Contact Geometry and Thermodynamics

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Contents

Abstract

We relate key elements of contact geometry to thermodynamics. We also investigate contact structures with metrics and their relationship to thermodynamic systems. In particular, we study the singularities of these metrics and compare them to the thermodynamic phase transitions of the Euler-Heisenberg-AdS black hole.

1. Introduction

Contact geometry concerns the study of smooth manifolds where each tangent space is suitably assigned a hyperplane. It originated in the work of Sophus Lie as a tool for studying differential equations [10]. Contact geometry has many applications in mathematics and physics, ranging from knot theory to quantum mechanics [4, 17, 33].

Contact geometry was used in thermodynamics by Gibbs [1, 12]. Later authors introduced metrics [32, 38], with some combining both contact structures and metrics [18, 29], to study thermodynamic interactions. The Ricci scalars of these metrics have been computed for various thermodynamic systems and their singularities are attributed with thermodynamic phase transitions, including the phase transitions of black holes [31].

Black holes are a feature of Einstein's theory of general relativity. They are extreme astronomical objects that, remarkably, turn out to be completely characterized by a few physical parameters, like mass, angular momentum, and charge (the so-called no hair theorems; see [7, 40, 41]). Of particular interest is the surface area of a black hole's event horizon. Hawking [13, 14] and Bekenstein [3] showed that the surface area behaves like an entropy in standard thermodynamics. As such, black holes have a history of being studied as thermodynamic objects. One of the earlier explorations of black hole thermodynamics was Hawking and Page's investigation of black holes in an Anti-de Sitter (AdS) space, where they identified phase transitions by analogy to standard thermodynamics [15]. Black hole thermodynamics is still an active area of study (see [8] for a helpful primer and [36] for a 2018 review article).

Accordingly, many authors subject black holes to investigations with thermodynamic metrics, where they try to associate the singularities of the Ricci scalars with thermodynamic phase transitions [18, 26, 31]. We will show, however, that not all singularities of these metrics correspond with phase transitions as obtained in standard thermodynamics, which are the points where the specific heat of a system diverge.

We begin by providing some first principles of contact geometry in Section 2. Section 3 identifies a contact structure for thermodynamics and introduces thermodynamic metrics. Section 4 applies the developments of Section 3 to a black hole.

2. Contact Geometry

Definition 2.1. Let M be a $(2n+1)$-dimensional smooth manifold. A *contact structure* on M is a smooth hyperplane distribution $\xi \subset TM$ such that any smooth defining 1-form α [23, p. 493] satisfies the *maximally nonintegrable* condition:

$$\alpha \wedge (d\alpha)^n \neq 0,$$

where $(d\alpha)^n = d\alpha \wedge \ldots \wedge d\alpha$ is the n-fold wedge product. A globally defined α is called a *contact form*, and the pair (M, ξ) is called a *contact manifold*.

Remark. A contact form α is not uniquely defined. One can multiply any such α by a nowhere vanishing smooth function f and still obtain a contact form for a given contact structure. This is because $f\alpha$ shares the same kernel as α and it is still maximally nonintegrable, which one can see with a calculation:

$$\begin{aligned}(f\alpha) \wedge (d(f\alpha))^n &= f\alpha \wedge (f\, d\alpha + df \wedge \alpha)^n \\ &= f^{n+1} \alpha \wedge (d\alpha)^n \neq 0.\end{aligned}$$

The following lemma captures a slightly stronger notion.

Lemma 2.2. Let (M, ξ) be a contact manifold. Suppose α_1 and α_2 are contact forms for the hyperplane distribution ξ. Then $\alpha_1 = f\alpha_2$ for some smooth nonvanishing function $f : M \to \mathbb{R}$.

Proof. Since α_1 and α_2 are both contact forms for ξ, we have $\ker \alpha_1 = \xi = \ker \alpha_2$. These 1-forms can be thought of as vectors in the cotangent space that are some scalar multiple of each other.

To construct f, let $p \in M$ and pick any nonzero vector $v_p \in T_pM \setminus \ker \alpha_1|_p$. Define $f : M \to \mathbb{R}$ pointwise with

$$f(p) = \frac{\alpha_1|_p(v_p)}{\alpha_2|_p(v_p)}.$$

The function f is independent of vector chosen in the 1-dimensional linear subspace $T_pM \setminus \ker \alpha_1|_p$ because any other nonzero vector u_p in the subspace is some scalar multiple of v_p. This factor cancels out by linearity of 1-forms and definition of f.

By construction, f is nonvanishing and $\alpha_1 = f\alpha_2$. Since α_1 and α_2 are smooth, the function f is smooth. $\square$

Example 2.3. Let us endow $\mathbb{R}^{2n+1} \ni (x^1, y^1, ..., x^n, y^n, z)$ with the 1-form

$$\alpha = dz - \sum_{i=1}^{n} y^i dx^i.$$

Together, $(\mathbb{R}^{2n+1}, \alpha)$ is a contact manifold. In the case of $\mathbb{R}^3$, the contact form $\alpha = dz - ydx$ defines the hyperplane distribution $\xi = \ker\alpha = \operatorname{span}\{\partial_y, y\partial_z + \partial_x\}$.

We can verify that α is maximally non-integrable by computing

$$\alpha \wedge (d\alpha)^n = -\left(dz - \sum_{i=1}^{n} x^i dy^i\right) \wedge \left(\sum_{j=1}^{n} dx^j \wedge dy^j\right)^n. \qquad (1)$$

The $2n$ wedge products only have nonvanishing terms of the form $dx^1 \wedge dy^1 \wedge ... \wedge dx^n \wedge dy^n$ and its permutations. By permuting the 1-forms in pairs $dx^i \wedge dy^i$, these terms never pick up a negative sign and thus do not cancel out. The sum ends up being $n!$. Thus (1) becomes

$$\alpha \wedge (d\alpha)^n = -n! dz \wedge dx^1 \wedge dy^1 \wedge ... \wedge dx^n \wedge dy^n,$$

which is a nonvanishing top form on $\mathbb{R}^{2n+1}$. //

Remark. The contact structure in the above example is sometimes called the *standard contact structure on* $\mathbb{R}^{2n+1}$. This contact structure is already of interest. For example, *Legendrian knots* are closed 1-dimensional immersed submanifolds [23, p. 108] in $\mathbb{R}^3$ which are tangent to the standard contact structure. Figure 1 shows a sampling of hyperplanes from this contact structure and Figure 2 shows a typical way of presenting these Legendrian knots.

Definition 2.4. Let (M, ξ) be a contact manifold. An immersed submanifold L of (M, ξ) is called *isotropic* if $T_pL \subset \xi_p$ for every $p \in L \subset M$.

