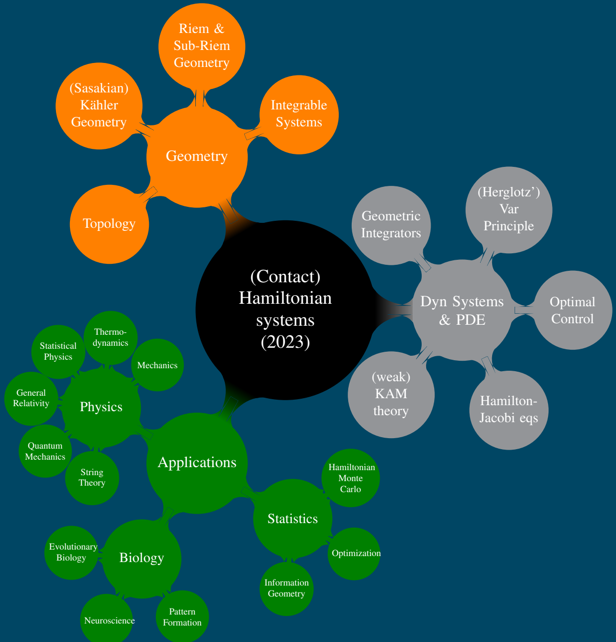
Thermostatted sys.

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -\frac{\partial V}{\partial q} - p\,w \\ \dot{w} &= p\frac{\partial H}{\partial p} - \frac{n}{\beta} \end{aligned}$$

Do they have some underlying geometric structure?

Can we use it to improve physical calculations?

Motivation: Geom., Dyn.Sys. & More



Contact Manifolds

Symplectic Vs Contact

Definitions: Nice Vs Ugly

Symplectic Manifold

$$(M^{2n}, \Omega),$$
$$\mathrm{d}\Omega = 0,\ V \equiv \Omega^n \neq 0$$

(General) Contact Manifold

$$(\mathcal{T}^{2n+1}, \mathcal{D}),$$
"$\mathcal{D}$ max. non-int."

Definition

A contact manifold is a $(2n+1)$-dimensional manifold $\mathcal{T}$, endowed with a contact structure, that is, a maximally non-integrable distribution $\mathcal{D} \subset T\mathcal{T}$ of hyperplanes

Symplectic Vs Contact
Definitions: Nice Vs Nice

Symplectic Manifold

$$(M^{2n}, \Omega),$$
$$\mathrm{d}\Omega = 0,\ V \equiv \Omega^n \neq 0$$

Theorem (Darboux)

In the neighborhood of any point on a symplectic manifold, it is always possible to find a set of local coordinates such that the 2-form Ω can be written

$$\Omega = \mathrm{d}p_a \wedge \mathrm{d}q^a$$

(Exact) Contact Manifold

$$(\mathcal{T}^{2n+1}, \mathcal{D} = \ker(\eta)),$$
$$V \equiv \eta \wedge (\mathrm{d}\eta)^n \neq 0$$

Theorem (Darboux)

In the neighborhood of any point on a contact manifold, it is always possible to find a set of local coordinates such that the 1-form η can be written

$$\eta = \mathrm{d}w - p_a \mathrm{d}q^a$$

Symplectic Vs Contact

Examples

Symplectic Manifold

$$(M^{2n}, \Omega),\ \mathrm{d}\Omega = 0,\ V \equiv \Omega^n \neq 0$$

Canonical coordinates:

$$(q, p) \qquad \Omega = \mathrm{d}p_a \wedge \mathrm{d}q^a$$

Examples:

- $\mathbb{R}^{2n}$ + standard symplectic

  $(\mathbb{R}^{2n}, \Omega),\ \Omega = \mathrm{d}p_a \wedge \mathrm{d}q^a$

Contact Manifold

$$(\mathcal{T}^{2n+1}, \eta),\ V \equiv \eta \wedge (\mathrm{d}\eta)^n \neq 0$$

Contact coordinates:

$$(q, p, w) \qquad \eta = \mathrm{d}w - p_a \mathrm{d}q^a$$

Examples:

