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Contact Hamiltonian Dynamics: The Concept and Its Use

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Abstract: We give a short survey on the concept of contact Hamiltonian dynamics and its use in several areas of physics, namely reversible and irreversible thermodynamics, statistical physics and classical mechanics. Some relevant examples are provided along the way. We conclude by giving insights into possible future directions.

Keywords: contact geometry; thermodynamics; statistical mechanics; dissipative systems

1. Introduction

Contact geometry is the "odd-dimensional cousin" of symplectic geometry [1,2]. Unlike her famous cousin, until recently, contact geometry has received much less attention in the physics literature, with some relevant exceptions being time-dependent Hamiltonian mechanics, thermodynamics and string theory [2–9].

One of the reasons why symplectic geometry appears everywhere in physical applications is the fact that Hamilton's equations on symplectic manifolds are the natural framework for classical mechanics and statistical physics and the starting point to derive their quantum counterparts. However, the standard (time-independent) Hamilton equations can only be used to model conservative mechanical systems, and in statistical mechanics, they only provide the dynamical basis for the microcanonical ensemble. Therefore, a major goal, at least in some areas, is that of finding generalizations of Hamilton's equations that apply to systems exchanging energy with an environment.

In contact geometry one has a direct generalization of Hamilton's equations, the so-called contact Hamiltonian equations. Again, such equations have not been considered as much as their symplectic counterparts in physics. Nevertheless, in recent years, several applications of contact Hamiltonian dynamics have been found, ranging from thermodynamics to classical and statistical mechanics. Unfortunately, such literature is quite dispersed, and we believe that a general treatment would be useful in order to highlight the common features and remark on the differences among the many applications of this research area of growing interest.

It is the purpose of this paper to give a brief survey of all these applications and to discuss possible future directions. In order to give a chronological introduction, we start with equilibrium thermodynamics, then we present the use of contact Hamiltonian systems in irreversible thermodynamics, and in the end, we investigate their use in statistical physics and classical mechanics of dissipative systems.

This work aims to give a concise introduction to the concept of contact Hamiltonian dynamics and its multiple uses in different disciplines, by collecting them all together for the first time and focusing on their common denominator: the fact that the system is not necessarily isolated, that is, contact Hamiltonian dynamics can help model open systems at all levels of description. However, we mention here only the main aspects of each application and select a few systems that are representative of each case, referring to the cited works for more details and examples.

2. Contact Hamiltonian Dynamics

We begin by introducing contact Hamiltonian dynamics and discussing in which way it generalizes the standard Hamiltonian equations. Throughout this work, we use the same definitions and sign conventions as in [10].

A contact manifold is a pair $(\mathcal{T}, \eta)$, where $\mathcal{T}$ is a $(2n+1)$-dimensional manifold and η is a one-form on $\mathcal{T}$, called the contact form, that satisfies the condition:

$$\eta \wedge (d\eta)^n \neq 0\,, \tag{1}$$

with $d\eta$ the exterior derivative of η and '$\wedge$' the wedge product. There is a more mathematical and more precise definition of a contact manifold, which considers the fact that the real relevant object in order to define a contact manifold is the distribution induced by the kernel of the one-form η (cf. [1,2]). For the purposes of this short survey, we can stick to the definition given above, which is more intuitive. However, in thermodynamic applications in which a change of representation, e.g., from entropy to internal energy, is considered, then this aspect becomes crucial (see [11–13] for related discussions). The left-hand side in (1) provides the standard volume form on $\mathcal{T}$, analogously to Ω^n for the symplectic case, where Ω is the symplectic two-form.

Let us define the dynamics in $\mathcal{T}$. One can associate with every differentiable function $\mathscr{H} : \mathcal{T} \to \mathbb{R}$, a vector field $X_{\mathscr{H}}$, called thecontact Hamiltonian vector field generated by $\mathscr{H}$, defined through the relations:

$$\pounds_{X_{\mathscr{H}}}\eta = f_{\mathscr{H}}\eta \qquad \text{and} \qquad \mathscr{H} = -\eta\left(X_{\mathscr{H}}\right)\,, \tag{2}$$

where $\pounds_{X_{\mathscr{H}}}$ is the Lie derivative along a vector field, $\mathscr{H}$ is called the contact Hamiltonian and $f_{\mathscr{H}} : \mathcal{T} \to \mathbb{R}$ is a function that turns out to be completely determined by $\mathscr{H}$ (see below). Associated with η, there is another fundamental object called the Reeb vector field ξ, which is defined intrinsically by the conditions:

$$\eta(\xi) = 1 \qquad \text{and} \qquad d\eta(\xi) = 0\,. \tag{3}$$

From the above Properties (2) and (3), it is easy to show that:

$$f_{\mathscr{H}} = -\xi(\mathscr{H})\,, \tag{4}$$

thus proving that $f_{\mathscr{H}}$ is completely determined by the contact Hamiltonian.