Remark. Note that L is isotropic if and only if $i^*\alpha = 0$, where i is the inclusion map $i : L \hookrightarrow M$. This is because for any $v \in T_pL$, $(i^*\alpha)_p(v) = \alpha_p(di_p v) = 0$ if and only if $v \in \xi_p$.

Contact geometry is closely related to its even-dimensional counterpart, called *symplectic geometry*. This is because the contact form induces a *symplectic tensor* on each contact hyperplane.

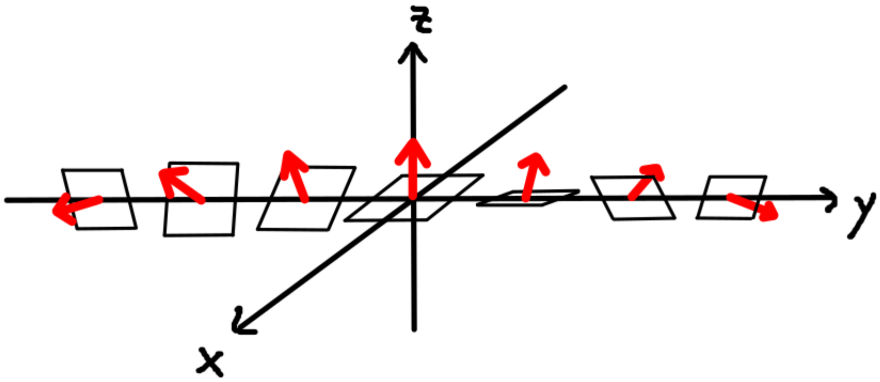

Figure 1: A selection of hyperplanes lying along the y-axis from the standard contact structure on $\mathbb{R}^3$. The planes are given by $\ker(dz - y\,dx) = \operatorname{span}(\partial_y, y\partial_z + \partial_x)$. Normal vectors $\partial_z - y\partial_x$ to the hyperplanes are drawn in red.

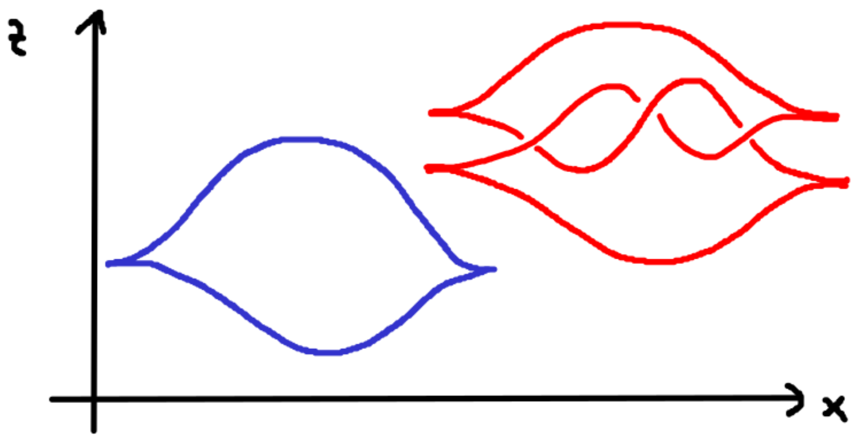

Figure 2: The "front projections" of two Legendrian knots from the standard contact structure on $\mathbb{R}^3$ onto the xz plane [33]. The blue knot is an unknot and the red knot is a trefoil. Given a point on the front projection, the y coordinate of a Legendrian knot is determined by the slope dz/dx at that point (see [33] and Example 2.10). More pictures of Legendrian knots may be found in [28, 33].

Definition 2.5. A 2-covector ω on a finite-dimensional vector space V is said to be *nondegenerate* if $\omega^n \neq 0$. A nondegenerate 2-covector is also called a *symplectic tensor* or a *symplectic bilinear form.* The data (V, ω) is called a *symplectic vector space* [23, p. 565].

Remark. That V must be even-dimensional can be derived from the nondegeneracy condition. There are also other equivalent definitions for nondegeneracy.

Lemma 2.6. Let (V, ω) be a symplectic vector space. The following are equivalent:

(a) $\omega^n \neq 0$.

(b) The linear map $\tilde{\omega} : V \to V^*$ defined by $\tilde{\omega}(v) = \omega(v, \cdot)$ is invertible.

(c) For every nonzero $v \in V$, there exists $w \in V$ such that $\omega(v, w) \neq 0$.

(d) There exists some (and therefore every) basis such that the matrix (ω_{ij}) representing ω is non-singular.

Proof sketch. We will show (b)$\Leftrightarrow$(c), (b)$\Leftrightarrow$(d), and (a)$\Leftrightarrow$(c).

- (b)$\Leftrightarrow$(c) By definition, $\tilde{\omega}$ is invertible if and only if it is injective (since it is a linear map between two finite-dimensional vector spaces of the same dimension), which is equivalent to ω having trivial kernel.

- (b)$\Leftrightarrow$(d) Let $\{e_i\}$ be a basis for V and $\{E^i\}$ be its dual basis for V^*. In this basis, the linear map can be written as

  $$\tilde{\omega}(e_i)e_j = \omega(e_i, e_j) = \omega_{ij}.$$

  Then

  $$\begin{aligned}
  \tilde{\omega} \text{ is invertible} &\Leftrightarrow \exists\ \tilde{\omega}^{-1} \text{ such that } \tilde{\omega}^{-1}(\tilde{\omega}(v)) = v \text{ for all } v \in V \\
  &\Leftrightarrow \text{for every } e_i,\ \tilde{\omega}^{-1}(\tilde{\omega}(e_i)) = e_i \\
  &\Leftrightarrow \tilde{\omega}^{-1}(\tilde{\omega}(e_i)e_jE^j) = e_i \qquad\qquad (\text{insert } 1 = \delta^j_j = e_jE^j) \\
  &\Leftrightarrow \tilde{\omega}(e_i)e_j\tilde{\omega}^{-1}(E^j)E^k = \delta^k_i \\
  &\Leftrightarrow \exists\ \omega^{ij} \text{ such that } \omega_{ij}\omega^{jk} = \delta^k_i \quad (\omega^{jk} = \tilde{\omega}^{-1}(E^j)E^k) \\
  &\Leftrightarrow \text{the matrix representing } \omega \text{ is nonsingular.}
  \end{aligned}$$

- (c)$\Leftrightarrow$(a) To satisfy ($\Rightarrow$), construct a *symplectic basis* [23, p. 566] for ω. Then by a similar calculation as in Example 2.3, $\omega^n \neq 0$. To satisfy ($\Leftarrow$), take the contrapositive. The negation of (c) implies that $\tilde{\omega}$ has nontrivial kernel, containing some nonzero $v \in V$. One can then extend v to a basis $(v, E^2, E^3, ..., E^{2n})$ for V, such that $\omega^n(v, E^2, ..., E^{2n}) = \iota_v \omega^n(E^2, ..., E^{2n}) = 0$ by definition of interior multiplication and $\omega(v) = 0$.