- $\mathbb{R}^{2n+1}$ + standard contact

  $(\mathbb{R}^{2n+1}, \eta),\ \eta = \mathrm{d}w - p_a \mathrm{d}q^a$

Symplectic Vs Contact
Reeb Vector Field

Symplectic Manifold

$$(M^{2n}, \Omega),\ \mathrm{d}\Omega = 0,\ V \equiv \Omega^n \neq 0$$

Canonical coordinates:

$$(q, p) \qquad \Omega = \mathrm{d}p_a \wedge \mathrm{d}q^a$$

Contact Manifold

$$(\mathcal{T}^{2n+1}, \eta),\ V \equiv \eta \wedge (\mathrm{d}\eta)^n \neq 0$$

Contact coordinates:

$$(q, p, w) \qquad \eta = \mathrm{d}w - p_a \mathrm{d}q^a$$

Reeb vector field:

$$\mathrm{d}\eta(\mathcal{R}, \cdot) = 0 \qquad \eta(\mathcal{R}) = 1$$

In contact coordinates:

$$\mathcal{R} = \frac{\partial}{\partial w}$$

Symplectic Vs Contact
Symmetries

Symplectic Manifold

$$(M^{2n}, \Omega),\ \mathrm{d}\Omega = 0,\ V \equiv \Omega^n \neq 0$$

Canonical coordinates:

$$(q, p) \qquad \Omega = \mathrm{d}p_a \wedge \mathrm{d}q^a$$

Canonical symmetries:

$$\begin{aligned} \tilde{\Omega} &= \mathrm{d}\tilde{p}_a \wedge \mathrm{d}\tilde{q}^a \\ &= \mathrm{d}p_a \wedge \mathrm{d}q^a \\ &= \Omega \end{aligned}$$

Contact Manifold

$$(\mathcal{T}^{2n+1}, \eta),\ V \equiv \eta \wedge (\mathrm{d}\eta)^n \neq 0$$

Contact coordinates:

$$(q, p, w) \qquad \eta = \mathrm{d}w - p_a \mathrm{d}q^a$$

Contact symmetries:

$$\begin{aligned} \tilde{\eta} &= \mathrm{d}\tilde{w} - \tilde{p}_a \mathrm{d}\tilde{q}^a \\ &= f\,(\mathrm{d}w - p_a \mathrm{d}q^a) \\ &= f\,\eta \end{aligned}$$

Advantage:
canonical + scaling

Contact Hamiltonian Dynamics

Symplectic Vs Contact
Dynamics: Definition

Hamiltonian:

$$H : M^{2n} \to \mathbb{R}$$

Dynamics:

$$\Omega(X_H, \cdot) = -\mathrm{d}H$$

Hamiltonian:

$$h : \mathcal{T}^{2n+1} \to \mathbb{R}$$

Dynamics:

$$\eta(X_h) = -h \qquad \pounds_{X_h}\eta = f_h\,\eta$$

Using Cartan:

$$\pounds_{X_h}\eta = f_h\,\eta$$

iif

$$-\mathcal{R}(h)\,\eta - \mathrm{d}\eta(X_h, \cdot) = -\mathrm{d}h$$

Symplectic Vs Contact
Dynamics: Hamilton's eqs

Hamiltonian:

$$H : M^{2n} \to \mathbb{R}$$

Dynamics:

$$\Omega(X_H, \cdot) = -\mathrm{d}H$$

Hamilton's eqs:

$$\begin{aligned} \dot{q}^i &= \frac{\partial H}{\partial p_i} \\ \dot{p}_i &= -\frac{\partial H}{\partial q^i} \end{aligned}$$

Hamiltonian:

$$h : \mathcal{T}^{2n+1} \to \mathbb{R}$$

Dynamics:

$$-\mathcal{R}(h)\,\eta - \mathrm{d}\eta(X_h, \cdot) = -\mathrm{d}h$$

Hamilton's eqs:

$$\begin{aligned} \dot{q}^i &= \frac{\partial h}{\partial p_i} \\ \dot{p}_i &= -\frac{\partial h}{\partial q^i} - p_i \frac{\partial h}{\partial w} \\ \dot{w} &= \frac{\partial h}{\partial p_a} p_a - h \end{aligned}$$

Symplectic Vs Contact
Dynamics: Example

Hamiltonian:

$$H = \frac{\|p\|^2}{2} + V(q)$$

Dynamics:

$$\Omega(X_H, \cdot) = -\mathrm{d}H$$

Hamilton's eqs:

$$\begin{aligned} \dot{q}^i &= p_i \\ \dot{p}_i &= -\frac{\partial V}{\partial q^i} \end{aligned}$$

Hamiltonian:

$$h = \frac{\|p\|^2}{2} + V(q) + \gamma\, w$$

Dynamics:

$$-\mathcal{R}(h)\,\eta - \mathrm{d}\eta(X_h, \cdot) = -\mathrm{d}h$$

Hamilton's eqs:

$$\begin{aligned} \dot{q}^i &= p_i \\ \dot{p}_i &= -\frac{\partial V}{\partial q^i} - \gamma\, p_i \\ \dot{w} &= \frac{\|p\|^2}{2} - V(q) - \gamma\, w \end{aligned}$$