It is always possible to find a set of local (Darboux) coordinates (x^a, y_a, z) for $\mathcal{T}$, with $a = 1, \ldots, n$, which we refer to as contact coordinates, such that the one-form η reads:

$$\eta = dz - y_a dx^a\,, \tag{5}$$

where Einstein's summation convention over repeated indices is assumed here and in the following. In these coordinates, the Reeb vector field is just $\xi = \partial/\partial z$, and the generic contact Hamiltonian vector field $X_{\mathscr{H}}$ takes the form:

$$X_{\mathscr{H}} = \left(y_a \frac{\partial \mathscr{H}}{\partial y_a} - \mathscr{H}\right)\frac{\partial}{\partial z} - \left(\frac{\partial \mathscr{H}}{\partial x^a} + y_a \frac{\partial \mathscr{H}}{\partial z}\right)\frac{\partial}{\partial y_a} + \left(\frac{\partial \mathscr{H}}{\partial y_a}\right)\frac{\partial}{\partial x^a}\,. \tag{6}$$

According to (6), the flow of $X_{\mathscr{H}}$ can be explicitly written in contact coordinates as:

$$\dot{x}^a = \frac{\partial \mathscr{H}}{\partial y_a}\,, \tag{7}$$

$$\dot{y}_a = -\frac{\partial \mathscr{H}}{\partial x^a} - y_a \frac{\partial \mathscr{H}}{\partial z}\,, \tag{8}$$

$$\dot{z} = y_a \frac{\partial \mathscr{H}}{\partial y_a} - \mathscr{H}\,. \tag{9}$$

The similarity of (7) and (8) with Hamilton's equations on symplectic manifolds:

$$\dot{q}^a = \frac{\partial H}{\partial p_a}, \quad \dot{p}_a = -\frac{\partial H}{\partial q^a}, \tag{10}$$

is clear. In fact, (7)–(9) are the generalization of Hamilton's equations to a contact manifold. In particular, when $\mathscr{H}$ does not depend on z, Equations (7) and (8) give exactly Hamilton's equations in the symplectic sub-space parametrized by x^a and y_a. Finally, (9) in this case is the usual definition of Hamilton's principal function [10,14].

An important difference between contact Hamiltonian dynamics and symplectic Hamiltonian dynamics is that in the contact case, the Hamiltonian $\mathscr{H}$ is not preserved along the evolution. In fact, using (7)–(9), it is straightforward to show that:

$$\dot{\mathscr{H}} = -\mathscr{H}\frac{\partial \mathscr{H}}{\partial z}. \tag{11}$$

Using (11), one can sometimes model the contact Hamiltonian (or appropriate functions thereof) as a Lyapunov function for the dynamics. This fact turns out to be extremely useful in irreversible thermodynamics, information geometry and control theory [15–18].

On contact manifolds, there is a distinguished class of submanifolds, namely Legendre submanifolds. These are defined as those submanifolds of maximal dimension whose tangent space is contained on the kernel of η at any point. More informally, they are solutions of the equation $\eta = 0$ of maximal dimension. Using Condition (1), one can prove [2] that the maximal dimension is n and that the general local form of a Legendre submanifold L is:

$$x^i = -\frac{\partial f}{\partial y_i}, \qquad y_j = \frac{\partial f}{\partial x^j}, \qquad z = f - y_i \frac{\partial f}{\partial y_i}, \tag{12}$$

where $I \cup J$ is a disjoint partition of the set of indices $\{1, \ldots, n\}$, $i \in I$, $j \in J$ and $f(y_i, x^j)$ is a function of n variables only, which we call the generating function of L. We remark that Legendre submanifolds are the contact counterparts of Lagrange submanifolds in symplectic geometry. Indeed, a Lagrange submanifold is defined as a submanifold of maximal dimension on which the symplectic form vanishes, and it turns out that Lagrangian submanifolds on a symplectic manifold of dimension $2n$ have dimension n [2].

A fundamental property of the dynamics (7)–(9) is that it can be shown [19] that a Legendre submanifold L is invariant (meaning that once the system enters such a submanifold, it remains on it) if and only if the contact Hamiltonian $\mathscr{H}$ vanishes on L, i.e.,

$$L \text{ invariant for } X_{\mathscr{H}} \quad \longleftrightarrow \quad \mathscr{H}|_L = 0. \tag{13}$$

3. Reversible Thermodynamics

The first appearance of contact Hamiltonian dynamics in physical applications is in [19,20], which deal with the definition of reversible thermodynamic processes by means of a Hamiltonian in the thermodynamic phase space. One starts with the first law for reversible processes written in the form:

$$dU - TdS + PdV - \mu dN = 0. \tag{14}$$

By defining the thermodynamic phase space to be a contact manifold $(\mathcal{T}^{\text{TD}}, \eta^{\text{TD}})$, one can always find local contact coordinates $(x^S, x^V, x^N, y_S, y_V, y_N, z)$ in which:

$$\eta^{\text{TD}} = dz - x^S dy_S - x^V dy_V - x^N dy_N. \tag{15}$$

Since all thermodynamic systems at equilibrium satisfy (14), one can then identify them as Legendre submanifolds of the thermodynamic phase space, cf. (12), by means of the natural embedding given by the relations $(x^S = S, x^V = V, x^N = N)$ and:

$$z|_{L^{\text{TD}}} = U(S, V, N)\,, \tag{16}$$

$$y_S|_{L^{\text{TD}}} = \left.\frac{\partial U}{\partial S}\right|_L = T\,, \tag{17}$$

$$y_V|_{L^{\text{TD}}} = \left.\frac{\partial U}{\partial V}\right|_L = -P\,, \tag{18}$$

$$y_N|_{L^{\text{TD}}} = \left.\frac{\partial U}{\partial N}\right|_L = \mu\,, \tag{19}$$

where $U(S, V, N)$ is the internal energy of the system, S, V and N are the extensive variables (entropy, volume and number of moles) and T, P and μ are the corresponding intensive variables (temperature, pressure and chemical potential); see, e.g., [21]. Notice that in this case, the generating function of the Legendre submanifold is given by the internal energy (16) of the system, and the remaining n equations are the equations of state (17)–(19). However, by (12), one can notice that any other representation of the system in terms of the various thermodynamic potentials and the corresponding equations of state can be equivalently used. Therefore, we can think of any thermodynamic system as a triple $(\mathcal{T}^{\text{TD}}, \eta^{\text{TD}}, L^{\text{TD}})$ where $(\mathcal{T}^{\text{TD}}, \eta^{\text{TD}})$ is the thermodynamic phase space and L^{TD} is the Legendre submanifold corresponding to the system.

