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Irreversible Processes and Dissipation in Mechanics and Hydrodynamics { without Statistics!

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Abstract

Cartan's magic formula is used as the link between mechanics and thermodynamics. Physical systems are de¯ned in terms of a di®erential 1-form of action, and processes are de¯ned in terms of vector ¯elds. The di®erential 1-form of virtual work is determined by both the process and the system. The concept of Pfa® dimension, or class, is used to identify equivalence classes of processes. When the Pfa® dimension of the virtual work 1-form is 4, the process is always irreversible. When the work 1-form is of Pfa® class 0, or 1, the processes are always reversible. The classes 0 and 1 include all Hamiltonian Extremal and Symplectic Processes. When the work 1-form is of Pfa® dimension 2, then exists a partition into reversible and irreversible parts. The reversible partition supports a fundamental (equilibrium?) constraint between 3 variables, (V, T, S) or (U,T,S)

I. INTRODUCTION

A major objective of this article is to establish a non-statistical link between mechanics and thermodynamics, with the particular goal of describing the di®erences between reversible and irreversible processes. Physical systems will be described by exterior di®erential forms constructed from covariant tensor ¯elds. Processes will be de¯ned in terms of contravariant vector ¯elds, which may or may not be generators of 1-parameter groups. The fundamental theme is that of continuous topological evolution. Such evolutionary processes are not invertible and do not admit unique deterministic prediction of tensor ¯elds from initial data. However, they do permit the deterministic retrodiction of tensor ¯elds by means of functional substitution and pullbacks. [1]

Cartan's "magic formula"

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

representing the "evolution" of the 1-form of Action, A, with respect to the "°ow" generated by the vector ¯eld, V, is the cornerstone of the development. The term $W = i(V)dA$ de¯nes the 1-form of "virtual work". The function $U = i(V)A$ de¯nes the "internal energy". The sum of these two terms de¯nes the result of the evolutionary process, and at the same time de¯nes the 1-form of "heat", Q. Both the heat and the work 1-forms are not necessarily exact, and therefore will lead to non-zero cyclic integrals. The symbol $L_{(V)}$ stands for the "Lie derivative" with respect to V;a term evidently coined by Slebodzinsky. The symbol dA stands for the "exterior derivative" of A; and the symbol i(V)A is used to designate the interior product of the covariant A with the contravariant V in a tensorial sense, producing a di®eomorphic invariant. However, no constraints of metric or connection are applied to the domain of de¯nition. For physical systems the fundamental domain (or base) of independent variables will be designated by the ordered quadruplet fx; y; z; tg. Most useful applications will be constructed from vector ¯elds over this base.

It is apparent that Cartan's equation of topological evolution is formally equivalent to the cohomological description of the ¯rst law of Thermodynamics. In this article this formal correspondence is taken seriously. Recall that Cartan proved that if the 1-form of Action is taken to be the classic $A = p_k dq^k + H(p_k; q^k; t)dt$, then his magical equation encompasses all of conservative Hamiltonian mechanics.[2] The necessary and su±cient condition was that the closed integrals of the Action $\oint A$ must be evolutionary invariants. This constraint thereby partitioned all possible vector ¯elds of evolution into two equivalence classes, those representing processes that were Hamiltonian, and those that were not Hamiltonian. Herein the idea is to exploit the Cartan concept to obtain a better understanding of the non-Hamiltonian processes, and how they represent dissipative and irreversible physical phenomena,

To repeat: the physical system is represented by the 1-form of Action, A; and the process by the vector ¯eld V. As the system (A) is propagated via the action of the Lie derivative with respect to the process, V, the outcome is to produce the heat 1-form, Q. Following the lead of thermodynamic experience, a process which is reversible it to be associated with a heat 1-form, Q, which admits an integrating factor. The integrating factor (in thermodynamics) de¯nes the concept of temperature. From a topological point of view, the heat 1-form admits an integrating factor if and only if Q satis¯es the conditions of the Frobenious integrability theorem, $Q\wedge dQ = 0$: Hence a simple test for irreversibilty of a process actiong on a system is given by the equations:

$$Q\wedge dQ = (L_{(V)}A)\wedge(L_{(V)}dA) = 0 \text{ ¾ the process is reversible:}$$

$$Q\wedge dQ = (L_{(V)}A)\wedge(L_{(V)}dA) \neq 0 \text{ ¾ the process is irreversible:}$$

The technique then is to start with a reasonable description of a physical system in terms of a 1-form of Action, and then for a given vector ¯eld, V, representing a process, construct Q from Cartan's formula, and test to see if the given process is reversible or not.

The processes represented by di®erent vector ¯elds V can be put into topological equivalence classes determined by the Pfa® dimension, or class, of the 1-form of virtual work, W: The Pfa® dimension of the virtual work 1-form, W, depends on both the process (V) and the system (A). Conservative Hamiltonian processes belong to the Pfa® class 0 or 1.

