

A Topological, Non-Statistical, Link between Mechanics and the Thermodynamics of Irreversible Processes

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Abstract

Cartan's magic formula is used as the fundamental link between mechanics and thermodynamics, expressing continuous topological evolution of physical systems, encoded by exterior differential forms, with respect to processes, defined by contravariant vector direction fields. Cartan's formula of continuous topological evolution is the dynamical equivalent of the first law, and permits the analysis of physical systems and processes based upon equivalence classes generated by the Pfaff topological dimensions of the 1-forms of Action, A , Work, W and Heat, Q . When the Pfaff dimension of the virtual work 1-form is 4 or more, the process is always irreversible,

Key Words: Thermodynamic irreversibility, Topological Torsion vector, Continuous Topological evolution, Pfaff dimension

1. INTRODUCTION

A major objective of this article is to establish a topological, non-statistical, link between mechanics and thermodynamics, with the particular goal of describing the differences between reversible and irreversible evolutionary processes. The

methods are based upon Cartan's techniques[1], which have been found capable of describing continuous topological evolution of exterior differential systems. The fundamental axioms are:

Axiom 1. *Physical systems can be described by exterior differential forms constructed from covariant tensor fields, A .*

Axiom 2. *Physical processes can be defined in terms of contravariant vector fields, \mathbf{V} , which may or may not be generators of 1-parameter groups.*

Axiom 3. *Equations of evolution describing processes acting on physical systems can be deduced from Cartan's magic formula :*

$$L_{(\mathbf{V})}A = i(\mathbf{V})dA + d(i(\mathbf{V})A). \quad (1.1)$$

Cartan's "magic formula" [2] representing the "evolution" of the 1-form of Action, A , with respect to the "flow" generated by the vector field, \mathbf{V} , is the cornerstone of the development. The Cartan formula does not depend upon the constraints of connection or metric imposed upon the base space of independent variables, and has been called the homotopy formula by Arnold [3]. The formula can be used to describe both those evolutionary processes which are homeomorphic and preserve topology, and those processes that represent continuous topological evolution. Hamiltonian processes are representatives of the homeomorphic category, and they are always thermodynamically reversible. Irreversible processes involve changing topology.

Herein, the following definitions are made:

1. The term $W = i(\mathbf{V})dA$ is defined as the inexact 1-form of "virtual work".
2. The function $U = i(\mathbf{V})A$ is defined as the "internal energy".
3. The sum of the two terms, $W + dU$, define the inexact 1-form of "heat", Q .

From these definitions, it is apparent that Cartan's magic formula not only represents an evolutionary process, where the process V acts on the physical system A to produce the 1-form of heat, Q , but also is formally equivalent to the cohomological description of the First Law of Thermodynamics.

$$\begin{aligned} L_{(\mathbf{V})}A &= i(\mathbf{V})dA + d(i(\mathbf{V})A) = Q \\ &= W + dU = Q. \end{aligned} \quad (1.2)$$

In this article this formal correspondence is taken seriously. The fundamental theme is to study processes that describe continuous topological evolution. Such evolutionary processes are not necessarily invertible and do not admit unique deterministic prediction of tensor fields from initial data. However, they do permit the deterministic retrodiction of tensor fields by means of functional substitution and pullback [4]. The magic in Cartan's formula is that it can be used to describe such evolutionary processes where the topology of the initial state is not the same as the topology of the final state, as well as for adiabatic processes for which the topology does not change.

Both the heat and the work 1-forms as defined above are not necessarily exact, and therefore can lead to non-zero cyclic integrals. The symbol $L_{(\mathbf{V})}$ stands for the "Lie derivative" with respect to \mathbf{V} , a term evidently coined by Slebodzinsky [5]. The symbol dA stands for the "exterior derivative" of A , and the symbol $i(\mathbf{V})A$ is used to designate the "interior product" of the contravariant \mathbf{V} with the covariant A in a tensorial sense, producing a diffeomorphic invariant. However, no constraints of metric or connection are applied a priori to the domain of definition. For more detail see [6].

For physical systems of measurement it is presumed that the ultimate or fundamental domain (or base) of independent variables will be designated by the ordered quadruplet $\{x, y, z, t\}$. Most useful applications will be constructed from both covariant and contravariant vector fields and functions ultimately defined over this base. However, an initial domain of definition may be conveniently of higher dimension; that is, the initial variety may consist of $2n+1$ or $2n+2$ independent variables. Note that the initial variety may consist of both "coordinates" and "parameters", and the notation is suitable for application of Fiber bundle theory.

1.1. The Pfaff Sequence and the Pfaff Dimension

Consider a physical system encoded by a single 1-form of Action, A . Construct the Pfaff sequence of ordered differential p-forms built from one exterior differential process combined with numerous exterior multiplications:

$$\text{Pfaff Sequence of } A : \{A, dA, A \wedge dA, dA \wedge dA, \dots\}. \quad (1.3)$$

For any given functional format of 1-form coefficients and differentials, the Pfaff sequence will consist of m terms. The p-form of highest degree in the sequence, $p = m$, is defined as the "top Pfaffian". The integer m defines the concept of the

Pfaff topological dimension, or class. The idea, due to Cartan, is associated with the fact that a given differential form, A , defined arbitrarily on a variety of, say, dimension $2n+2$ independent variables, may require only $m \leq 2n+2$ independent functions for its description. This lesser number of (differentiable) functions (a projection) may be used to describe the topological features of the system. By using functional substitution and the "pullback" of the projection, the results of investigations on the lower dimensional space can be retrodicted back to the initial higher dimensional manifold. Note that the projection will not have an inverse map, yet the 1-form on the target space, m , is functionally well defined on the $2n+2$ dimensional space used in the original formulation, if the projection is C^1 differentiable. This fact is a remarkable result that demonstrates that Cartan's exterior differential forms are not necessarily tensors, which by definition are well behaved with respect to diffeomorphisms. Cartan's exterior differential forms are well behaved with respect to differentiable maps without inverse, and therefore are appropriate for the study of irreversible thermodynamic processes. Problems of non-differentiable functions are not considered in this current article.

Of key importance for any particular physical system is the choice of the "correct" 1-form of Action, A . Experience (guesswork) and the degree of agreement with measurement will satisfy the working scientist. By measurement, it is meant that certain geometrical and topological features will be "observable" evolutionary invariants of a process, or of an equivalence class of processes. In physics, the equivalence class of processes is often specified as solutions to a system of partial differential equations; herein, the alternative view is taken that the equivalence class is generated by an exterior differential system of constraints.