Symplectic Vs Contact
Liouville Theorem

H is conserved:

$$\dot{H} = X_H H = 0$$

Canonical transformations:

$$\pounds_{X_H} \Omega = 0$$

Liouville Theorem:

$$\pounds_{X_H} \Omega^n = 0$$

h is NOT conserved:

$$\dot{h} = X_h h = -\frac{\partial h}{\partial w}\, h$$

Contact transformations:

$$\pounds_{X_h} \eta = -\frac{\partial h}{\partial w}\, \eta$$

Contact Liouville Theorem:

$$\pounds_{X_h} \left(|h|^{-(n+1)} \eta \wedge (\mathrm{d}\eta)^n \right) = 0$$

[Bravetti & Tapias, JPA 48, 245001, (2015)]

[Bravetti & Tapias, PhysRevE 93, 022139, (2016)]

Symplectic Vs Contact
Variational Principles

Lagrange-Hamilton (∼1800):

$$s = \int_0^T L(q, \dot{q}) \mathrm{d}t \to \text{extr.}$$

E-L equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} = 0$$

Recall:

Noether theorem:

Canonical Symmetries
⇓
Conserved quantities

Herglotz (∼1930):

$$\dot{w} = L(q, \dot{q}, w) \to \text{extr.}$$

Generalized E-L equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} - \frac{\partial L}{\partial w}\frac{\partial L}{\partial \dot{q}^i} = 0$$

Advantage:

Generalized Noether:

Canonical + Scaling
⇓
Conserved + dissipated

Symplectic Vs Contact

Hamilton–Jacobi

Stationary:

$$H\left(q,\partial_q s\right)=c$$

Evolutionary:

$$H\left(q,\partial_q s\right)=\frac{\partial s}{\partial t}$$

Characteristic eqs:

$$\begin{aligned}\dot{q}^i &= \frac{\partial H}{\partial p_i}\\ \dot{p}_i &= -\frac{\partial H}{\partial q^i}\end{aligned}$$

Stationary:

$$h\left(q,\partial_q w,w\right)=c$$

Evolutionary:

$$h\left(q,\partial_q w,w\right)=\frac{\partial w}{\partial t}$$

Characteristic eqs:

$$\begin{aligned}\dot{q}^i &= \frac{\partial h}{\partial p_i}\\ \dot{p}_i &= -\frac{\partial h}{\partial q^i}-p_i\frac{\partial h}{\partial w}\\ \dot{w} &= \frac{\partial h}{\partial p_a}p_a-h\end{aligned}$$

Symplectic Vs Contact
Hamilton–Jacobi

Stationary:

$$H\left(q, \partial_q s\right) = c$$

Evolutionary:

$$H\left(q, \partial_q s\right) = \frac{\partial s}{\partial t}$$

Stationary:

$$h\left(q, \partial_q w, w\right) = c$$

Evolutionary:

$$h\left(q, \partial_q w, w\right) = \frac{\partial w}{\partial t}$$

Advantage:
More general (all)

[Wang, Wang & Yan, Nonlinearity, 30(2):492, (2016)]

[Wang, Wang & Yan, Comm Math Phys 366, 3, 981–1023 (2019)]

Symplectic Vs Contact
Algebraic Structures

Poisson bracket:

$$\{F, G\} := \Omega(X_F, X_G)$$

In coords:

$$\{F, G\} = \frac{\partial F}{\partial q^a}\frac{\partial G}{\partial p_a} - \frac{\partial G}{\partial q^a}\frac{\partial F}{\partial p_a}$$

Then:
Integrable Systems
Heisenberg Algebra

Jacobi bracket:

$$\{f, g\} := \eta([X_f, X_g])$$

In coords:

$$\{f, g\} = \frac{\partial f}{\partial q^a}\frac{\partial g}{\partial p_a} - \frac{\partial g}{\partial q^a}\frac{\partial f}{\partial p_a} + p_a\left(\frac{\partial f}{\partial w}\frac{\partial g}{\partial p_a} - \frac{\partial g}{\partial w}\frac{\partial f}{\partial p_a}\right) + f\frac{\partial g}{\partial w} - g\frac{\partial f}{\partial w}$$

Then:
Contact Integrable Systems
Contact Heisenberg Algebra

Symplectic Vs Contact
Algebraic Structures

Poisson bracket:

$$\{F, G\} := \Omega(X_F, X_G)$$

Recall:

$$(\mathcal{C}^\infty(M), \{,\}) \to \left(\mathfrak{X}^H(M), [,]\right)$$

homomorphism

Jacobi bracket:

$$\{f, g\} := \eta([X_f, X_g])$$

Advantage:

$$(\mathcal{C}^\infty(\mathcal{T}), \{,\}) \to \left(\mathfrak{X}^h(\mathcal{T}), [,]\right)$$

isomorphism

[Bravetti, García-Chung & Tapias, JPA 50(10):105203, (2017)]