A. The Pfaff Dimension of the Work 1-form

Given any 1-form, W, it is always possible to construct its Pfaff sequence from the form, W, its exterior differential, dW, and algebraic exterior products of these objects; $\{W, dW, W \wedge dW, dW \wedge dW, \ldots\}$. The Pfaff dimension, or class, of the form is the largest number of non-zero terms that form this sequence.

1. When the Pfaff Dimension of the Virtual Work = 0

When the virtual work 1-form vanishes, $W = i(V)dA = 0$, then such processes, V, are defined as extremals (a word borrowed from the calculus of variations). The vector field, or process, that generates this result is uniquely defined by the Action (to within a projective factor) on odd dimensional spaces of dimension $2n+1$. Any closed integral of the Action, $\oint A$, is a (relative) integral invariant of the evolutionary process generated by V of this equivalence class.

$$L_{(V)} \oint A = \oint Q = 0.$$

Such unique 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 addtion the internal energy is a constant, $dU = 0$, then such processes are trivially adiabatic, $Q = W + dU = 0 + 0 = 0$.

Extremal processes on odd dimensional spaces are said to be Hamiltonian in the sense there exists a function, $H(p, q, t)$, such that $dp - (-\partial H/\partial q)dt = 0$ and $dq - (\partial H/\partial p)dt = 0$. By constucting the exterior derivative of Cartan's magic formula,

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

and as $dW = 0$, which implies that $dQ = 0$, for all elements of the class 0, or 1, it is apparent that all even dimensional elements of the Pfaff sequence generated by the Action, $\{A, dA, A \wedge dA, dA \wedge dA \ldots\}$, and their integrals, are absolute invariants of the equivalence class of extremal fields, a result kn own to Poincare.

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

2. When the Pfaff Dimension of the Virtual Work = 1

When the virtual work 1-form is closed, $W \neq 0; dW = 0$, the process V is defined as a symplectomorphism. The Pfaff dimension, or class, of the work 1-form is equal to 1. In the special case when $W = -dU$; the process is again trivially adiabatic ($Q = 0$). When the work 1-form is exact, such that

$$W = i(V)dA = d\Theta;$$

then the function Θ is defined as a Bernouilli-Casimir function, and is an invariant (first integral) of those evolutionary process, V; that belong to the Pfaff class = 1.

$$L_{(V)}\Theta = i(V)d\Theta = i(V)(i(V)dA) = 0.$$

However, when the work 1-form in not exact, then the process is not cyclically adiabatic, and there will exist non-zero cyclic contributions to the work and heat. The ratio of these integrals is rational [deRham].

The evolutionary vector field is again said to be "Hamiltonian", for $dp - (-\partial\Theta/\partial q)dt = 0$ and $dq - (\partial\Theta/\partial p)dt = 0$. If the Action is written in the Cartan format,

$$A = pdq - H(p, q, t, \sigma)dt);$$

then the Hamiltonian energy, $H(p, q, t, \sigma)$; is not neccessarily an invariant of the flow generated by the Bernouilli-Casimir function, Θ. The Bernoulli-Casimir is, however, an evolutionary invariant, and its gradient is transversal to the evolutionary process.

However, when the work 1-form in not exact, but may have harmonic components, γ; representing topological obstructions. In these cases, the process is not adiabatic in a cyclic sense, for

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

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

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

3. When the Pfa® Dimension of the Virtual Work = 2

When the Work 1-form is not closed, $dW \neq 0$; but the 3-form vanishes, $W \wedge dW = 0$; the Pfa® dimension or class of the work 1-form is 2. Locally, the work 1-form can be formulated (by the Darboux theorem) in terms of two functions; e.g., (symbolically)

$$W = P\,dV.$$

There are two possible situations: either $Q \wedge dQ = 0$ or $Q \wedge dQ = -d(U\,dQ) = -d(U\,dW)$.

The Reversible Class 2 Case (The Ideal Gas) First consider the reversible case, for then locally, $Q \equiv T\,dS$. It follows that for reversible processes,

$$(P/T)dV + (1/T)dU = dS$$

By taking the exterior derivative of both sides,

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

A simple class of solutions would impose the "quadrature" conditions that each of the two forms vanish separately. It follows 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 in the format

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

These representations are not the only possibilities for the reversible processes of Pfa® class = 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.

The Irreversible Case In this situation the three form, $Q \wedge dQ$, must be exact but non-zero.

4. When the Pfaff Dimension of the Virtual Work = 3

For the process to be reversible, it must be true that $Q \wedge dQ = 0$; which implies that

$$W \wedge dW + dU \wedge dW = Q \wedge dQ = 0$$

By exterior differentiation, a necessary condition for reversibility is that

$$dW \wedge dW = dQ \wedge dQ = 0$$

Hence reversibility requires that both the heat 1-form and the work 1-form be of Pfaff dimension less than 4. It is also necessary that the heat 1-form be of Pfaff dimension less than 3. Not so for the work 1-form, for if the 3-form of work $W \wedge dW \neq 0$; then reversibility implies that it is exact,

$$W \wedge dW = -d(UdW) \neq 0$$

Hence if the work generated 3-form is closed and exact then there exists an exceptional possibility of a reversible process. But if the work 3-form is closed but not exact, then the topological obstructions generated by the closed but not exact 3-form imply irreversibility. .