$\square$

We can extend these definitions of symplectic bilinear forms on vector spaces to a *symplectic structure* on smooth manifolds.

Definition 2.7. Let M be a smooth manifold. A *nondegenerate* 2-form on M is a 2-form ω such that ω_p is a nondegenerate 2-covector on T_pM for every $p \in M$ (making T_pM into a symplectic vector space). The 2-form ω is also called a *symplectic form* or symplectic structure. The data (M, ω) is called a symplectic manifold [23].

Remark. Since its tangent spaces must be even-dimensional, the manifold M is also even-dimensional. While contact manifolds are odd-dimensional, the contact structure assigns an even-dimensional hyperplane in each tangent space. The contact form then induces a symplectic bilinear form on each hyperplane.

Lemma 2.8. Let $(M, \xi = \ker \alpha)$ be a contact manifold. Then $(\xi_p, d\alpha|_{\xi_p})$ is a symplectic vector space, where $d\alpha|_{\xi_p}$ is defined by

$$\begin{aligned} d\alpha|_{\xi_p} : \xi_p &\to \xi_p^* \\ v &\mapsto d\alpha(v, \cdot). \end{aligned}$$

Proof. The maximally non-integrable condition $\alpha \wedge (d\alpha)^n \neq 0$ requires that $(d\alpha)^n \neq 0$ everywhere. Thus $d\alpha|_{\xi_p}$ satisfies the nondegeneracy condition by construction and we conclude that $(\xi_p, d\alpha|_{\xi_p})$ is a symplectic vector space. $\square$

The existence of a symplectic bilinear form on a vector space provides a generalized notion of orthogonality, much like how regular inner products do, with the distinction being that symplectic tensors are antisymmetric products. Given a linear subspace S of a symplectic vector space (V, ω), the *symplectic complement* of S, denoted $S^\perp$, is the subspace

$$S^\perp = \{v \in V \mid \omega(v, w) = 0 \text{ for all } w \in S\}.$$

All of these symplectic notions come together to prove this following result in contact geometry.

Proposition 2.9. Let $(M^{2n+1}, \xi = \ker \alpha)$ be a contact manifold. If L is an isotropic submanifold of M, then $\dim L \leq n$. In the case where $\dim L = n$, we call L a *Legendrian* submanifold of M.

Proof. [11, p. 13] For every $p \in L$, since $T_pL \subset \xi_p$, $\iota^*\alpha = 0$ (Definition 2.4). Since the exterior derivative commutes with pullbacks, we have $\iota^* d\alpha = 0$. Thus, for every $u, v \in T_pL$, $d\alpha|_{\xi_p}(u, v) = 0$.

Since the hyperplanes are symplectic vector spaces, let us consider the symplectic complement of T_pL, the linear subspace $(T_pL)^\perp \subset \xi_p$ given by

$$(T_pL)^\perp = \{v \in \xi_p \mid d\alpha|_{\xi_p}(u, v) = 0 \ \text{ for every } u \in T_pL\}.$$

Note that $T_pL \subset (T_pL)^\perp$ since $d\alpha|_{\xi_p}(u, v) = 0$ for every $u, v \in T_pL$. Thus $\dim T_pL \leq \dim(T_pL)^\perp$. We would like use these two spaces T_pL and $(T_pL)^\perp$ alongside a rank-nullity theorem argument to identify $\dim T_pL$ and therefore $\dim L$.

To this end, construct the linear map $\varphi : \xi_p \to T_p^*L$ by

$$\varphi(v)(w) = d\alpha(v, w),$$

where $v \in \xi_p$ and $w \in T_pL$. By Lemma 2.8, $d\alpha|_{\xi_p}$ is nondegenerate. Thus by Lemma 2.6(b), for any $w \in T_p^*L \subset \xi_p^*$, there exists $v \in \xi_p$ such that $d\alpha(v, \cdot) = w$. Thus the map is surjective and im $\varphi = T_p^*L \cong T_pL$. Next, $\ker \varphi = (T_pL)^\perp$ by construction of $\varphi(v)$. Hence we have a linear map between vector spaces and the rank-nullity theorem gives

$$\begin{aligned} \dim \xi_p &= \dim \mathrm{im}\ \varphi + \dim \ker \varphi \\ 2n &= \dim T_pL + \dim(T_pL)^\perp. \end{aligned}$$

Since $\dim T_pL \leq \dim(T_pL)^\perp$, we have $\dim T_pL \leq n$ such that $\dim L \leq n$. $\square$

Remark. This proposition and its proof illustrates two key ideas about contact geometry. Firstly, the hyperplane distribution ξ fails to admit an integral manifold (an immersed submanifold S satisfying $T_pS = \xi_p$ for every $p \in S$) . The immersed submanifolds tangent to the distribution have half the distribution's dimension at most. Secondly, contact geometry is closely related to symplectic geometry (see Example 2.13); one could even use the data of a symplectic manifold to create a contact manifold [11, p. 8].

Example 2.10. Smooth functions on a manifold can be used to create a contact manifold [1]. This example uses Euclidean space for clarity, but the construction is generalizable to smooth manifolds.

Let q be a point in $\mathbb{R}^n$ and $\varphi : \mathbb{R}^n \to \mathbb{R}$ a smooth function. The *1-jet at q of φ*, denoted $J^1_q(\varphi)$, is the truncated first order Taylor polynomial of φ; explicitly, it is

$$J^1_q(\varphi) = \varphi(q) + \frac{\partial \varphi}{\partial x^i}(q)x^i$$

where $q = (x^1, ..., x^n) \in \mathbb{R}^n$. This data of a 1-jet at q of φ is in 1-1 correspondence with a point in $\mathbb{R}^{2n+1}$. For example, labeling $p_i = \partial\varphi/\partial x^i$, the 1-jet $J^1_q(\varphi)$ labels the point $(q, \varphi(q), p) \in \mathbb{R}^{2n+1}$. As such, there is a notion of a natural contact structure [1, p. 163] that one can give to the space of 1-jets, thought of as $\mathbb{R}^{2n+1}$.