[Zadra, Bravetti, García-Chung, & Seri, JPA 56(38), 385206, (2023)]

Applications

Symplectic Vs Contact: Applications

Damped sys.

$$\ddot{q} = -\frac{\partial V}{\partial q} - \gamma\,\dot{q}$$

Damped-driven sys.

$$\ddot{q} = -\frac{\partial V(q,t)}{\partial q} - f(t)\,\dot{q}$$

Thermostatted sys.

$$\begin{aligned}
\dot{q} &= p \\
\dot{p} &= -\frac{\partial V}{\partial q} - p\,w \\
\dot{w} &= p\frac{\partial H}{\partial p} - \frac{n}{\beta}
\end{aligned}$$

Do they have some underlying geometric structure?

Can we use it to improve physical calculations?

Symplectic Vs Contact: Damped sys

$$H = \mathrm{e}^{-\gamma t}\, \tfrac{1}{2}\, \|p_*\|^2 + \mathrm{e}^{\gamma t}\, V(q_*)$$

$$q_* := q, \quad p_* := \mathrm{e}^{\gamma t}\, p$$

$$\ddot{q} = -\frac{\partial V}{\partial q} - \gamma\, \dot{q}$$

Disadvantages:

Time-dependent, non-canonical variables, hard to generalize

[Caldirola, Il Nuovo Cimento, 18(9), 393-400, (1941)]

[Kanai, Progr. Theor. Phys., 3(4), 440-442, (1948)]

$$h = \tfrac{1}{2}\, \|p\|^2 + V(q) + \gamma\, w$$

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -\frac{\partial V}{\partial q} - \gamma\, p \\ \dot{w} &= \frac{1}{2} \|p\|^2 - V(q) - \gamma\, w \end{aligned}$$

Advantages:

Autonomous, canonical variables, new Noether, easy to generalize

[Bravetti, Cruz & Tapias, AnnPhys 376 1739, (2017)]

[Bravetti & García-Chung, JPA 54(9), 095205, (2021)]

Symplectic Vs Contact: Damped-driven sys

$$H = \frac{1}{2}\|I\|^2 + V(q, t(\tau))\left(\frac{\mathrm{d}t}{\mathrm{d}\tau}\right)^2$$

$$I := \frac{\mathrm{d}q}{\mathrm{d}\tau}, \quad \frac{\mathrm{d}^2 t}{\mathrm{d}\tau^2} - f(t)\left(\frac{\mathrm{d}t}{\mathrm{d}\tau}\right)^2 = 0$$

$$\ddot{q} = -\frac{\partial V(q,t)}{\partial q} - f(t)\,\dot{q}$$

[Gkolias, et al., Commun Nonlinear Sci Numer Simulat 51 (2017) 2338]

$$h = \frac{1}{2}\|p\|^2 + V(q,t) + f(t)\,w$$

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -\frac{\partial V(q,t)}{\partial q} - f(t)\,p \\ \dot{w} &= \frac{1}{2}\|p\|^2 - V(q,t) - f(t)\,w \end{aligned}$$

[Vermeeren, Bravetti, Seri, JPA(52): 445206, (2019)]
[Bravetti, Seri, Vermeeren & Zadra, CMDA, 132(1), 1-29, (2020)]

Symplectic Vs Contact: Damped-driven sys

$$H = \frac{1}{2}\|I\|^2 + V(q, t(\tau)) \left(\frac{\mathrm{d}t}{\mathrm{d}\tau}\right)^2$$

$$I := \frac{\mathrm{d}q}{\mathrm{d}\tau}, \quad \frac{\mathrm{d}^2 t}{\mathrm{d}\tau^2} - f(t) \left(\frac{\mathrm{d}t}{\mathrm{d}\tau}\right)^2 = 0$$

- Advantages:
  - Geometric structure
  - Numerical Integration
- Disadvantages:
  - $t(\tau)$ difficult to solve
  - Case-by-case scenario

[Gkolias, et al., Commun Nonlinear Sci Numer Simulat 51 (2017) 2338]

$$h = \frac{1}{2}\|p\|^2 + V(q,t) + f(t)\, w$$

- Advantages:
  - Geometric structure
  - Numerical Integration
- More advantages:
  - No eq. to be solved
  - General scenario

[Bravetti, Seri, Vermeeren & Zadra, CMDA, 132(1), 1-29, (2020)]