Note that the Cartan Magic formula defines two other 1-forms, W and Q , and each will have its own Pfaff dimension, which will refine the topological equivalence classes established by the 1-form, A . The top Pfaffian is a global concept on the space of independent variables, defining a domain of support. Subspace regions can exist as singularities, where the Top Pfaffian vanishes, and the Pfaff sequence of a given 1-form, A , terminates at a smaller integer. Continuous processes exist such that irreversible dissipation can cause the physical system to be attracted to the singular regions. Such evolutionary processes are not homeomorphisms, for the process causes a change in the topology: the Pfaff dimension changes as the topology "decays".

It was demonstrated by Caratheodory [7] that the "singular" states of Pfaff dimension 2 or less correspond to "equilibrium" systems, as they satisfy the Frobenius theorem of unique integrability. There can exist singular states of odd Pfaff

dimension greater than 2 which support unique physical (extremal) processes that are "conservative" and do not topologically decay. These long lived states give a formal definition to the meaning of "stationary states far from equilibrium".

1.2. Cartan's development of Hamiltonian processes.

Recall that Cartan proved that if the 1-form of Action is taken to be of the classic format, $A = p_k dq^k + H(p_k, q^k, t)dt$, on a $2n+1$ dimensional domain of variables $\{p_k, q^k, t\}$, then a subset of all vector fields, V , that satisfy his magical equation would generate "Hamiltonian flows" of classical mechanics [8]. The necessary and sufficient constraint established by Cartan for the vector field to be of the Hamiltonian format was that the closed integrals of the Action $\int_{z_1} A$ must be evolutionary invariants of the process, V .

$$\text{Cartan's Constraint: } L_{(\mathbf{v})} \int_{z_1} A \Rightarrow 0. \quad (1.4)$$

The symbol, \int_{z_1} , is used to designate that the integration chain is a closed cycle, z_1 ; \int_{z_2} , would be used to designate a two dimensional closed cycle; etc.. The cycle may or may not be a boundary. When the cycle is not a boundary, the invariant constraint becomes a topological period integral in the sense of deRham. In other words, the Cartan constraint implies that Hamiltonian extremal processes preserve topology.

The Cartan criteria does not constrain the Hamiltonian function $H(p_k, q^k, t)$ to be independent from time, but as will be described below, it does insure that the Cartan topology of the initial state is the same as the Cartan topology of the final state. The same criteria to generate "Hamiltonian flows" can be used on $2n+2$ dimensional domains, (p_k, q^k, t, s) . The key difference is that on the odd dimensional domain (a contact manifold) the Hamiltonian flow is a unique "extremal" field. The generator of the flow is the Hamiltonian function, $H(p_k, q^k, t)$. On the $2n+2$ dimensional domain (a symplectic manifold), a unique extremal field does not exist. There do exist (many) "Hamiltonian flows", but they are generated, not from $H(p_k, q^k, t, s)$, but from other functions, known as Bernoulli-Casimir functions, Θ .

There does, however, exist a unique vector direction field of evolution on the symplectic $2n+2$ domain, but it is not equivalent to a Hamiltonian flow. In fact, it will be demonstrated below that this unique vector field (defined as the Topological Torsion current) represents thermodynamically irreversible processes.

1.3. Thermodynamic Irreversibility $Q \wedge dQ = 0$

The Cartan constraint ($L_{(\mathbf{V})} \int_{z1} A = 0$) thereby partitions all possible vector fields of evolution into two equivalence classes, those representing processes that are "Hamiltonian", and those that are not Hamiltonian. Herein the idea is to exploit Cartan's magic formula to obtain a better understanding of the non-Hamiltonian processes ($L_{(\mathbf{V})} \int_{z1} A \neq 0$), and how they may represent dissipative and irreversible physical phenomena. Hamiltonian processes may be time-dependent, hence decaying energy alone is not a sufficient criteria to insure thermodynamic irreversibility.

Following the lead of thermodynamic experience, a thermodynamic process which is reversible it to be associated with a heat 1-form, Q , which admits an integrating factor. The integrating factor (in thermodynamics) defines the concept of temperature. Therefore, if the heat 1-form does not admit an integrating factor, the thermodynamic process is irreversible [9]. From a topological point of view, the heat 1-form admits an integrating factor if and only if Q satisfies the conditions of the Frobenius integrability theorem, $Q \wedge dQ = 0$. The Pfaff dimension of the Heat 1-form is 2 or less for reversible processes. This definition of thermodynamic irreversibility, when combined with Cartan's magic formula, permits the link to be made between thermodynamics and mechanical systems.

To repeat: It is subsumed that the physical system can be represented by a 1-form of Action, A , and a physical process can be represented by the vector field \mathbf{V} . As the system (A) is propagated via the action of the Lie derivative with respect to the process, \mathbf{V} , the outcome is to produce the heat 1-form, Q . Hence a simple test for thermodynamic irreversibility of a process acting on a system is given by the equations:

$$Q \wedge dQ = (L_{(\mathbf{V})}A) \wedge (L_{(\mathbf{V})}dA) = 0 \supset \text{the process is reversible.} \quad (1.5)$$

$$Q \wedge dQ = (L_{(\mathbf{V})}A) \wedge (L_{(\mathbf{V})}dA) \neq 0 \supset \text{the process is irreversible.} \quad (1.6)$$

The technique is as follows: First start with a reasonable description of a physical system in terms of a 1-form of Action, A , and then for a given vector field, \mathbf{V} , representing a process, construct Q from Cartan's formula. Finally, use the Frobenius test to see if the given process is reversible or not.

Rather than applying the method to many examples, it is possible to consider equivalence classes determined by the Pfaff dimension, or class, $Pfaff(W)$, of the 1-form of virtual work, W . The Pfaff dimension of the virtual work 1-form, $W = i(\mathbf{V})dA$, depends on both the process (\mathbf{V}) and the system (A). Conservative

Hamiltonian processes belong to the class, $Pfaff(W) = 0$ or $Pfaff(W) = 1$. Processes that belong to the $Pfaff(W) = 4$ are always irreversible.