Considering this fact and the invariance property (13), in [19,20], it has been argued that thermodynamic transformations of a system like, e.g., an ideal gas can be defined as a quadruple $(\mathcal{T}^{\text{TD}}, \eta^{\text{TD}}, L^{\text{TD}}, \mathscr{H}^{\text{TD}})$, where $\mathscr{H}^{\text{TD}}$ is a contact Hamiltonian that vanishes on L^{TD}. In this way, the dynamics automatically preserves L^{TD}, i.e., the thermodynamic properties of the system, expressed by (16)–(19). For instance, an ideal gas with gas constant R undergoing an isothermal and isochoric transformation can be given by the Legendre submanifold L^{IG} defined by (16)–(19), where:

$$U^{\text{IG}}(S, V, N) = U_0\, \mathrm{e}^{S/cNR} V^{-1/c} N^{1+1/c} \tag{20}$$

is the internal energy of the gas, with U_0 an arbitrary positive constant and c the heat capacity at constant volume (e.g., $c = 3/2$ for a monatomic ideal gas), together with the contact Hamiltonian:

$$\mathscr{H}^{\text{IG}} = z - y_S x^S + R y_S x^N - y_N x^N\,. \tag{21}$$

Notice that $\mathscr{H}^{\text{IG}}$ restricted to L^{IG} reads:

$$\mathscr{H}^{\text{IG}}|_{L^{\text{IG}}} = U - TS + NRT - \mu N = 0\,, \tag{22}$$

where in the last equality, we have used the ideal gas equation of state $PV = NRT$, which can be easily derived from (17)–(18) and (20) and the fact that (20) is a homogeneous function of degree one; thus by Euler's theorem, it satisfies $U = TS - PV + \mu N$ [21]. We conclude that $\mathscr{H}^{\text{IG}}$ fulfills the invariance property (13) for the Legendre submanifold representing an ideal gas, and thus, its contact Hamiltonian vector field preserves the thermodynamic relations of the ideal gas. Finally, a direct calculation from (7)–(9) shows that the flow of $\mathscr{H}^{\text{IG}}$ is given by,

$$\dot{S} = -S + NR, \quad \dot{V} = 0, \quad \dot{N} = -N, \quad \dot{T} = 0, \quad \dot{P} = -P, \quad \dot{\mu} = -RT, \quad \dot{U} = U\,. \tag{23}$$

thus inducing an isothermal and isochoric transformation, as anticipated.

Several other cases have been investigated in [6,19,20,22], including that of transformations deforming an ideal gas into a van der Waals gas (see also [23]). For an analysis of equilibrium thermodynamics using symplectic structures and the Dirac formalism for constrained systems, see [12,24].

4. Irreversible Thermodynamics

4.1. The Work of Grmela and Öttinger on Mesoscopic Dynamics

While looking for a general equation for the non-equilibrium reversible-irreversible coupling (GENERIC), Grmela and Öttinger immediately realized that it could be cast in the form of a contact Hamiltonian system [25]. Later, in [26], a "contact geometry formulation of nonequilibrium thermodynamics" had been put forward. We report here from [26] the contact formulation of the Onsager-Casimir (OC) dynamics for a system that approaches equilibrium in the linear regime. Considering the state variables x^a to be the extensive equilibrium variables, the OC dynamics reads:

$$\dot{x}^a = (T_0 J^{ab} - D^{ab}) \frac{\partial \phi}{\partial x^b}, \tag{24}$$

with T_0 the equilibrium temperature, J a skew-symmetric matrix defining the reversible part of the evolution, D a symmetric nonnegative matrix responsible for the irreversible part of the evolution and $\phi(x^a)$ the potential function defining the thermodynamic properties. Thus, $\phi(x^a)$ is the generating function of the Legendre submanifold L^{OC} defined by:

$$z|_{L^{\mathrm{OC}}} = \phi(x^a), \tag{25}$$

$$y_a|_{L^{\mathrm{OC}}} = \frac{\partial \phi}{\partial x^a}, \tag{26}$$

in the contact phase space $\mathcal{T}^{\mathrm{OC}}$ with coordinates (x^a, y_a, z), which entails the equilibrium thermodynamic properties of the system, exactly in the same sense as in the previous section. The next step in the construction is to reproduce (24) on L^{OC}. The contact Hamiltonian suggested in [26] is of the form:

$$\mathscr{H}^{\mathrm{OC}} = -\frac{1}{2} y_a D^{ab} y_b + \frac{1}{2} \frac{\partial \phi}{\partial x^a} D^{ab} \frac{\partial \phi}{\partial x^b} + T_0 y_a J^{ab} \frac{\partial \phi}{\partial x^b}. \tag{27}$$

One can directly show that $\mathscr{H}^{\mathrm{OC}}$ vanishes on L^{OC}, thus ensuring by (13) that the thermodynamic relations at equilibrium are preserved. Moreover, $\mathscr{H}^{\mathrm{OC}}$ is constructed so that the dynamics for the extensive variables (cf. (7)) restricted to L^{OC} gives exactly the Onsager-Casimir evolution (24). Thus, the contact dynamics given by $\mathscr{H}^{\mathrm{OC}}$ is the proper lift to $\mathcal{T}^{\mathrm{OC}}$ of the Onsager-Casimir dynamics, meaning that it extends it to the contact phase space, and reduces to it on the invariant Legendre submanifold L^{OC} representing the thermodynamic system of interest.