[Bravetti, Daza-Torres, Flores-Arguedas & Betancourt, InfoGeom, 1-23, (2023)]

Symplectic Vs Contact: Thermostatted sys

Nosé–Hoover

$$\dot{q} = \frac{\partial H}{\partial p}$$

$$\dot{p} = -\frac{\partial V}{\partial q} - p\,w$$

$$\dot{w} = p\frac{\partial H}{\partial p} - \frac{n}{\beta}$$

[Tuckerman, *Statistical mechanics: theory and molecular simulation*, Oxford University Press, (2010)]

$$h = \left[e^{-\beta H(q,p)}\rho(w)\right]^{-1/(n+1)}$$

$$\dot{q} = \frac{\beta h}{n+1}\frac{\partial H}{\partial p}$$

$$\dot{p} = \frac{\beta h}{n+1}\left(-\frac{\partial V}{\partial q} - p\frac{\rho'(w)}{\rho(w)}\right)$$

$$\dot{w} = \frac{\beta h}{n+1}\left(p\frac{\partial H}{\partial p} - \frac{(n+1)}{\beta}\right)$$

[Bravetti & Tapias, PhysRevE 93, 022139, (2016)]

Symplectic Vs Contact: Thermostatted sys

...

General algorithm

Given $\rho(q,p)$, choose $\rho(w)$ and let

$$h = [\rho(q,p)\rho(w)]^{-1/(n+1)}$$

Remind: Contact Liouville Th.

$$\mathrm{d}\mu_h = |h|^{-(n+1)}\eta \wedge (\mathrm{d}\eta)^n$$

Obtain the desired invariant measure:

$$\mathrm{d}\mu_h = \rho(q,p)\rho(w)\,\mathrm{d}p\,\mathrm{d}q\,\mathrm{d}w$$

[Bravetti & Tapias, PhysRevE 93, 022139, (2016)]

Symplectic Vs Contact: Thermostatted sys

...

General algorithm

$$h = [\rho(q,p)\rho(w)]^{-1/(n+1)}$$

Advantages:

- Hamiltonian formulation
- Geometric integrators
- Freedom in $\rho(w)$
- Valid for any $\rho(q,p)$
- It can be implemented in Hamiltonian Monte Carlo

[Bravetti & Tapias, PhysRevE 93, 022139, (2016)]

Conclusions & Further Subjects

(Some) Conclusions

1. Worth having a look at contact Hamiltonian systems

   [Manuel Lainz Valcázar, Contact Hamiltonian Systems, ICMAT, (2022)]

   [Federico Zadra, Topics in contact Hamiltonian systems: analytical and numerical perspectives, University of Groningen, (2023)]
2. Very similar to their symplectic (Poisson) counterparts
   ($\Rightarrow$ similar theoretical & numerical tools)
3. New symmetries (rescalings, dynamical similarities)
   ($\Rightarrow$ new Noether, new reductions)
4. Particularly suitable for (some class of) dissip sys
   ($\Rightarrow$ classical & quantum mechanics)
5. Extremely useful for inverse problems of dynamics
   ($\Rightarrow$ optimization, HMC, ...)

(Some) Further subjects

- CHS & Field theories

  [Gaset, et al. AnnPhys, 414, 168092, (2020)]
- CHS & Gravity

  [Paiva, et al. PhysRevD, 105(12), 124023, (2022)]
- CHS in Cosmology

  [Sloan, PhysRevD, 97(12), 123541, (2018)]
- CHS in Quantum Mechanics

  [Ciaglia, Cruz, & Marmo, AnnPhys, 398, 159-179, (2018)]
- CHS in Optimization

  [Bravetti, et al. InfoGeom, 1-23, (2023)]
- CHS in Hamiltonian Monte Carlo

  [Betancourt, arXiv:1405.3489]

(Some) Interesting conjectures

Grmela Conjecture
"Legendre (contact) transformations are the basic dynamical laws for irreversible phenomena"

[Grmela, M., Entropy, 16(3), 1652-1686, (2014)]

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is every irreversible. sys. a contact Ham. sys.?

[Esen, Grmela, & Pavelka, JMathPhys, 63(12), (2022)]

Shape Dyn. Conjecture
"Scale is surplus"
(Only relational degrees of freedom are observable)

[Gryb, S., & Sloan, D., When scale is surplus, Synthese 199.5 (2021): 14769-14820.]

⇓

is the universe a contact Ham. sys.?

[Bravetti, Jackman, & Sloan, JPA, to appear, (2023)]

Announcement

- Joint PhD projects with Prof. Seri

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Thank you!

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