2. The Pfaff Dimension of the 1-form of Virtual Work

In a manner similar to that used to construct the Pfaff sequence for a given 1-form of Action, A , it is possible to construct the Pfaff sequence for the 1-form of Work, $W = i(\mathbf{V})dA$. The sequence, $W, dW, W \wedge dW, dW \wedge dW, \dots$ defines the Pfaff dimension, or class, $Pfaff(W)$ of the form, W . The 1-form of Work is composed of both those functions which encode the physical system, A , and those functions which encode the process, \mathbf{V} . As the 1-form of Work is constructed from the 1-form of Action, A , the number of contravariant components of a vector field, V , required to define the 1-form of virtual work, W , need not exceed the Pfaff dimension of the Action 1-form. However, the components of an arbitrary contravariant vector field on the original domain of definition may not be fully expressible in terms of projected functions of the 1-form of Action. In other language, the Pfaff dimension of the 1-form of Action determines the base, but the contravariant vector field has additional components along the fibers of the vector bundle.

Cartan's magic formula takes note of this difference, for the 1-form of virtual work, W , is transversal to the process, \mathbf{V} , while the 1-form of heat, Q , is not.

$$i(\mathbf{V})W = i(\mathbf{V})i(\mathbf{V})dA = 0, \quad \text{but} \quad i(\mathbf{V})Q = i(\mathbf{V})d(i(\mathbf{V})A) \neq 0. \quad (2.1)$$

This result gives a precise definition to the differences between the concepts of work and heat. Heat can have components along the fibers, work does not.

In that which follows, the features of the various equivalence classes defined by the Pfaff dimension of the 1-form of virtual work are explored. In all classes considered, the trivial case $dA = 0$, is ignored, for then every vector field representing a process on such physical systems is such that the virtual work vanishes. All such cyclic processes are adiabatic, and if the process is such the internal energy is constant, $dU = d(i(\mathbf{V})A) = 0$, then such processes are locally and globally adiabatic. If the process is an associated vector, (such the $U = i(\mathbf{V})A \Rightarrow 0$) then the process resides on the "equipotential" surface defined by the Pfaffian equation, $dA = 0$.

2.1. Reversible Case 1: Pfaff(W) = 0. Cyclically adiabatic extremal processes.

When $dA \neq 0$, the constraint, $Pfaff(W) = 0$, implies that the virtual work 1-form vanishes, $W = i(\mathbf{V})dA = 0$, and the 2-form $dW \Rightarrow 0$. Recall that the 2-form of "vorticity", or field intensities, dA , consists of an anti-symmetric matrix of coefficients. Hence, only when the Pfaff dimension of the Action is an odd-integer, $2n+1$, is it possible for work 1-form to vanish. In such cases the processes, \mathbf{V} , are defined as extremals (a word borrowed from the calculus of variations) and are *uniquely* determined (to within a projective factor) as the null eigen vector of the anti-symmetric matrix of functions that are used to represent the coefficients of the 2-form dA . As this extremal constraint determines the "equations of motion", it should be noted that there is a large equivalence class of physical systems that will have similar orbital motion. In the extremal case the 1-form of Action is not unique, for any closed 1-form, γ , with $d\gamma = 0$, may be added to the initial 1-form, A , without changing the structure of the 2-form, dA . It is the form dA that determines the virtual work, W .

$$dA = d(A_0 + \gamma) = dA_0 + d\gamma = dA_0. \quad (2.2)$$

The "equations of motion" are said to be "gauge" invariant in the sense that the virtual work 1-form is the same for all physical systems which are elements of the large equivalence class of Actions which differ from one another by a closed 1-form (the "gauge"). Note that the gauge differences between the elements of different actions are not necessarily exact differentials; the class of actions that produce gauge invariant fields, or equations of motion, can belong to different cohomology classes. In short, the same W can have many precursors A

However, from a thermodynamic point of view, the heat 1-form, Q , and how the system interacts with its surroundings, is sensitive to the closed 1-form additions to the Action 1-form. The heat 1-form, Q , and the internal energy, U , are **not** necessarily gauge invariant, but the work 1-form is always gauge invariant. For a closed 1-form, $dA = 0$, modified by gauge additions, $A = A_0 + \gamma$:

$$\begin{aligned} L_{(\mathbf{V})}A &= i(\mathbf{V})dA + d(i(\mathbf{V})A) \\ &= 0 + dU = d\{i(\mathbf{V})A_0 + (i(\mathbf{V})\gamma)\} = Q. \end{aligned} \quad (2.3)$$

However, what is remarkable, is that any closed integral of the Action, $\int_{z_1} A$, is a (relative) integral invariant of the extremal evolutionary processes generated by

\mathbf{V} of this equivalence class.

$$L_{(\mathbf{v})} \int_{z_1} A = \int_{z_1} Q = 0 \quad (W = 0). \quad (2.4)$$

Hence, any cyclic integral of the heat 1-form is "gauge" invariant. During portions of the cycle, Q may be positive and negative, such that over the cycle, the net Q is zero. (Such systems are sometimes called "breathers" and can be related to limit cycles that occur in dissipative systems.)

If Q vanishes identically, the process is said to be locally adiabatic. For a given system, the constraint that the process be locally adiabatic, can be satisfied by an extremal vector field, which is also "associated". The two constraints,

$$i(\mathbf{V})A = 0 \quad (\textit{associated}) \quad (2.5)$$

$$i(\mathbf{V})dA = 0 \quad (\textit{extremal}) \quad (2.6)$$

form a subclass of processes defined as "characteristic" processes. It follows that such characteristic processes are locally adiabatic¹.

The extremal evolutionary processes form the basis for classical mechanics on state-space. It is apparent that the net heat around any closed path is cyclically zero. If in addition the internal energy is a constant, $dU = 0$, then such processes are locally adiabatic, as $Q = W + dU = 0 + 0 = 0$. As the extremal vector field is determined only up to a factor, ρ , it is possible to choose this function such that the internal energy is a constant,

$$U = \rho(i(\mathbf{V})A) = \textit{Const}. \quad (2.7)$$

For such choices of ρ the extremal process is locally adiabatic.

As an example, suppose the initial domain of independent variables $\{E, t, p_k, q^k\}$ is of dimension $2n+2$, with a Darboux representation for the 1-form of Action given by the expression

$$A = p_k dq^k - E dt. \quad (2.8)$$

The top Pfaffian, $dA \wedge dA \dots$ is a $2n+2$ form

$$dA \wedge dA \dots = dE \wedge dt \wedge dp_1 \dots \wedge dp_n \wedge dq^1 \dots \wedge dq^n. \quad (2.9)$$

¹It is remarkable that characteristic processes can propagate discontinuities.