A further generalization of this dynamics has been made in [26], by removing the restriction that the variables x^a are the equilibrium extensive variables and with a choice similar to (27) for the contact Hamiltonian. This generalization has been called rate thermodynamics, and it has been proven that when restricted to the corresponding invariant Legendre submanifold, it reduces to GENERIC, from which one can further deduce that by an appropriate choice of the independent variables x^a and of the Legendre submanifold, a number of mesoscopic dynamical descriptions such as, e.g., Boltzmann kinetic theory and Navier-Stokes-Fourier hydrodynamics can be recovered (see [25–27]).

4.2. The Work of Eberard, Maschke and van der Schaft on Conservative Contact Systems

A strictly related formulation is that of [28]. Again, the authors define a class of contact Hamiltonian systems representing both the invariance of the thermodynamic properties of the system and the fluxes due to nonequilibrium conditions, dubbed as conservative contact systems. The construction of conservative contact systems proceeds along the same steps as in the work of Grmela, the main difference being in the specification of the state variables and hence of the contact phase space.

A conservative contact system (CCS) is a quadruple $(\mathcal{T}^{\mathrm{CCS}}, \eta^{\mathrm{CCS}}, L^{\mathrm{CCS}}, \mathscr{H}^{\mathrm{CCS}})$, where $(\mathcal{T}^{\mathrm{CCS}}, \eta^{\mathrm{CCS}})$ is a contact manifold defining the extended phase space of the system, possibly including mechanical, as well as thermodynamical variables, L^{CCS} is a Legendre submanifold encoding the thermodynamic properties of the system and the mechanical relations between conjugate variables and $\mathscr{H}^{\text{ccs}}$ is a contact Hamiltonian satisfying the invariance condition (13) and generating the vector field that corresponds to dynamical phenomena due to nonequilibrium conditions. The physical equations of motion are obtained by the restriction of the contact Hamiltonian Equations (7)–(9) to the Legendre submanifold L^{ccs}.

As an example, we report here from [28] the case of an ideal gas in a cylinder under a piston. The properties of the piston are encoded in its mechanical Hamiltonian:

$$H_0 = \frac{1}{2m}(x^{\text{kin}})^2 + mgx^{\text{pot}}\,, \tag{28}$$

with x^{kin} the momentum and x^{pot} the height of the piston. The thermodynamic properties of the ideal gas are defined by, e.g., the internal energy $U(S,V,N)$, cf. (20). Therefore, the physical properties of the total system are given in an 11-dimensional phase space $\mathcal{T}^{\text{ccs}}$ with local coordinates:

$$(x^S, x^V, x^N, x^{\text{pot}}, x^{\text{kin}}, y_S, y_V, y_N, y_{\text{pot}}, y_{\text{kin}}, z) \tag{29}$$

by means of the Legendre submanifold defined by the generating function:

$$f(S,V,N,x^{\text{pot}},x^{\text{kin}}) = U(S,V,N) + H_0(x^{\text{pot}},x^{\text{kin}})\,, \tag{30}$$

i.e., the Legendre submanifold L^{ccs} that satisfies the relations $x^S = S, x^V = V, x^N = N$ and:

$$z|_{L^{\text{CCS}}} = f(S,V,N,x^{\text{pot}},x^{\text{kin}})\,, \tag{31}$$

$$y_S|_{L^{\text{CCS}}} = \frac{\partial f}{\partial S} = T\,, \tag{32}$$

$$y_V|_{L^{\text{CCS}}} = \frac{\partial f}{\partial V} = -P\,, \tag{33}$$

$$y_N|_{L^{\text{CCS}}} = \frac{\partial f}{\partial N} = \mu\,, \tag{34}$$

$$y_{\text{pot}}|_{L^{\text{CCS}}} = \frac{\partial f}{\partial x^{\text{pot}}} = mg = F\,, \tag{35}$$

$$y_{\text{kin}}|_{L^{\text{CCS}}} = \frac{\partial f}{\partial x^{\text{kin}}} = \frac{x^{\text{kin}}}{m} = v\,. \tag{36}$$

Now, let us consider for instance a nonadiabatic transformation due to friction, in which the dissipated mechanical energy is converted entirely into a flow of heat in the gas. To do so, one defines the contact Hamiltonian:

$$\mathscr{H}^{\text{CCS}} = K_{\text{mec}} + (y_V + P)Av + (y_{\text{kin}} - v)AP - \left(y_{\text{kin}} - \frac{y_S}{T}v\right)\gamma v\,, \tag{37}$$

where γ is the friction coefficient, A denotes the area of the piston, P, v, T and F are defined in (31)–(36) and:

$$K_{\text{mec}} = y_{\text{pot}}v - y_{\text{kin}}F\,. \tag{38}$$

One can directly check that $\mathscr{H}^{\text{ccs}}$ satisfies the invariance property (13) and that the contact dynamics (7) of the extensive variables restricted to L^{ccs} reads:

$$\dot{S}|_{L^{\text{CCS}}} = \frac{\partial \mathscr{H}^{\text{CCS}}}{\partial y_S} = \frac{1}{T}\gamma v^2\,, \tag{39}$$

$$\dot{V}|_{L^{\text{CCS}}} = \frac{\partial \mathscr{H}^{\text{CCS}}}{\partial y_V} = Av\,, \tag{40}$$

$$\dot{N}|_{L^{\text{CCS}}} = \frac{\partial \mathscr{H}^{\text{CCS}}}{\partial y_N} = 0\,, \tag{41}$$

$$\dot{x}^{\text{pot}}|_{L^{\text{CCS}}} = \frac{\partial \mathscr{H}^{\text{CCS}}}{\partial y_{\text{pot}}} = v\,, \tag{42}$$

$$\dot{x}^{\text{kin}}|_{L^{\text{CCS}}} = \frac{\partial \mathscr{H}^{\text{CCS}}}{\partial y_{\text{kin}}} = -mg + AP\,. \tag{43}$$