5. When the Pfaff Dimension of the Virtual Work = 4

In this case $dW \wedge dW \neq 0$ and the process is never reversible.

B. SUMMARY

When is dW related to dA?? There is a case where $Q = -A = W$
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1. FORMS

Consider a physical system that can be defined in terms of the Cartan-Hilbert 1-form

$$A = L(t, q, v)dt + p(dq - vdt);$$

defined on the 3n+1 variety $\{t, q, v, p\}$. Do not assume that p is constrained to be a jet; e.g., $p \neq \partial L/\partial v$. Instead, consider p to be a Lagrange multiplier to be determined later. It follows that the exact two form dA satisfies the equations

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

The actual formula for the top Pfaffian (which is of dimension 2n+2 and not 3n+1) is:

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

It is to be noted that the top Pfaffian is always symplectic, but not of the maximum dimension of the space of the 3n+1 variables. For n = 3 degrees of freedom the top dimension $\Rightarrow$ 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 form dA is not symplectic on its maximal dimension 2n+2, but becomes a contact structure on 2n+1 with the formula

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

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

Consider evolutionary processes defined interms of a vector field $\gamma W = \gamma\{1, v, a, f\}$, relative to $\{t, q, v, p\}$. 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

$$W = i(W)dA = \{p - \partial L/\partial v\}\Delta v + \{f - \partial L/\partial x\}\Delta q.$$

where

$$\Delta v = dv - a dt \neq 0$$

and

$$\Delta q = dq - v dt \neq 0.$$

In the symplectic case, the work 1-form has two terms for any n; the first involves Δv and the second involves Δq. The work 1-form cannot vanish in the symplectic space, for there are no null eigenvectors of an anti-symmetric matrix of maximal rank. Hence none of the factors in the expression for virtual work can be zero in pairs. In contrast, for the contact case, there can exist one unique null eigen vector, defined as the extremal vector field, which is the basis for the classical theorems that are based on zero virtual work. As $p - \partial L/\partial v = 0$ for a domain with contact structure, then the work 1-form reduces to

$$W = \{f - \partial L/\partial x\}\Delta q \Rightarrow 0 \text{ in the extremal case.}$$

The extremal constraint is satisfied when the bracket factor vanishes, which is then the equivalent of the Lagrange-Euler equations of classical mechanics.

Of current interest are those situations when the work one form is closed, but not zero. Such constraints define symplectic (not extremal) evolutionary processes. Locally, $W = i(W)dA = d\Theta$, and it can be shown that such evolutionary fields belong to Lie groups, and that the non-constant functions, Θ, are Casimirs. A hydrodynamicist would describe the Casimir as a Bernoulli function, a function which is constant along a particular flow line, but 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, but the system can decay to singular points where the symplectic structure condition fails. Such points will be defined as "equilibrium" points of a symplectic process. An example is given in reference [5] 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 [6]

If Δv is interpreted as "anholonomic differential fluctuations" in velocity, and Δq is interpreted as "anholonomic differential fluctuations" in position, then it is intuitive that the first term in the expression for W 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 100 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 becomes

$$L(W)A = W + dU = \{p - \partial L/\partial v\}\cdot v + \{f - \partial L/\partial x\}\cdot q + dU \Rightarrow d(-TS + PV + U) = Q,$$

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.

$$L(W)(G - U) = i(W)d(G - U) = i(W)i(W)dA = 0.$$

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. These ideas stem from Cartan's definition of an evolutionary process in terms of the equation,

$$L(W)A = i(W)dA + d(i(W)A) = W + dU = Q,$$

and the equation of closure,

$$L(W)dA = di(W)dA = dW = dQ.$$

Note that Cartan's equation (of topological evolution) is equivalent to the cohomological statement of the First Law of Thermodynamics. To test for irreversibility, the usual engineering requirement is that the heat 1-form Q does not admit an integrating factor. Hence by the Frobenious theorem a given process, W, acting on a physical system, A, is irreversible (and not symplectic) when

$$Q \wedge dQ = L(W)A \wedge L(W)dA \neq 0.$$

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 interpretation of the fact that the top Pfa±an 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.

References

R. M. Kiehn, J. Math Phys. 5, 9 (1974) "Extensions of Hamilton's Principle to include Dissipative Systems"

Kiehn, R. M. (1992) "Topological Defects, Coherent Structures and Turbulence in Terms of Cartan's Theory of Di®erential Topology" in Developments in Theoretical and Applied Mathematics, Proceedings of the SECTAM XVI conference, B. N. Antar, R. Engels, A.A. Prinaris and T. H. Moulden, Editors, The University of Tennessee Space Institute, Tullahoma, TN 37388 USA.