If the Pfaff dimension of the Action 1-form is to be $2n+1$, then this $2n+2$ form must vanish. Hence the variable, E , cannot be functionally independent from the remaining (presumed to be independent) variables; it follows that $E = H\{p, q, t\}$ on the $2n+1$ dimensional domain. The Action 1-form is then written in the Cartan-Hilbert-Hamiltonian format

$$A = p_k dq^k - H\{p, q, t\} dt. \quad (2.10)$$

Relative to the $2n+1$ "coordinates" $[p_k, q^k, t]$, consider the vector field $\mathbf{V} = [f_k, V^k, 1]$ and find the solution to the equation, $W = i(\mathbf{V})dA = 0$. The result is

$$\mathbf{V} = [f_k = -\partial H/\partial q, V^k = \partial H/\partial p, 1]. \quad (2.11)$$

and the extremal field is said to be Hamiltonian.

By computing the exterior derivative of Cartan's magic formula, it follows that,

$$\begin{aligned} L_{(\mathbf{V})}dA &= di(\mathbf{V})dA + dd(i(\mathbf{V})A) \\ &= dW + 0 = dQ. \end{aligned} \quad (2.12)$$

As $dW = 0$ for $Pfaff(W) = 0$, it follows that $dQ = 0$. Hence, all even dimensional elements of the Pfaff sequence generated by the Action, $\{dA, dA \wedge dA, \dots\}$, and their integrals, are absolute invariants of the equivalence class of Hamiltonian extremal fields, a result known to Poincare.

Note that all processes for which the work 1-form is of Pfaff class zero are reversible, for then $Q \wedge dQ = 0$.

2.2. Reversible Case 2: Pfaff(W) = 1. Symplectic processes.

When the virtual work 1-form is closed but not zero, $W \neq 0, dW = 0$, then the Pfaff dimension of W is equal to 1. The closure constraint forces the virtual work 1-form to be composed of a perfect differential and/or a harmonic part. When the virtual work 1-form is exact, such that

$$W = i(\mathbf{V})dA = d\Theta(x, y, z, t), \quad (2.13)$$

then the function Θ is defined as a Bernoulli-Casimir function. The function $\Theta(x, y, z, t)$ satisfies the equation,

$$L_{(\mathbf{V})}\Theta = i(\mathbf{V})d\Theta = i(\mathbf{V})(i(\mathbf{V})dA) = 0, \quad (2.14)$$

from which it is determined that the Bernoulli-Casimir function is an evolutionary invariant, and its gradient is transversal to the evolutionary process, when the Work 1-form is of Pfaff dimension 1, and exact. In hydrodynamics, the Bernoulli function is a constant along any streamline, but neighboring streamlines will have different values for the Bernoulli function. When the virtual work 1-form is exact, the processes are not only reversible ($dQ = 0$), but they are also cyclically adiabatic.

If the Action, A , is written in the Cartan format,

$$A = p_k dq^k - H(p_k, q^k, t, \sigma)dt, \quad (2.15)$$

then the Hamiltonian energy, $H(p, q, t, \sigma)$, is not necessarily an invariant of the flow generated by the Bernoulli-Casimir function, Θ . However, the evolutionary vector field is again said to be "Hamiltonian", for $dp - (-\partial\Theta/\partial q)dt = 0$ and $dq - (\partial\Theta/\partial p)dt = 0$.

When the Work 1-form is non-zero but exact, an adiabatic solution for the process can be determined from the exterior differential system,

$$\text{adiabatic constraint: } W = -dU \Rightarrow i(\mathbf{V})dA = -d(i(\mathbf{V})A), \quad (2.16)$$

for then

$$L_{(\mathbf{V})}A = W + dU = -dU + dU = Q = 0. \quad (2.17)$$

The adiabatic exterior differential system is equivalent to a system of partial differential equations recognizable in both hydrodynamic and electromagnetic language. As an example consider the domain $\{x, y, z, t\}$ and the Action, $A = \mathbf{A} \bullet d\mathbf{r} - \phi dt$. The adiabatic condition becomes the partial differential system,

$$-\partial\mathbf{A}/\partial t - \text{grad}\phi + \mathbf{V} \times \text{curl}\mathbf{A} = -\text{grad}(\mathbf{V} \cdot \mathbf{A} - \phi), \quad (2.18)$$

$$\mathbf{V} \cdot (-\partial\mathbf{A}/\partial t - \text{grad}\phi) = \partial(\mathbf{V} \cdot \mathbf{A} - \phi)/\partial t. \quad (2.19)$$

The first equation, in EM language, is a statement defining the Lorentz force in terms of the gradient of the interaction energy. In hydrodynamics, the first equation is a statement that describes an Eulerian fluid.

When the Work 1-form is not exact, but closed, the domain may support harmonic components, γ , representing topological obstructions. In these cases, the process is not adiabatic in a cyclic sense, for

$$\int_{z_1} Q = \int_{z_1} W + d(U) = \int_{z_1} \{d(\Theta + U) + \gamma\} = 0 + \int_{z_1} \gamma \neq 0$$

There will exist non-zero cyclic contributions to the work and heat. The ratio of these cyclic integrals is rational [10].

Note that all processes for which the Work 1-form is of Pfaff dimension 1, or less, are reversible, for $Q \wedge dQ = 0$.

2.3. Reversible Case 3: Pfaff(W) = 2 or 3

In the exercise that follows, topological arguments will be used to deduce the ideal gas law. For when $Q \wedge dQ = 0$, but $dQ = dW \neq 0$, the first law implies that

$$W \wedge dW + dU \wedge dW = 0. \quad (2.20)$$

Then either $W \wedge dW = 0$ (and the Pfaff dimension of W is 2) or $W \wedge dW \neq 0$, but $dW \wedge dW = 0$ (and the Pfaff dimension of W is 3). Consider the case of an ideal gas, where the work 1-form is defined as $W = PdV$ and is of Pfaff dimension 2. It follows that

$$dU \wedge dW = dU \wedge dP \wedge dV = 0. \quad (2.21)$$

The result implies that the internal energy U is a function of the pressure and volume: $U = U(P, V)$.