Here, the last equation is Newton's law for the motion of the piston; the fourth equation is the definition of the velocity; the third equation indicates that the system is closed; the second equation is the relation between the motion of the piston and the change in volume of the gas; and the first equation is the entropy balance, stating that the irreversible entropy production due to friction is converted into an entropy flow in the gas.

Several other examples, concerning also the generalization to open systems (called control contact systems) can be found in [28] and also in subsequent works, e.g., [29–34]. Further (and different) approaches to the use of contact Hamiltonian dynamics in irreversible thermodynamics can be found in [12,15,16,35–37].

5. Equilibrium Statistical Mechanics

Recently, in [38], another application of contact Hamiltonian dynamics has been proposed, namely in equilibrium statistical mechanics (SM). A major problem for the dynamical simulations of systems in an equilibrium ensemble different from the microcanonical one is that of finding equations of motion that generate the correct equilibrium distribution for the positions and momenta of the physical system (see, e.g., [39–41]).

Let us start by considering the phase space of a (possibly open) mechanical system to be a contact manifold $(\mathcal{T}^{\text{SM}}, \eta^{\text{SM}})$ with local contact coordinates (q^a, p_a, S) given by the canonical positions and momenta of the system and by the additional variable S. In this case, η^{SM} takes the form:

$$\eta^{\text{SM}} = dS - p_a dq^a\,. \tag{44}$$

The key to find the correct equations of motion that give any invariant distribution on the physical phase space (with variables (q^a, p_a) only) is to use contact Hamiltonian dynamics and take advantage of a theorem called Liouville's theorem for nonconservative systems from contact geometry [14] (see also [42,43]). The theorem says that for a general contact Hamiltonian $\mathscr{H}^{\text{SM}}$, there is only one invariant measure, which depends only on $\mathscr{H}^{\text{SM}}$, given by:

$$d\mu = \rho\, \eta^{\text{SM}} \wedge (d\eta^{\text{SM}})^n = \frac{|\mathscr{H}^{\text{SM}}|^{-(n+1)}}{\mathcal{Z}} dq^a \wedge dp_a \wedge dS\,, \tag{45}$$

where $\mathcal{Z}$ is a normalization factor and n is the number of degrees of freedom of the physical system of interest. We emphasize that for a general choice of $\mathscr{H}^{\text{SM}}$, the distribution in (45) may not be integrable. However, we are interested here only in those cases where such an integral exists. Besides, due to the property (11), the contact Hamiltonian does not change its sign along the dynamics, and thus, if it is positive at the initial condition, it will stay positive along the evolution, and we can then omit the absolute value in (45). In particular, choosing $\mathscr{H}^{\text{SM}}$ of the form:

$$\mathscr{H}^{\text{SM}} = \rho_t(q^a, p_a, S)^{-\frac{1}{n+1}}\,, \tag{46}$$

with $\rho_t(q^a, p_a, S)$ any distribution on $\mathcal{T}^{\text{SM}}$, then the contact Hamiltonian Equations (7)–(9) take the form:

$$\dot{q}_i = \frac{\mathscr{H}^{\text{SM}}}{n+1}\frac{\partial\Theta(p,q,S)}{\partial p_i}, \tag{47}$$

$$\dot{p}_i = \frac{\mathscr{H}^{\text{SM}}}{n+1}\left[-\frac{\partial\Theta(p,q,S)}{\partial q_i} - \frac{\partial\Theta(p,q,S)}{\partial S}p_i\right], \tag{48}$$

$$\dot{S} = \frac{\mathscr{H}^{\text{SM}}}{n+1}\left[p_i\frac{\partial\Theta(p,q,S)}{\partial p_i} - (n+1)\right], \tag{49}$$

with $\Theta = -\ln\rho_t$. Using the above-mentioned Liouville theorem, it follows that the invariant measure of the dynamics has the distribution $\rho_t(q^a, p_a, S)$ [38]. Therefore, one is free to choose ρ_t from the onset to be any distribution in $\mathcal{T}^{\text{SM}}$. A particularly convenient choice for the problem of generating target equilibrium distributions in q^a and p_a is:

$$\rho_t = \rho_{\text{target}}(q^a, p_a)f(S), \tag{50}$$

where ρ_{target} is the desired distribution for the momenta and positions of the physical system of interest and $f(S)$ is an independent distribution for the additional variable S. In fact, in this case, the additional variable S can then be integrated out using the fact that ρ_t is separable and one ends up with the desired distribution ρ_{target} for the physical system. For example, it has been shown both analytically and with numerical simulations that when ρ_{target} and $f(S)$ are a canonical and a logistic distribution, respectively, then Equations (47)–(49) correctly simulate the equilibrium properties of systems in the canonical ensemble (see [38,44,45]).