Given a smooth function φ, its differential induces Legendrian submanifolds in the following sense. The so-called 1-graph of a function φ is the subset

$$\Gamma(\varphi) = \left\{ \left(q, \varphi(q), \frac{\partial \varphi}{\partial x}(q) \right) \right\} \subset J^1(\mathbb{R}^n, \mathbb{R})\,.$$

The 1-form $\alpha = dy - p\,dx$, where y is the $(n+1)$th coordinate corresponding to $\varphi(q)$, is pulled back to zero on every 1-graph by the inclusion map $\iota : \Gamma(\varphi) \to J^1(\mathbb{R}^n, \mathbb{R})$:

$$\iota^*\alpha = \iota^*(dy - p\,dx) = d\varphi - \frac{\partial \varphi}{\partial x}\,dx = 0\,.$$

Here, α is the contact form from Example 2.3 up to renaming coordinates. The 1-graphs of smooth functions are thus Legendrian submanifolds. //

Example 2.11. Given any B^{n+1} dimensional smooth manifold, one can create a contact manifold with the following construction [1].

A *contact element* at a point $p \in B$ is a hyperplane H_p in the tangent space T_pB. One can think of a contact element as the specification of the n partial derivatives in a 1-jet from Example 2.10. The data of a hyperplane H_p is equivalent to an equivalence class of covectors $\alpha_p \in T^*_pB$ which annihilates every vector in H_p. The equivalence relation is obtained by using the fact that two covectors which are scalar multiples of each other determine the same hyperplane. Thus contact elements at $p \in B$ are also equivalence classes of covectors in T^*_pB.

The space of all contact elements at every $p \in B$ can be shown to be the projectivized cotangent bundle PT^*B. This space has a fiber bundle structure, where a model fiber at p is the space of rays in T_p^*B. In coordinates, a point in PT^*B can be labeled by $(u, x^1, ..., x^n, p^1, ..., p^n)$, where $u, x^1, ..., x^n$ are coordinates for B and $p^1, ..., p^n$ are covector coefficients. In light of the 1-jets example, u are the possible values that a real-valued function of $x^1, ..., x^n$ can take on, and $p^1, ..., p^n$ are the possible partial derivatives. //

Having seen some examples of contact structures and contact forms, let us introduce a method of comparing two structures and seeing whether or not they are the same.

Definition 2.12. Let (M_1, α_1) and (M_2, α_2) be contact manifolds. A diffeomorphism $f : M_1 \to M_2$ is called a *contact transformation* or *contactomorphism* if there exists a smooth nowhere vanishing function $\lambda : M_1 \to \mathbb{R}$ such that

$$f^*\alpha_2 = \lambda\alpha_1.$$

If $\lambda = 1$, we call this a *strict* contactomorphism.

Example 2.13. Contact geometry shows up in various ways in physics. For example, the Lagrangian formulation of classical mechanics postulates that classical systems can be described by an action S, defined by

$$S[\gamma(t)] = \int_\gamma L(q, \dot{q}, t)\, dt.$$

Here, S is a functional of a path γ in some phase space and L is the Lagrangian for the system, where q, $\dot{q}$, and t are coordinates for the system, which can be thought of as positions, velocities, and time respectively. The classical solution to the equations of motion is the path $\gamma(t)$ that extremizes S.

The Hamiltonian formulation is related to the Lagrangian formulation through a Legendre transform (see §3.2.1). Taking $H(q, p, t)$ as a Hamiltonian, where p is the momentum, its corresponding Lagrangian $L(q, \dot{q}, t)$ is given by

$$H(q, p, t) = p\dot{q} - L(q, \dot{q}, t).$$

We can thus rewrite the action as

$$S = \int_\gamma (p\dot{q} - H)\, dt.$$

The integrand is a local expression for the pullback of the contact form $\alpha = p\,dq - H\,dt$ defined on some manifold M with local coordinates q, p, and t. Thus we can write

$$S = \int_\gamma \alpha\,.$$

This is one method of producing classical mechanics using contact geometry. Other formulations can be found in [6, 11]. For an application to quantization, see [17]. //

3. Thermodynamics

> Every mathematician knows that it is impossible to understand any elementary course in thermodynamics.
>
> *Contact Geometry: the Geometrical Method of Gibbs's Thermodynamics*
>
> V.I. Arnold [1]

Contact geometry naturally describes thermodynamics. We will begin with an observation about Legendrian submanifolds of a contact manifold before identifying a general contact structure for thermodynamic systems.

3.1 Constructing Legendrian Submanifolds

Recall from our 1-jets example (Example 2.10) that smooth functions on $\mathbb{R}^n$ can induce Legendrian submanifolds in $\mathbb{R}^{2n+1}$ with the standard contact structure. However, given a smooth function f on $\mathbb{R}^n$, there are other ways of constructing a Legendrian submanifold in $\mathbb{R}^{2n+1}$.

Proposition 3.1. [2, 6] Let $(\mathbb{R}^{2n+1}, \alpha)$ be the contact manifold from Example 2.3. Let $I \sqcup J$ be a disjoint partition of $\{1, ..., n\}$ with $i \in I$ and $j \in J$. The coordinates $(x^I, x^J, y_I, y_J, z) \in \mathbb{R}^{2n+1}$ are the same coordinates as in Example 2.3, but with some specific indices identified.

Suppose $f(x^J, y_I)$ is a smooth function of only n coordinates $p = (x^J, y_I)$. Define the smooth embedding

$$\varphi :\ \mathbb{R}^n \to \mathbb{R}^{2n+1}$$

where $\varphi(p) = (x^I(p), x^J, y_I, y_J(p), z(p))$ and

$$x^i(p) = -\frac{\partial f}{\partial y_i}(p), \quad y_j(p) = \frac{\partial f}{\partial x^j}(p), \quad \text{and} \quad z = f(p) - y_i \frac{\partial f}{\partial y_i}(p). \tag{2}$$

The image of φ, denoted $L \subset \mathbb{R}^{2n+1}$, is a Legendrian submanifold.

Remark. Example 2.10 is the $I = \emptyset$ case of this proposition.

Proof. To see that the map φ is a smooth embedding, note that its differential is injective; its Jacobian is a $(2n+1) \times n$ matrix that contains the $n \times n$ identity as a block due to the $\partial x^J/\partial x^J$ and $\partial y_I/\partial y_I$ terms. Furthermore, it is a homeomorphism onto its image since f is smooth and φ is an invertible map between $\mathbb{R}^n$ and L. Therefore its image is an embedded (and thus immersed) submanifold [23, p. 99].