Next consider the case where both the Pfaff dimension of W and Q are equal to 2. Then as $Q \wedge dQ = 0$ the heat 1-form can be expressed in terms of two functions as, $Q = TdS$. It follows from the first law that

$$(P/T)dV + (1/T)dU = dS. \quad (2.22)$$

By taking the exterior derivative of both sides,

$$d(P/T) \wedge dV + d(1/T) \wedge dU = 0. \quad (2.23)$$

A simple class of solutions would impose the "quadrature" conditions that each of the two forms vanish separately. It follows for this simple class that V must be a

function of (T/P) , alone, and U must be a function of T , alone. Such conditions establish the equivalence class of the "ideal gas" with a linear representation

$$V = nRT/P \quad \text{and} \quad U = nC_v T. \quad (2.24)$$

The moral to the story is that the ubiquitous ideal gas law (like the laws of Maxwell electrodynamics) has foundations in a set of topological constraints which are independent from size and shape.

These representations are not the only possibilities for the reversible processes where the Pfaff dimension of the work 1-form is 2. Another realization implies that $dU \wedge dT \wedge dS = 0$, such that the internal energy, U , is not a function of temperature alone, but unlike the ideal gas, the internal energy, in this reversible situation, also depends upon the entropy function, S .

2.4. Case 4 : The Pfaff dimension of the Work 1-form is 4.

When the Pfaff dimension of the work 1-form is 4, then $dW \wedge dW = dQ \wedge dQ \neq 0$ and the process is never reversible. The Frobenius integrability conditions for Q are not satisfied. In such cases it is necessary to examine the case where $dA \wedge dA \neq 0$, on an even dimensional domain of 4 dimensions. Then there exists a unique direction field \mathbf{T} such that

$$A \wedge dA = i(\mathbf{T})dx \wedge dy \wedge dz \wedge dt = i(\mathbf{T})\Omega. \quad (2.25)$$

The components of \mathbf{T} are completely determined from the functional components of the physical system encoded as a 1-form of Action, A . This vector field \mathbf{T} is defined as the Topological Torsion vector. As $A \wedge A \wedge dA = 0$ the Topological Torsion vector is "associated with" or "orthogonal to" the 1-form of Action:

$$i(\mathbf{T})A = 0. \quad (2.26)$$

By direct calculation of the Work 1-form it is possible to show that

$$W = i(\mathbf{T})dA = \Gamma A, \quad (2.27)$$

such that

$$L_{(\mathbf{T})}A = \Gamma A, \quad (2.28)$$

$$\text{and } L_{(\mathbf{T})}\Omega = di(\mathbf{T})\Omega = (div \mathbf{T})dx \wedge dy \wedge dz \wedge dt \quad (2.29)$$

$$= 2 \cdot \Gamma(x, y, z, t)\Omega = dA \wedge dA. \quad (2.30)$$

In other words, depending upon the sign of the 4-divergence of the Topological Torsion vector, the 4D volume element is either expanding or contracting, unless the divergence vanishes. The 1-form of virtual work is proportional to the 1-form of Action. As the 2-form, dA , is of maximal rank, $\Gamma(x, y, z, t) \neq 0$, and the 4D manifold is symplectic. Cartan's magic formula has become the extension of Euler's formula for homogeneous functions to p-forms.

It follows that evolution in the direction of the Torsion Vector yields

$$Q \wedge dQ = L_{(\mathbf{T})} A \wedge L_{(\mathbf{T})} dA = \Gamma^2 A \wedge dA \neq 0, \quad (2.31)$$

which implies that the process is thermodynamically irreversible, independent upon whether or not the volume element is expanding ($\Gamma > 0$) or contracting ($\Gamma < 0$). The process becomes reversible only when $Q \wedge dQ = 0$, which implies that $A \wedge dA \Rightarrow 0$, or $\Gamma^2 \Rightarrow 0$. Then the Pfaff dimension of W cannot be 4, contrary to hypothesis for the class under study.

This is a remarkable development for several reasons.

1. The development demonstrates the topological foundations of thermodynamically irreversible processes, and the relationship to expanding or contracting space time volume elements.
2. The development demonstrates that there exists an irreversible direction field that can be inferred from the functional properties used to define the physical system.
3. The development demonstrates that the irreversible direction field acts on the physical system in a homogeneous manner [11]. The homogeneous degree need not be an integer, which indicates the association of thermodynamic irreversibility and fractal evolution [4].

Dissipative evolution in the direction of the torsion current on the $2n+2$ (symplectic) domain can topologically decay to a $2n+1$ (contact) domain. On the contact Action manifold of the attractor, the evolution can be described by a Hamiltonian system, where with minimal fluctuations and perturbations, the physical system can enjoy a relatively long lifetime, in a state that may be far from equilibrium.

3. Anholonomic Constraints and Fluctuations.

The methods described above can be extended to systems with higher degrees of freedom. Consider a physical system that can be defined in terms of the Cartan-Hilbert 1-form

$$A = L(t; q^k, v^k)dt + p_k(dq^k - v^k dt), \quad (3.1)$$

defined on the $3n+1$ variety of functions, $\{t; q^k, v^k, p_k\}$. At first, do not assume that the p_k are constrained to be jets; e.g., $p_k \neq \partial L/\partial v^k$. Instead, consider the p_k to be a Lagrange multipliers to be determined later. Construct the Pfaff sequence for the 1-form of Action, A . It follows that the exact two form dA satisfies the equations

$$(dA)^{n+1} \neq 0, \text{ but } A \wedge (dA)^{n+1} = 0, \quad (3.2)$$

hence the Pfaff dimension of the Action 1-form is $2n+2$ which is considerably less than the $3n+1$ functions used to construct the Cartan- Hilbert 1-form. The $2n+2$ dimensional space will be defined as the thermodynamic space. The actual formula for the top Pfaffian ($p = 2n+2$) is:

$$(dA)^{n+1} = (n+1)! \{ \sum_{k=1}^n (\partial L/\partial v^k - p_k) \bullet dv^k \} \wedge dp_1 \wedge \dots \wedge dp_n \wedge dq^1 \wedge \dots \wedge dq^n \wedge dt. \quad (3.3)$$

It is to be noted that the unconstrained top Pfaffian of the Cartan-Hilbert Action is always associated with a symplectic (even dimensional) manifold, but not of the maximum dimension of the space of the $3n+1$ variables. For $n = 3$ degrees of freedom, the top Pfaffian indicates that the topological of Pfaff dimension of the 2-form, dA is $2n + 2 = 8$.