6. Classical Mechanics

Once one realizes that contact Hamiltonian dynamics provides a useful framework for simulating the equilibrium statistical mechanics of open systems by virtue of the dynamical friction mechanism given in (48)–(49), a natural question arises as to whether it can also describe the motion of a simple dissipative system in classical mechanics (CM). In [10], it has been shown that considering the mechanical phase space of a system to be a contact manifold $(\mathcal{T}^{\text{CM}}, \eta^{\text{CM}})$, the contact Hamiltonian Equations (7)–(9) extend the standard Hamiltonian equations to include cases where dissipation is considered. As an example, considering the (on-dimensional) contact Hamiltonian:

$$\mathscr{H}^{\text{CM}} = H_{\text{mec}}(q,p) + \gamma S, \tag{51}$$

where:

$$H_{\text{mec}}(q,p) = \frac{p^2}{2m} + V(q) \tag{52}$$

is the mechanical energy of the system and γ is a constant, from (7)–(9), it follows that the dynamics of the system in the contact phase space is:

$$\dot{q} = \frac{p}{m}, \tag{53}$$

$$\dot{p} = -\frac{\partial V(q)}{\partial q} - \gamma p, \tag{54}$$

$$\dot{S} = \frac{p^2}{2m} - V(q) - \gamma S. \tag{55}$$

By the first two equations, one has that the equation for the position of the system is:

$$\ddot{q} + \gamma\dot{q} + \frac{1}{m}\frac{\partial V}{\partial q} = 0, \tag{56}$$

which is the standard Newtonian equation for mechanical systems with a dissipation linear in the velocity, with γ being the friction coefficient. Moreover, from the third equation, one can see that S (whose dynamics decouples from that of q and p in this case) is Hamilton's principal function.

Furthermore, it is possible to extend contact Hamiltonian systems to the time-dependent case and to show that several results from symplectic mechanics carry over to the contact setting. For instance, contact transformations generalize canonical transformations, and one can find a contact version of the Hamilton-Jacobi theory, equivalent to the dynamics (7)–(9) (cf. [10,46]).

7. Conclusions and Future Directions

The main purpose of this work has been to review and collect in a unified framework different novel applications of contact Hamiltonian dynamics in various areas of physics. The two main points we want to stress are on the one side that contact Hamiltonian dynamics is just as ubiquitous as its symplectic 'cousin', and on the other side that from all the applications presented here, it seems that it is a natural candidate for the extension of standard Hamiltonian dynamics to systems governed by irreversible phenomena. Indeed, there is a general belief that a full knowledge of the degrees of freedom and of the dynamics of a system corresponds to a symplectic Hamiltonian evolution, i.e., a time-reversible dynamics for which energy is conserved. On the contrary, dissipation and irreversibility are usually associated with effective or averaged descriptions and hence with a dimensional reduction of the phase space of the problem. In this work, we have shown that contact Hamiltonian dynamics plays a role at all levels of representation whenever an effective description is taken into account: from classical mechanics of dissipative systems, to mesoscopic dynamics, up to equilibrium statistical mechanics and thermodynamics.

Since the contact Hamiltonian equations are Legendre transformations (meaning that they preserve the contact structure), our analysis seems to provide further motivation for the program proposed in [25–27] of considering Legendre transformations as the basic dynamical laws for irreversible phenomena, motivated by the fact that they correspond to maximization of eta-functions (like, e.g., the entropy) subject to constraints. This aspect certainly deserves further investigation. It is also worth trying to understand precisely the mechanism of dimensional reduction by which the reversible symplectic Hamiltonian dynamics converts into an irreversible contact Hamiltonian evolution at the various levels of description (for this purpose, a comparison with different approaches may be useful [47]).

Related to contact Hamiltonian mechanics, a direction that needs to be addressed is that of the quantization of contact Hamiltonian systems. In this sense, a naive proposal has been sketched already in [10], whereas in [48–50], one can find more formal approaches.

In equilibrium thermodynamics, one can codify fluctuations by means of another geometric object, namely a metric structure. Such a metric on the Legendre submanifolds representing systems at equilibrium takes the form of a Hessian metric of the thermodynamic potential (see, e.g., [12,51,52]). This Hessian metric can be lifted naturally to the thermodynamic phase space, and one can prove that its lift is as well adapted to the contact structure as it can be, i.e., it defines a (para-)Sasakian structure (see [15,53]), which is the analogue in odd-dimensional spaces of a (para-)Kähler structure. It is natural then to ask whether such geometry plays any role in the other areas presented in this work or if on the contrary contact Hamiltonian dynamics can be relevant for theories using similar geometric structures such as, e.g., string theory [8,9] and the geometric description of quantum mechanics [54–57].

In this work, we have deliberately focused only on physical applications. However, contact geometry and contact Hamiltonian dynamics appear also in the theory of the optimal control of systems [58,59]. Other areas where contact geometry has been used and which have not been covered in this survey are fluid mechanics [60], electromagnetism [61], electric circuits theory [37,62] and black hole thermodynamics [7,63]. Moreover, recently, a novel application of contact geometry in order to obtain a generally covariant approach to quantum mechanics has been presented in [64]. We consider that these can be fruitful areas for further research.

Finally, from our analysis, it should be clear that contact Hamiltonian dynamics provides a formal framework to describe systems undergoing irreversible phenomena at all scales. Therefore, an interesting direction is that of finding new systems and new effective theories starting from contact Hamiltonian dynamics.