Next we check if L is isotropic. Computing the pullback of α under the inclusion map, we obtain

$$\begin{aligned}
\iota^*\alpha &= \iota^*(dz - y_a dx^a) = \iota^*(dz - y_i dx^i - y_j dx^j) \\
&= d\left(\varphi - y_i \frac{\partial \varphi}{\partial y_i}\right) + y_i d\left(\frac{\partial \varphi}{\partial y_i}\right) - \frac{\partial \varphi}{\partial x^j}\, dx^j \\
&= \frac{\partial \varphi}{\partial y_i}\, dy_i + \frac{\partial \varphi}{\partial x^j}\, dx^j - y_i d\left(\frac{\partial \varphi}{\partial y_i}\right) - \frac{\partial \varphi}{\partial y_i}\, dy_i + y_i d\left(\frac{\partial \varphi}{\partial y_i}\right) - \frac{\partial \varphi}{\partial x^j}\, dx^j \\
&= 0.
\end{aligned}$$

Thus L is a maximal dimension isotropic immersed submanifold, a Legendrian submanifold. □

For those familiar with standard thermodynamics, the defining formulas (2) specify a *Legendre transformation* between different *thermodynamic potentials*, constructing a new potential z from f. Given a generating function, its associated Legendrian submanifold is the *space of equilibrium states* where all the equations of state are satisfied. Let us clarify these ideas by identifying a contact structure for thermodynamics.

3.2 Thermodynamic Contact Structure

We will start with the full thermodynamic phase space[1] and introduce a contact structure for it [6, 18, 29].

Definition 3.2. A *thermodynamic system* is the data of

(i) a $(2n+1)$-dimensional smooth manifold $\mathcal{T}$ called the thermodynamic phase space, with coordinates Φ, E^a, and I^a where $a \in \{1, ..., n\}$, and

(ii) a real-valued function called a *fundamental equation* $\Phi = \Phi(E^a)$, also called a thermodynamic potential.

[1] There are other methods that start with the smaller space of equilibrium states and constructs a contact manifold [27] as in Example 2.11.

The manifold $\mathcal{T}$ is given the *Gibbs 1-form* Θ, defined by

$$\Theta = d\Phi - \delta_{ab} I^a dE^b.$$

Remark. The variables E^a and I^a are sometimes called *extensive* and *intensive parameters* respectively. Fixing an index a, E^a and I^a are said to be *conjugate* to each other. A general thermodynamic potential Φ is a function of n of these parameters such that no two parameters are a conjugate pair. For example, one can think of the y_i's in Proposition 3.1 as extensive parameters, the x^j's as intensive parameters, and the function f as a thermodynamic potential. The variables which f depends on we call *defining* variables.

Lemma 3.3. The pair $(\mathcal{T}, \Theta)$ is a contact manifold.

Proof. The structure given above is the same as the one in Example 2.3. $\square$

Definition 3.4. Given the data of a thermodynamic system, the space of equilibrium states $\mathcal{E}$ is the subspace of the thermodynamic phase space $\mathcal{T}$ defined as the image of the smooth embedding $\varphi : \mathcal{E} \to \mathcal{T}$, where

$$\varphi : (E^a) \mapsto (\Phi(E^a), E^a, I^a(E^a)) \quad \text{and} \quad \varphi^*(\Theta) = 0.$$

Recall that $\Phi = \Phi(E^a)$ the thermodynamic potential was specified by the thermodynamic data.

Lemma 3.5. On the space of equilibrium states $\mathcal{E} \subset \mathcal{T}$ with a given thermodynamic potential $\Phi = \Phi(E^a)$, we have

$$\frac{\partial \Phi}{\partial E^a} = \delta_{ab} I^b.$$

The equations are also called equations of state.

Proof. We compute the pullback condition $\varphi^*(\Theta) = 0$. Given $p \in \mathcal{E} \subset \mathcal{T}$, we have

$$\begin{aligned}
\varphi_p^*(\Theta) &= \varphi_p^*(d\Phi - \delta_{ab} I^a dE^b) \\
&= d\Phi_p - \delta_{ab} I^a(p) dE_p^b \\
&= \frac{\partial \Phi}{\partial E^a}(p) dE_p^a - \delta_{ab} I^a(p) dE_p^b = 0\,.
\end{aligned}$$

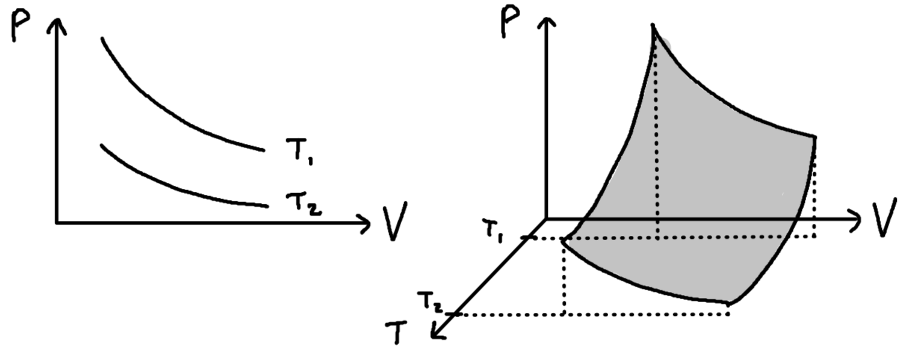

Figure 3: On the left, a PV diagram with two isotherms (constant temperature lines) plotted at temperatures T_1 and T_2. Each point on the line labels an equilibrium state of the ideal gas. On the right, a sheet of isotherms between T_1 and T_2 for the ideal gas. The grey sheet is a slice of the immersed submanifold L. The other two axes U and S have been suppressed.

This gives us

$$\frac{\partial \Phi}{\partial E^a}(p) = \delta_{ab} I^b(p)$$

as desired. □

Remark. There are two useful ways of thinking about $\mathcal{E}$. One can choose to think of it as just the n-dimensional space with the defining parameters (E^a) as the coordinates or, as Proposition 3.1 and Lemma 3.5 show, a Legendrian submanifold of $\mathcal{T}$.

Example 3.6. The classical ideal gas model describes the behavior of dilute gases. Its thermodynamic phase space $\mathcal{T}$ is coordinatized by five thermodynamic parameters: total internal energy U, temperature T, entropy S, pressure P, and volume V.

There are various fundamental equations that we can choose for this system. Each choice is called a *representation*. In the internal energy representation, the fundamental equation is given by $U = U(S, V)$, which gives internal energy as a function of entropy and volume. The explicit formula can be found in [19, p. 140].

Our thermodynamic phase space is the contact manifold $(\mathcal{T}, \Theta)$. In the energy representation, the Gibbs 1-form Θ is

$$\Theta = dU - T\, d + P\, dV.$$

By Lemma 3.5, T and P are defined by

$$T = \frac{\partial U(S,V)}{\partial S} \quad \text{and} \quad -P = \frac{\partial U(S,V)}{\partial V} \tag{3}$$

on the space of equilibrium states. The negative sign is by convention. We see that we recover the definitions of temperature and pressure in standard thermodynamics. Evaluating the partial derivatives, we obtain the equations of state:

$$T = \frac{2}{3}\frac{U(S,V)}{Nk} \quad \text{and} \quad P = \frac{2}{3}\frac{U(S,V)}{V}. \tag{4}$$

The classical ideal gas law $PV = NkT$ follows from the above. It is also often called an equation of state. Here, N is particle number and k is Boltzmann's constant.