If the domain of definition is constrained such that the momenta are defined canonically, $\partial L/\partial v^k - p_k = 0$, then the 2-form dA is not symplectic on its maximal dimension $2n+2$, but defines a contact structure on $2n+1$ with the formula

$$A \wedge (dA)^n = n! \{ v^k p_k - L(t, q^k, v^k) \} dp_1 \wedge \dots \wedge dp_n \wedge dq^1 \wedge \dots \wedge dq^n \wedge dt. \quad (3.4)$$

The coefficient in brackets is the Legendre transform of the Lagrangian producing the format of the classic Hamiltonian energy. The resulting $2n+1$ dimensional (state) space always has a contact structure if the "total energy" is never zero, and the momenta are canonically defined. The state space is reducible to a $2n$ phase space only if the Lagrangian is homogeneous of degree 1 in the v^k ,

$$v^k p_k - L(t, q, v) = v^k \partial L / \partial v^k - L(t, q, v) \Rightarrow 0; \quad (3.5)$$

otherwise the top Pfaffian defines a contact structure of dimension $2n+1$. The sequence of Pfaff reductions, representing topological decay, brings to mind a possible evolutionary process that starts on a symplectic manifold (thermodynamic space) which irreversibly decays to a contact manifold (state space), and then further evolves into a symplectic homogeneous space.

Consider evolutionary processes defined in terms of a vector field $\gamma \mathbf{W} = \gamma[1, v^k, a^k, f_k]$, relative to $[t; q^k, v^k, p_k]$. Construct the 1-form W of virtual work by contracting the exact two form dA with the vector field. For every case, the 1-form of virtual work has the format

$$W = i(\mathbf{W})dA = \{p_k - \partial L / \partial v^k\} \Delta v^k + \{f_k - \partial L / \partial x^k\} \Delta q^k. \quad (3.6)$$

where

$$\Delta v^k = dv^k - a^k dt \neq 0 \quad (3.7)$$

and

$$\Delta q^k = dq^k - v^k dt \neq 0. \quad (3.8)$$

If Δv is interpreted as representing "anholonomic differential fluctuations" in velocity, and Δq is interpreted as representing "anholonomic differential fluctuations" in position, then it is intuitive to assume that fluctuations in velocity relate to temperature and fluctuations in position relate to temperature in a kinematic sense.

When the 2-form dA is symplectic, the work 1-form (which can not vanish) has two terms for any n ; the first involves Δv and the second involves Δq . The work 1-form cannot vanish if dA is symplectic for there are no null eigenvectors of an anti-symmetric matrix of maximal rank. This fact implies that the following 4 situations are NOT allowed when dA is symplectic:

1. $\Delta v = 0$ and $\Delta q = 0$.

(Zero kinematic fluctuations in velocity and zero kinematic fluctuations in position are not permitted.)

2. $\{p_k - \partial L / \partial v^k\} = 0$ and $\Delta q = 0$.

(Canonical momentum, combined with zero kinematic fluctuations in position are not permitted.)

3. $\{f_k - \partial L/\partial x^k\} = 0$ and $\Delta v = 0$.

(Exact gradient forces, combined with zero kinematic fluctuations in velocity are not permitted.)

4. $\{p_k - \partial L/\partial v^k\} = 0$ and $\{f_k - \partial L/\partial x^k\} = 0$.

(Canonical momentum, combined with gradient forces are not permitted. Fluctuations of both position (pressure) and velocity (temperature) permitted .

Conversely, when dA generates a contact manifold, one of the four cases above must be true.

- The first classic elementary case is based upon the assumption that there exists a kinematic description of the process at both the first and the second order. That is, there are no fluctuations, and the kinematics is perfect. The velocity and acceleration fields admit expressions in terms of a single parameter, t .
- The second case which satisfies the contact conditions is based on the assumption that the momentum is canonically defined, and there are no fluctuations in position (pressure). Fluctuations in velocity (temperature) are admitted.
- The third case presumes that the forces are exact gradient fields, and there are no fluctuations in velocity (temperature). Fluctuations in position (pressure) are admitted.
- The fourth case assumes that Then, for the Contact extremal case to exist, and as $\{p_k - \partial L/\partial v^k\} = 0$, it is necessary that the work 1-form reduces to vanishing expression $W = \{f_k - \partial L/\partial x^k\}\Delta q^k \Rightarrow 0$ in the extremal case. There can be fluctuations from kinematic perfection in both the position (pressure) and velocity (temperature) terms.

These observations lead to the theorem

Theorem 3.1. *The extremal constraint is satisfied when the 1-form of virtual work vanishes, which can happen only on a contact manifold of odd Pfaff dimension. In the classic case of no fluctuations, the resulting extremal fields are the equivalent of the Lagrange-Euler equations of classical mechanics. However, the Contact constraints are also satisfied when the force is a gradient field, or there exist zero fluctuations in position, or the non-zero components of the force (the otherwise dissipative components) are orthogonal to the kinematic fluctuations in position.*

Also of current interest [?] are those situations when the work one form is closed, but not zero. Such constraints define symplectic (not extremal) evolutionary processes which occur on even dimensional symplectic manifolds. Locally, as $W = i(\mathbf{W})dA = d\Theta$, it can be shown that such evolutionary fields belong to Lie groups, and that the non-constant functions, Θ , are Casimirs. A hydrodynamicist would use a different set of words. He would describe the Casimir as a Bernoulli function, a function which is constant along a particular flow line, but a constant which will vary from flow line to flow line. Symplectic processes create conservation theorems of the Helmholtz type (conservation of vorticity, conservation of angular momentum,...). In such systems, the Hamiltonian energy need not be an evolutionary invariant, and the system can decay to singular points or regions where the symplectic structure condition fails. Such regions, will be defined as "equilibrium" points of a symplectic process. An example is given in reference [12] to show how the Navier-Stokes equations generate evolutionary vector fields of the symplectic type, but the Euler equations (without pressure) generate extremal vector fields. Numerical studies indicating such phenomena appear in [13]