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References

1. Geiges, H. *An Introduction to Contact Topology*; Cambridge University Press: Cambridge, UK, 2008; Volume 109.
2. Arnold, V.I. *Mathematical Methods of Classical Mechanics*; Springer: New York, NY, USA, 1989; Volume 60.
3. Abraham, R.; Marsden, J.E.; Marsden, J.E. *Foundations of Mechanics*; Benjamin/Cummings Publishing: Reading, MA, USA, 1978.
4. Mrugała, R. Geometrical formulation of equilibrium phenomenological thermodynamics. *Rep. Math. Phys.* **1978**, *14*, 419–427.
5. Mrugała, R.; Nulton, J.D.; Schön, J.C.; Salamon, P. Statistical approach to the geometric structure of thermodynamics. *Phys. Rev. A* **1990**, *41*, 3156–3160.
6. Mrugała, R. On contact and metric structures on thermodynamic spaces. *RIMS Kokyuroku* **2000**, *1142*, 167–181.
7. Quevedo, H. Geometrothermodynamics. *J. Math. Phys.* **2007**, *48*, 13506.
8. Martelli, D.; Sparks, J. Toric geometry, Sasaki–Einstein manifolds and a new infinite class of AdS/CFT duals. *Commun. Math. Phys.* **2006**, *262*, 51–89.
9. Martelli, D.; Sparks, J.; Yau, S.T. Sasaki–Einstein manifolds and volume minimisation. *Commun. Math. Phys.* **2008**, *280*, 611–673.
10. Bravetti, A.; Cruz, H.; Tapias, D. Contact Hamiltonian Mechanics. *Ann. Phys.* **2017**, *376*, 17–39.
11. Bravetti, A.; Lopez-Monsalvo, C.S.; Nettel, F. Conformal gauge transformations in thermodynamics. *Entropy* **2015**, *17*, 6150–6168.
12. Balian, R.; Valentin, P. Hamiltonian structure of thermodynamics with gauge. *Eur. Phys. J. B* **2001**, *21*, 269–282.
13. Pollettini, M. Nonequilibrium thermodynamics as a gauge theory. *Europhys. Lett.* **2012**, *97*, 30003.
14. Bravetti, A.; Tapias, D. Liouville's theorem and the canonical measure for nonconservative systems from contact geometry. *J. Phys. A Math. Theor.* **2015**, *48*, 245001.
15. Bravetti, A.; Lopez-Monsalvo, C.; Nettel, F. Contact symmetries and Hamiltonian thermodynamics. *Ann. Phys.* **2015**, *361*, 377–400.
16. Goto, S.I. Legendre submanifolds in contact manifolds as attractors and geometric nonequilibrium thermodynamics. *J. Math. Phys.* **2015**, *56*, 73301.
17. Maschke, B. About the lift of irreversible thermodynamic systems to the Thermodynamic Phase Space. *IFAC-PapersOnLine* **2016**, *49*, 40–45.
18. Ramirez, H.; Maschke, B.; Sbarbaro, D. Partial stabilization of input-output contact systems on a Legendre submanifold. *IEEE Trans. Autom. Control* **2017**, *62*, 1431–1437.
19. Mrugała, R.; Nulton, J.D.; Schön, J.C.; Salamon, P. Contact structure in thermodynamic theory. *Rep. Math. Phys.* **1991**, *29*, 109–121.
20. Mrugała, R. On a special family of thermodynamic processes and their invariants. *Rep. Math. Phys.* **2000**, *46*.
21. Callen, H.B. *Thermodynamics and an Introduction to Thermostatistics*; Wiley: New Delhi, India, 2006.
22. Mrugała, R. Structure group $U(n) \times 1$ in thermodynamics. *J. Phys. A Math. Gen.* **2005**, *38*, 10905.
23. Hernández, G.; Lacomba, E.A. Contact Riemannian geometry and thermodynamics. *Differ. Geom. Appl.* **1998**, *8*, 205–216.
24. Baldiotti, M.; Fresneda, R.; Molina, C. A Hamiltonian approach to Thermodynamics. *Ann. Phys.* **2016**, *373*, 245–256.
25. Grmela, M.; Öttinger, H.C. Dynamics and thermodynamics of complex fluids. I. Development of a general formalism. *Phys. Rev. E* **1997**, *56*, 6620–6632.