Points on the Legendrian submanifolds are equilibrium states. Let L be a 2-dimensional subspace of $\mathcal{T}$ defined by

$$L = \{(U(P,V), T(P,V), S(P,V), P, V)\} \subset \{(U,T,S,P,V)\} = \mathcal{T}$$

where

$$U(P,V) = \frac{3}{2}PV, \quad T(P,V) = \frac{Nk}{PV}, \quad \text{and} \quad S = S(P,V)\,.$$

In the remark after Definition 3.2, we claimed that the thermodynamic potential (generating function) is not a function of both extensive and intensive variables in a conjugate pair, yet here the internal energy is a function of both P and V.

This discrepancy is resolved by our equations of state and repeated variable substitution using equations (3) and (4). For entropy in particular, the first equation of (3) gives temperature $T = T(S,V)$ which can be inverted to find $S(T,V)$. Then substituting in the ideal gas law gives $S(P,V)$. This is then substituted into $U(S,V)$ to obtain $U(P,V)$. Figure 3 illustrates the Legendrian submanifold L. //

Remark. Note that the Gibbs 1-form Θ recovers the first law of thermodynamics on the space of equilibrium states. The smooth embedding pulls back Θ to zero, so one could write

$$0 = dU - T\, dS + P\, dV \quad \Rightarrow \quad dU = T\, dS - P\, dV,$$

which is the usual presentation of the first law for the ideal gas as the differential of a function.

Generic thermodynamic potentials are convex functions of the extensive variables, such that

$$\frac{\partial^2 \Phi}{\partial E^a \partial E^b} \geq 0.$$

This enables us to perform Legendre transformations to obtain new thermodynamic potentials.

3.2.1 Legendre Transformations

Whenever we are given a convex function, we can consider an equivalent description of the function in terms of its first derivative because first derivative values are in 1-1 correspondence with points in the function's domain. This encapsulates the idea of a Legendre transformation [2, pp. 61-62].

Definition 3.7. Let $f : \mathbb{R} \to \mathbb{R}$ be a smooth, convex function, i.e., $f''(x) > 0$. The Legendre transformation of f is a new function $g : \mathbb{R} \to \mathbb{R}$ defined as follows. Construct the function $F : \mathbb{R}^2 \to \mathbb{R}$ by

$$F(x, p) = f(x) - px.$$

For $p \in \mathbb{R}$, define $x(p) \in \mathbb{R}$ by

$$0 = \frac{\partial F}{\partial x}(x(p), p) = f'(x(p)) - p.$$

Then $g(p) = F(x(p), p) = f(x(p)) - px(p)$.

Remark. Given p, the point in the original function's domain, $x(p)$ is uniquely defined since f is convex.

Example 3.8. Consider again our ideal gas example in the energy representation $U = U(S, V)$. Internal energy is convex with respect to entropy. Thus we can perform a Legendre transform to a new potential $F(T, V)$. We follow the construction in Definition 3.7.

Let $\tilde{F}(S, T, V) = U(S, V) - TS$. The entropy $S(T)$ is uniquely defined by convexity of U. Thus

$$F(T, V) = \tilde{F}(S(T), T, V) = U(S(T), V) - TS(T),$$

or $F = U - TS$ for short. This potential is called the Helmholtz free energy [19, p. 22]. In terms of Proposition 3.1, F is another generating function for a Legendrian submanifold. //

Remark. As in Definition 3.7 where we exchange a point x in the domain of f for the corresponding derivative value p, here we exchange a defining variable S for its conjugate T.

Staying in the energy representation, there are two more potentials that can be obtained by repeatedly applying Legendre transforms to the internal energy U. These are

$$H = U + PV \quad \text{and} \qquad G = U - TS + PV,$$

the enthalpy and Gibbs free energy respectively. These potentials are used in chemistry and physics to characterize equilibrium states of various thermodynamic systems. For example, a closed system, like a box of gas, kept at constant temperature will be in an equilibrium state when the Helmholtz free energy is minimized [19, p. 23], which is equivalent to the vanishing of the pulled-back Gibbs 1-form. Furthermore, some thermodynamic variables, like entropy, are not easily measurable in a laboratory, so Legendre transformations can give equivalent descriptions of the system in terms of more easily measurable quantities, like temperature.

For general thermodynamic systems we define Legendre transforms as follows, which turn out to be a set of strict contactomorphisms.

Definition 3.9. Given a thermodynamic system, let $(\mathcal{T}, \Theta)$ and $(\tilde{\mathcal{T}}, \tilde{\Theta})$ be two thermodynamic phase spaces coordinatized by Φ, E^a, I^a and $\tilde{\Phi}, \tilde{E}^a, \tilde{I}^a$ respectively. A *partial* Legendre transformation of the thermodynamic system is a map $\varphi : \tilde{\mathcal{T}} \to \mathcal{T}$ given by

$$\varphi : (\tilde{\Phi}, \tilde{E}^a, \tilde{I}^a) \mapsto (\Phi, E^a, I^a)$$

such that

$$\Phi = \tilde{\Phi} - \delta_{k\ell} \tilde{I}^k \tilde{E}^\ell, \quad E^i = -\tilde{I}^i, \quad E^j = \tilde{E}^j, \quad I^i = \tilde{E}^i, \quad I^j = \tilde{I}^j,$$

$I \sqcup J$ is a disjoint partition of $\{1, ..., n\}$, $i, k, \ell \in I$, and $j \in J$. The identity and *total* Legendre transformations have $I = \emptyset$ and $I = \{1, ..., n\}$ respectively.

Example 3.10. Let us return to the ideal gas system, with the phase spaces $\mathcal{T}$ and $\tilde{\mathcal{T}}$ coordinatized by $\{\Phi, E^1, E^2, I^1, I^2\}$ and $\{\tilde{U}, \tilde{S}, \tilde{V}, \tilde{T}, -\tilde{P}\}$ respectively. A partial Legendre transformation with $i = \{1\}$ gives

$$E^1 = -\tilde{T}, \quad E^2 = \tilde{V}, \quad I^1 = \tilde{S}, \quad I^2 = -\tilde{P} \quad \Rightarrow \quad \Phi = \tilde{U} - \tilde{T}\tilde{S}.$$

Here we recognize Φ as the Helmholtz free energy. If $i = \{1, 2\}$ we have the following total Legendre transformation

$$E^1 = -\tilde{T}, \quad E^2 = \tilde{P}, \quad I_1 = \tilde{S}, \quad I_2 = \tilde{V} \quad \Rightarrow \quad \Phi = \tilde{U} - \tilde{T}\tilde{S} + \tilde{P}\tilde{V}$$

giving us the Gibbs free energy. Taking $i = \{2\}$ will similarly give enthalpy.