Following the train of thought that associates fluctuations in position with pressure and fluctuations of velocity with temperature, implies that the first term in the expression for W (see 3.6) must be related to Enthalpy (functions of the type $-TS$ that involve temperature) and the second term to Helmholtz free energy (functions of the type $+PV$ that involve pressure). The combination defines the Gibbs free energy (functions of the type $-TS + PV$) of closed thermodynamic systems, and reversible processes. These thermodynamic ideas, more than 150 years old, are essentially the Casimirs of the symplectic vector fields of irreducible dimension $2n+2$, and are not evident in extremal systems. When the evolutionary vector fields are symplectic, such that $dW = dQ = 0$, they define thermodynamic reversible processes. The Cartan evolutionary equation of a symplectic process becomes

$$L_{(\mathbf{w})}A = W + dU = d\Theta + dU \quad (3.9)$$

$$= \{p - \partial L/\partial v\}\Delta v + \{f - \partial L/\partial x\}\Delta q + dU \quad (3.10)$$

$$\Rightarrow d(-TS + PV + U) = d(G) = Q, \quad (3.11)$$

which defines the heat 1-form Q as the "gradient" of the Gibbs free energy, $G = TS - PV + U$. The Gibbs function is an evolutionary invariant by construction, for all Bernoulli-Casimir functions have transversal gradients.

$$L_{(\mathbf{w})}(G - U) = i(\mathbf{W})d(G - U) = i(\mathbf{W})i(\mathbf{W})dA = 0. \quad (3.12)$$

Under the classic assumption that $dU - TdS + PdV = Q$, it follows that the symplectic evolution generates a Pfaffian form of the type $-SdT + VdP = 0$, which if integrated yields Gibbs version of an equation of state.

When the work 1-form is not closed, then the process can become thermodynamically irreversible. In this case, the evolution is on a symplectic manifold, but the process is not symplectic (as $dW \neq 0$). To test for irreversibility, the usual engineering requirement is that the heat 1-form Q does not admit an integrating factor. Hence, as described above, a given process, \mathbf{W} , acting on a physical system, A , is irreversible when

$$Q \wedge dQ = L_{(\mathbf{w})}A \wedge L_{(\mathbf{w})}dA \neq 0. \quad (3.13)$$

It is remarkable that the symplectic systems of irreducible dimension $2n+2$ seem to solve the Boltzmann - Loschmidt-Zermelo paradox of why canonical Hamiltonian mechanics does not seem to be able to describe the decay to an equilibrium state, and why the usual (extremal) methods of Hamiltonian mechanics do not give any insight into the concept of Pressure, Temperature, or the Gibbs free energy. It is extraordinary that answers to these 150 year old paradoxes of physics seem to follow without recourse to statistics if one utilizes Gromov's [?] work on symplectic systems.

The practical utilization of the fact that the top Pfaffian is of dimension $2n+2$ and not $3n+1$ is an open problem. The implication is that there must exist $3n+1-2n+2 = n-1$ topological invariants in these systems.

3.1. The Skidding-Slipping Bowling Ball example.

As an application of the topological theory of irreversibility and anholonomic fluctuations, consider the experiment of a bowling ball given an initial amount of

translational energy and given amount of rotational energy. Upon contact with the bowling alley, the ball slips or skids irreversibly dissipating both its translational and rotational, momentum and energy (the dissipative force is obscurely defined as friction). The dissipation process continues until a condition is reached where by the translational velocity of the center of mass is equal to the instantaneous tangential velocity of the contact point relative to the center of mass (equal to the product of the angular velocity and the radius of the ball). This condition is defined in engineering textbooks as rolling without slipping. Once the condition of rolling without slipping is reached, the motion proceeds (essentially) without further dissipation (neglecting air resistance, etc.). The objective of this section is demonstrate how these observations can be put into correspondence with the idea that the irreversible portion of the evolution begins on a symplectic manifold of dimension $2n+2$, follows an irreversible trajectory in the direction of the Topological Torsion vector, and topologically decays into (or is attracted to) a contact manifold of dimension $2n+1$, where the subsequent evolution can be described by a conservative Hamiltonian process.

So, consider a mechanical system with initial rotational energy $\beta m \lambda^2 \omega^2 / 2$ and a translational energy $mv^2 / 2$. Define a Lagrange function,

$$L(x, \theta, t, v, \omega) = \{\beta m \lambda^2 \omega^2 / 2 - mv^2 / 2\}, \quad (3.14)$$

where m is a constant mass, β is a numeric factor representing the geometrical features of the moment of inertia, and λ is characteristic constant length of the extended rotating and translating object (e.g., the radius of a ball). Initial conditions $\{v_0, \omega_0\}$ determine the initial relative amounts of rotational and translational energy. Now place the spinning ball on a surface that exerts a pressure on the boundary (on a surface orthogonal to a uniform gravitational field). Empirically it is observed that the initial amounts of kinetic energy and momentum decay irreversibly until the "no-slip" condition $\{dx - \lambda d\theta = 0\}$ is achieved. (The no-slip condition is an anholonomic constraint.) From this point on the ball rolls "without slipping" and without further reduction of translational and rotational energy. It is also noted that depending upon the initial conditions there can be a reversal of the direction of the translational motion, or there can be a reversal of the sense of rotation. The problem at hand is to define a dynamical system that replicates these observations.

Sophomoric analysis explains the decay of rotational and translational energy as being due to "frictional forces" whose magnitude and direction "adjust" such as to achieve the desired result. The Hamiltonian extremal technique does not

seem to apply to the irreversible state, but does seem to apply to the steady state of no-slip.

The 1-form of Action is presumed to be of the form

$$A = (L(x, \theta, t, v, \omega)dt + p_v(dx - vdt) + p_\omega(d\theta - \omega dt) + s(\lambda d\theta - dx)). \quad (3.15)$$

The coefficients $\{p_v, p_\omega, s\}$ are to be considered as prolongation variables, or Lagrange multipliers. Re-arranging the $3n+1=9$ variables $\{t; x, \theta, v, \omega, p_v, p_\omega, s, L\}$, and substituting the assumption for the functional form of the Lagrangian given above, yields the Cartan format in terms of 8 independent variables, $\{x, \theta, t, s, v, \omega, p_v, p_\omega\}$,

$$A = (p_v - s)dx + (p_\omega + \lambda s)d\theta - \{p_v v + p_\omega \omega - (\beta m \lambda^2 \omega^2 / 2 - mv^2 / 2)\}dt. \quad (3.16)$$

By direct computation of the Pfaff sequence on the set of 8 independent variables, $\{x, \theta, t, s, v, \omega, p_v, p_\omega\}$ the form

$$A \wedge dA \wedge dA \wedge dA \Rightarrow 0, \quad (3.17)$$

which implies that the Pfaff dimension of the 1-form, A , is six. By comparison to the Darboux theorem, it is also apparent that this 1-form is of $Pfaff((A)) = 6$.