26. Grmela, M. Reciprocity relations in thermodynamics. *Phys. A Stat. Mech. Appl.* **2002**, *309*, 304–328.
27. Grmela, M. Contact geometry of mesoscopic thermodynamics and dynamics. *Entropy* **2014**, *16*, 1652–1686.
28. Eberard, D.; Maschke, B.; Van Der Schaft, A. An extension of Hamiltonian systems to the thermodynamic phase space: Towards a geometry of nonreversible processes. *Rep. Math. Phys.* **2007**, *60*, 175–198.
29. Favache, A.; Martins, V.S.D.S.; Dochain, D.; Maschke, B. Some properties of conservative port contact systems. *IEEE Trans. Autom. Control* **2009**, *54*, 2341–2351.
30. Favache, A.; Dochain, D.; Maschke, B. An entropy-based formulation of irreversible processes based on contact structures. *Chem. Eng. Sci.* **2010**, *65*, 5204–5216.
31. Ramirez, H.; Maschke, B.; Sbarbaro, D. Feedback equivalence of input-output contact systems. *Syst. Control Lett.* **2013**, *62*, 475–481.
32. Wang, L.; Maschke, B.; van der Schaft, A. Stabilization of Control Contact Systems. *IFAC-PapersOnLine* **2015**, *48*, 144–149.
33. Hudon, N.; Dochain, D.; Guay, M. Representation of irreversible systems in a metric thermodynamic phase space. *IFAC-PapersOnLine* **2015**, *48*, 1070–1074.
34. Merker, J.; Krüger, M. On a variational principle in Thermodynamics. *Contin. Mech. Thermodyn.* **2013**, *25*, 779–793.
35. Dolfin, M.; Francaviglia, M. A geometric perspective on Irreversible Thermodynamics. Part I: General concepts. *Commun. Appl. Ind. Math.* **2011**, *1*, 135–152.
36. Dolfin, M.; Francaviglia, M.; Preston, S.; Restuccia, L. Entropy form and the contact geometry of the material point model. *Int. J. Geom. Methods Mod. Phys.* **2012**, *9*, 1250013.
37. Goto, S.I. Contact geometric descriptions of vector fields on dually flat spaces and their applications in electric circuit models and nonequilibrium statistical mechanics. *J. Math. Phys.* **2016**, *57*, 102702.
38. Bravetti, A.; Tapias, D. Thermostat algorithm for generating target ensembles. *Phys. Rev. E* **2016**, *93*, 22139.
39. Tuckerman, M.E. *Statistical Mechanics: Theory and Molecular Simulation*; Oxford Graduate Texts; Oxford University Press: Oxford, UK, 2010.
40. Evans, D.; Morriss, G. *Statistical Mechanics of Nonequilirium Liquids*; Cambridge University Press: Cambridge, UK, 2008.
41. Sergi, A. Non-Hamiltonian equilibrium statistical mechanics. *Phys. Rev. E* **2003**, *67*, 21101.
42. Lacomba, E.A.; Losco, L. Variational characterization of contact vector fields in the group of contact diffeomorphisms. *Phys. A Stat. Mech. Appl.* **1982**, *114*, 124–128.
43. Lacomba, E.; Losco, L. Caractérisation variationnelle globale des flots canoniques et de contact dans leurs groupes de difféomorphismes. *Ann. l'IHP Physique Théorique* **1986**, *45*, 99–116. (In French)
44. Tapias, D.; Sanders, D.P.; Bravetti, A. Geometric integrator for simulations in the canonical ensemble. *J. Chem. Phys.* **2016**, *145*, 84113.
45. Tapias, D.; Bravetti, A.; Sanders, D.P. Ergodicity of one-dimensional systems coupled to the logistic thermostat. *Comput. Methods Sci. Technol.* **2017**, *23*, 11–18.
46. De León, M.; Sardón, C. A geometric approach to solve time dependent and dissipative Hamiltonian systems. *arXiv* **2016**, arXiv:1607.01239.
47. Bianucci, M. Large Scale Emerging Properties from Non Hamiltonian Complex Systems. *Entropy* **2017**, *19*, 302.
48. Rajeev, S.G. Quantization of contact manifolds and thermodynamics. *Ann. Phys.* **2008**, *323*, 768–782.
49. Fitzpatrick, S. On the geometric quantization of contact manifolds. *J. Geom. Phys.* **2011**, *61*, 2384–2399.
50. Bravetti, A.; Garcia-Chung, A.; Tapias, D. Exact Baker-Campbell-Hausdorff formula for the contact Heisenberg algebra. *J. Phys. A Math. Theor.* **2017**, *50*, 105203.
51. Ruppeiner, G. Riemannian geometry in thermodynamic fluctuation theory. *Rev. Mod. Phys.* **1995**, *67*, 605–659.
52. Weinhold, F. *Classical and Geometrical Theory of Chemical and Phase Thermodynamics*; Wiley: Hoboken, NJ, USA, 2009.
53. Bravetti, A.; Lopez-Monsalvo, C. Para-Sasakian geometry in thermodynamic fluctuation theory. *J. Phys. A Math. Theor.* **2015**, *48*, 125206.
54. De León, M.; Marrero, J.C.; Padrón, E. On the geometric quantization of Jacobi manifolds. *J. Math. Phys.* **1997**, *38*, 6185–6213.
55. Carinena, J.F.; Clemente-Gallardo, J.; Marmo, G. Geometrization of quantum mechanics. *Theor. Math. Phys.* **2007**, *152*, 894–903.

56. Facchi, P.; Kulkarni, R.; Man'ko, V.; Marmo, G.; Sudarshan, E.; Ventriglia, F. Classical and quantum Fisher information in the geometrical formulation of quantum mechanics. *Phys. Lett. A* **2010**, *374*, 4801–4803.
57. Cariñena, J.F.; Ibort, A.; Marmo, G.; Morandi, G. *Geometry from Dynamics, Classical and Quantum*; Springer: Dordrecht, The Netherlands, 2015.
58. Ohsawa, T. Contact geometry of the Pontryagin maximum principle. *Automatica* **2015**, *55*, doi:10.1016/j.automatica.2015.02.015.
59. Jóźwikowski, M.; Respondek, W. A contact covariant approach to optimal control with applications to sub-Riemannian geometry. *Math. Control Signals Syst.* **2016**, *28*, doi:10.1007/s00498-016-0176-3.
60. Ghrist, R. On the contact topology and geometry of ideal fluids. In *Handbook of Mathematical Fluid Dynamics*; Friedlander, S., Serre, D., Eds; Elsevier: Amsterdam, The Netherlands, 2007.
61. Dahl, M. Contact geometry in electromagnetism. *Prog. Electromagn. Res.* **2004**, *46*, 77–104.
62. Eberard, D.; Maschke, B.M.; Schaft, A.J. Energy-conserving formulation of RLC-circuits with linear resistors. In Proceedings of the 17th International Symposium on Mathematical Theory of Networks and Systems, Kyoto, Japan, 24–28 July 2006.
63. Quevedo, H. Geometrothermodynamics of black holes. *Gen. Relativ. Gravit.* **2008**, *40*, 971–984.
64. Herczeg, G.; Waldron, A. Contact Geometry and Quantum Mechanics. *arXiv* **2017**, arXiv:1709.04557.