Lemma 3.11. Let $(\mathcal{T}, \Theta)$ and $(\tilde{\mathcal{T}}, \tilde{\Theta})$ be two thermodynamic phase spaces of a thermodynamic system. Then the map $\varphi : \tilde{\mathcal{T}} \to \mathcal{T}$ given by Definition 3.9 is a strict contactomorphism.

Proof. The map φ is invertible; the defining and conjugate variables are either mapped to themselves or exchanged with their conjugates, which can be inverted by contracting with a kronecker delta. The potential is inverted by substituting in the conjugates for the $\delta_{k\ell}\tilde{I}^k\tilde{E}^\ell$ term. Furthermore, φ is smooth since it is a map from coordinate functions to sums and products of coordinate functions. Thus φ is a diffeomorphism.

Next, let us compute $\varphi^*(\Theta)$. We have

$$\begin{aligned}
\varphi^*(\Theta) &= \varphi^*(d\Phi - \delta_{ab}I^a dE^b) \\
&= d\tilde{\Phi} - \delta_{k\ell}\tilde{I}^k d\tilde{E}^\ell - \delta_{k\ell}\tilde{E}^k d\tilde{I}^\ell - (\delta_{rs}\tilde{I}^r d\tilde{E}^s + \delta_{k\ell}I^k dE^\ell) \\
&= d\tilde{\Phi} - \delta_{k\ell}\tilde{I}^k d\tilde{E}^\ell - \delta_{k\ell}\tilde{E}^k d\tilde{I}^\ell - \delta_{rs}\tilde{I}^r d\tilde{E}^s - \delta_{k\ell}\tilde{E}^k d(-\tilde{I}^\ell) \\
&= d\tilde{\Phi} - \delta_{ab}\tilde{I}^a d\tilde{E}^b = \tilde{\Theta}.
\end{aligned}$$

Here, $k, \ell \in I$ and $r, s \in J$ as originally defined, and a, b range over all n. Thus φ is a strict contactomorphism. ☐

3.3 Thermodynamic Metrics

There have been various approaches to studying thermodynamics by introducing metrics (both Riemannian and pseudo-Riemannian) on either the space of equilibrium states or thermodynamic phase space [32, 38]. By analogy to Einstein's theory of general relativity, the Ricci scalars of those metrics are often interpreted as a measure of thermodynamic interaction. Of particular interest are singularities in the curvature scalars, which are often interpreted as phase transitions [30].

This section will provide coordinate expressions for metrics on the space of equilibrium states, which are obtained by pulling back metrics defined on the thermodynamic phase space using the smooth embedding of Definition 3.4. With these coordinate expressions, we will then compute curvature scalars in the following section, enabling us to investigate whether or not curvature singularities come in 1-1 correspondence with phase transitions.

3.3.1 Metrics and Contact Structures

Given a contact manifold, there is a notion of an *associated* metric to the contact structure. It is the contact geometry analogue of an *almost complex structure* from symplectic geometry [5, 34].

Definition 3.12. Let (M, η) be a contact manifold and R the Reeb vector field. Let X, Y be arbitrary vector fields on M. A Riemannian metric G is said to be an associated metric if

$$\eta(X) = G(X, R) \tag{5}$$

and there exists a $(1, 1)$-tensor field ϕ such that

$$\phi^2 = -\mathrm{Id} + \eta \otimes R \tag{6}$$

and

$$d\eta(X, Y) = G(X, \phi Y). \tag{7}$$

Here Id is the identity. The data (ϕ, R, η, G) where G is an associated metric is said to be a *contact metric structure*.

Remark. Any vector X in the distribution is orthogonal to the Reeb with respect to the metric G by virtue of (6). Furthermore, the (1,1)-tensor maps arbitrary vectors to a vector in the distribution; given an arbitrary vector field Y, the vector field ϕY is orthogonal to the Reeb with respect to G:

$$0 = \ d\eta(R, Y) = G(R, \phi Y) = \eta(\phi Y)\,. \tag{8}$$

Thus ϕY is in the distribution. When restricted to vectors in the distribution, we also recover the almost complex structure $\phi^2 = -\mathrm{Id}$.

Let us give a coordinate expression for ϕ. By Darboux's theorem, there exists a neighborhood with coordinates (x^i, y_i, z), $i \in \{1, ..., n\}$, such that the contact form becomes $\eta = dz - y_i\, dx^i$. The hyperplanes of the contact structure in this neighborhood are thus spanned by the $2n$ vectors ∂_{y_i} and $y_i\partial_z + \partial_{x^i}$. Including the Reeb vector ∂_z, these $2n + 1$ vectors span the tangent spaces at each point in the neighborhood. One possible ϕ is defined by the following action on basis vectors:

$$\phi(\partial_z) = 0, \quad \phi(\partial_{y_i}) = (y_i\partial_z + \partial_{x^i}), \quad \phi(y_i\partial_z + \partial_{x^i}) = -\partial_{y_i}\,.$$

For other constructions, see [24]. Locally ϕ can be written as

$$\phi = \sum_{i=1}^{n} \left[dy_i \otimes (y_i\partial_z + \partial_{x^i}) - dx^i \otimes \partial_{y_i} \right]. \tag{9}$$

Example 3.13. Given a contact structure, there are infinitely many associated metrics; an explicit construction can be found in [5, p. 47]. The construction is far from canonical due to a choice of arbitrary starting Riemannian metric. Here is one possible associated metric on the contact manifold $(\mathbb{R}^{2n+1}, \eta)$ where η is the standard contact form (Example 2.3) [4, 5, 24]. Given arbitrary vector fields X and Y, define the metric G by

$$G(X,Y) = \eta(X)\eta(Y) + d\eta(\phi X, Y).$$

The (1,1)-tensor ϕ is given by Equation (9), where the Darboux coordinates are identified with global coordinates on $\mathbb{R}^{2n+1}$. Let us check that G is an associated metric. Let R be the Reeb vector field. The metric G readily satisfies Equation (5):

$$G(X,\xi) = \eta(X) \otimes \eta(R) + 0 = \eta(X).$$

We now check the orthogonality requirement (7):

$$\begin{aligned} G(X,\phi Y) &= G(\phi Y, X) \\ &= \eta(\phi Y)\eta(X) + d\eta(\phi^2 Y, X) \\ &= \eta(\phi Y)\eta(X) + d\eta(-Y + \eta(Y)R, X) \\ &= d\eta(-Y, X) + \eta(Y)d\eta(R, X) + \eta(\phi Y)\eta(X) \\ &= d\eta(X,Y) + \eta(\phi Y)\eta(X). \end{aligned}$$