Now redefine the Action 1-form in terms of new momenta

$$\pi_x = (p_v - s), \quad (3.18)$$

$$\pi_\theta = (p_\omega + \lambda s), \quad (3.19)$$

$$e_t = \{p_v v + p_\omega \omega - (\beta m \lambda^2 \omega^2 / 2 - mv^2 / 2)\}, \quad (3.20)$$

The 1-form of Action becomes

$$A = \pi_x dx + \pi_\theta d\theta - e_t dt \quad (3.21)$$

which is of the standard Cartan form and is of Pfaff dimension $2n + 2 = 6$, with a volume element

$$\Omega = d\pi_x \wedge d\pi_\theta \wedge de_t \wedge dx \wedge d\theta \wedge dt. \quad (3.22)$$

On this $2n+2$ space the unique Topological Torsion vector direction field can be computed from the definition,

$$i(\mathbf{T})\Omega = A \wedge dA \wedge dA, \quad (3.23)$$

and will have non-zero components only in the momentum (or vertical) subspace $\{d\pi_x \wedge d\pi_\theta \wedge de_t\}$. The Topological Torsion vector is orthogonal to the coordinate (or horizontal) subspace, $\{dx \wedge d\theta \wedge dt\}$.

For the problem at hand the algebra becomes simplified if the two Lagrange multipliers (momentum components), p_v and p_ω are assumed to be canonical, but the Lagrange multiplier, s , is presumed to be non-canonical. In this case, for $m = \text{constant}$, $\beta = \text{constant}$, $\lambda = \text{constant}$,

$$p_v = -mv, \quad (3.24)$$

$$p_\omega = \beta m \lambda^2 \omega. \quad (3.25)$$

The Action 1-form becomes

$$A = \beta m \lambda^2 \omega d\theta - m v dx - (\beta m \lambda^2 \omega^2 / 2 - m v^2 / 2) dt + s(\lambda d\theta - dx) \quad (3.26)$$

with a 6D volume element (Top Pfaffian)

$$\Omega = dA \wedge dA \wedge dA = -6m^2 \beta \lambda^2 (v - \lambda \omega) dx \wedge d\theta \wedge dt \wedge dv \wedge d\omega \wedge ds$$

The unique Torsion vector has 6 components

$$\mathbf{T} = [0, 0, 0, T_v, T_\omega, T_s,] \quad (3.27)$$

$$\text{with respect to } \mathbf{R} = [x, \theta, t, v, \omega, s]. \quad (3.28)$$

The functional components are proportional to:

$$T_v = m^2 \lambda (-2\beta \lambda^2 \omega v + \lambda \beta v^2 + \lambda^3 \beta^2 \omega^2) \quad (3.29)$$

$$T_\omega = -m^2 \lambda (-2\beta \lambda \omega v + v^2 + \lambda^2 \beta \omega^2) \quad (3.30)$$

$$T_s = -m^2 \lambda (-2\beta \lambda^2 \omega v + \lambda m \beta v^2 - \lambda^3 m \beta^2 \omega^2 + 2\lambda \beta v s - 2\lambda^2 \beta s \omega) \quad (3.31)$$

Relative to motion along the direction field of the unique Topological Torsion vector, the components of the work 1-form become

$$i(\mathbf{T})dA = W = \Gamma A = m^2\beta\lambda^2(v - \omega\lambda)A, \quad (3.32)$$

$$\text{with } i(\mathbf{T})A = U = 0, \quad (3.33)$$

$$L_{(\mathbf{T})}dA = W = \Gamma A = m^2\beta\lambda^2(v - \omega\lambda)A, \quad (3.34)$$

It is apparent that the virtual work 1-form, W , is not zero except at the point when the system satisfies the "no-slip" condition:

$$\text{No slip condition : } (v - \omega\lambda) = 0. \quad (3.35)$$

For motion in this unique direction not only is the work 1-form not zero, it also is non-integrable.

Hence, before the system decays to the "no-slip" condition, the process is thermodynamically irreversible, as

$$Q \wedge dQ = L_{(\mathbf{T})}A \wedge L_{(\mathbf{T})}dA = W \wedge dW = (m^2\beta\lambda^2(v - \omega\lambda))^2 A \wedge dA \neq 0.$$

The heat 1-form does not admit an integrating factor. However, after the system decays to the "no-slip" condition, the evolutionary process becomes adiabatic, for then $L_{(\mathbf{T})}A = Q = 0$.

It is apparent that the Torsion vector is completely determined by the system. That is the 1-form of Action is either of even or odd Pfaff dimension. If odd, there exists a unique extremal field, and a Hamiltonian representation. If the Pfaff dimension is even, there is a unique Torsion field, which is either expanding or contracting. (The sign of Γ determines the dilatation). The evolutionary process proceeds irreversibly until (possibly) the divergence of the Torsion vector vanishes ($\Gamma \Rightarrow 0$). From then on the system evolution proceeds in an adiabatic fashion. (This remark must be modified if the system momenta are not canonical, for then there will be temperature effects, not just pressure effects).

The Torsion vector generates a dynamical system that describes the irreversible evolutionary process.

$$\frac{dv}{Tv} = \frac{d\omega}{T\omega} = \frac{ds}{Ts} = d\tau \equiv \frac{dt}{\gamma}$$

$$\frac{dx}{v} = \frac{d\theta}{\omega} = \frac{dt}{1}$$

The torsion coefficients are the dissipative forces and torques. The singular set $6m^2\beta\lambda^2(v - \lambda\omega) \Rightarrow 0$ reduces the top Pfaffian to a contact manifold, which has a unique extremal.

4. Summary

It is apparent that a topological perspective establishes the long sought for, non-statistical, connection between dynamic mechanical systems and thermodynamic irreversibility. The principal point of departure from the classic methods is to enlarge the domain of dynamics to include continuous topological evolution. Such methods require the use of mathematical objects, such as exterior differential forms, and non-invertible differentiable maps, that go beyond the mathematical objects of tensor analysis, which are constrained by the homeomorphic property of diffeomorphisms.

5. References

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