It may seem by virtue of Equation (8) that $\eta(\phi Y) = 0$ depends on the metric. It turns out that this is not the case; that $\eta \circ \phi = 0$ is a consequence of (5) [5, p. 43]. Thus $G(X, \phi Y) = d\eta(X,Y)$, so G is an associated metric. Using Equation (9) and evaluating $d\eta$, one can write down G in coordinates:

$$G = \eta \otimes \eta + \sum_{i=1}^{n} [(dx^i)^2 + (dy_i)^2] \,.$$

//

While we are interested in associated metrics because we will use them to study thermodynamics, it is worth mentioning some related structures derived from the contact form. For example, an *almost contact structure* on an odd-dimensional smooth manifold is the data of (ϕ, R, η), where η is a contact form, R is the Reeb vector field, and ϕ is a $(1,1)$-tensor field satisfying $\phi^2 = -\mathrm{Id} + \eta \otimes \xi$. A *compatible* metric g to the almost contact structure is a metric that satisfies

$$g(\phi X, \phi Y) = g(X,Y) - \eta(X)\eta(Y) \,.$$

Altogether, (ϕ, R, η, g) is said to be an *almost contact metric structure*. A compatible metric does not necessarily satisfy the associated metric condition $d\eta(X,Y) = g(X, \phi Y)$.

A *para-contact metric structure* [24] (φ, R, η, G) is defined the same as in Definition 3.12, but the $(1,1)$-tensor field φ instead satisfies

$$\varphi^2 = \mathrm{Id} - \eta \otimes R\,.$$

The metric G is still said to be an associated metric and the triplet (φ, R, η) is said to be an *almost para-contact structure*.

3.3.2 Distances Between Equilibrium States

As we have stated, to study equilibrium states, we need to pull these associated metrics back to the space of equilibrium states using the smooth embedding (Definition 3.4). However, the first attempts to use metrics to study thermodynamics introduced metrics only on the space of equilibrium states without regard to the overall thermodynamic phase space and its contact structure. The following two ad hoc metrics

$$g^R = -\frac{\partial^2 S}{\partial E^a \partial E^b}\, dE^a\, dE^b$$
$$g^W = \frac{\partial^2 U}{\partial E^a \partial E^b}\, dE^a\, dE^b$$

by Ruppeiner [32] and Weinhold [38] respectively are metrics on the equilibrium space, using either entropy or internal energy as a distinguished thermodynamic potential.

These metrics were derived from physical arguments and offer some intuition about thermodynamic metrics. For example, Ruppeiner's metric g^R is derived from fluctuation arguments [32]. An equilibrium state of a thermodynamic system is characterized by some $x = (x^1, ..., x^n)$ variables on the space of equilibrium states, but it can fluctuate to some other state x' on the space of equilibrium states. One can characterize the probability distribution obtained after many measurements of this thermodynamic system with a Gaussian distribution $w(\Delta x)$ [22, p. 343], where $\Delta x = x' - x$ is the fluctuation, i.e., the difference between two points. The second moment of w is then taken as the inverse of g^R. The components of g^R can thus be thought of as an "inverse variance." Given a neighboring point x' of the mean x, if the distribution has a high variance, then g^R will think that x' and x are closer together than if the distribution has a low variance.

It turns out that these two metrics are related in the sense that they can both be obtained from pulling back a covariantly defined metric of a para-contact metric structure. Let $(\mathcal{T}, \Theta)$ be a thermodynamic phase space. Given arbitrary vectors X and Y on $\mathcal{T}$, define the metric G with

$$G(X, Y) = \Theta(X)\Theta(Y) - \, d\Theta(\varphi X, Y)$$

where the $(1,1)$-tensor φ satisfies $\varphi^2 = \mathrm{Id} - \eta \otimes \xi$. Take φ in coordinates to be

$$\varphi = dE^i \otimes \frac{\partial}{\partial E^i} - dI^i \otimes \frac{\partial}{\partial I^i}$$

in local coordinates and $i \in \{1, ..., n\}$ [24]. The metric G is an associated metric to the almost para-contact structure (φ, R, Θ) by similar reasoning to Example 3.13. In coordinates, G becomes

$$G = \Theta \otimes \Theta - \delta_{ab} \, dI^a \, dE^b$$

where a and b are indices running from 1 to n. The smooth embedding pulls G back to the metric

$$g = -\frac{\partial^2 \Phi}{\partial E^a \partial E^b} \, dE^a \, dE^b \tag{10}$$

on the space of equilibrium states. The metrics of Ruppeiner and Weinhold are thus specific cases of this metric.

3.3.3 Legendre Invariant Metrics

Given a metric on the thermodynamic phase space, one could also ask about Legendre transformations acting on the metric.

Example 3.14. Let us write the associated Riemannian metric from Example 3.13 in the coordinates of a thermodynamic phase space:

$$G^a = \Theta \otimes \Theta + \delta_{ab}(\, dE^a \, dE^b + \, dI^a \, dI^b). \tag{11}$$

A feature of this metric is that it is *Legendre invariant*, i.e., the Legendre transform φ of Definition 3.9 induces the following isometry.

Let $(\mathcal{T}, \Theta, G^a)$ be the phase space and metric as defined above, let $(\tilde{\mathcal{T}}, \tilde{\Theta})$ be a thermodynamic phase space for the same thermodynamic system, and take φ to be a Legendre transform $\varphi : \tilde{\mathcal{T}} \to \mathcal{T}$. We give $\tilde{\mathcal{T}}$ the metric

$$\tilde{G}^a = \tilde{\Theta} \otimes \tilde{\Theta} + \delta_{ab}(\, d\tilde{E}^a \, d\tilde{E}^b + \, d\tilde{I}^a \, d\tilde{I}^b).$$

Lemma 3.11 gives $\varphi^*\Theta = \tilde{\Theta}$. The remaining forms we can compute:

$$\begin{aligned}
&\varphi^*(\delta_{ab}(\, dE^a\, dE^b + \, dI^a\, dI^b)) \\
&\quad = \varphi^* \left(\sum_{i\in I} (dE^i)^2 + \sum_{j\in J} (dE^j)^2 + \sum_{i\in I} (dI^i)^2 + \sum_{j\in J} (dI^j)^2 \right) \\
&\quad = \sum_{i\in I} (d\tilde{I}^i)^2 + \sum_{j\in J} (d\tilde{E}^j)^2 + \sum_{i\in I} (d\tilde{E}^i)^2 + \sum_{j\in J} (d\tilde{I}^j)^2 \\
&\quad = \sum_{a}^{n} [(d\tilde{E}^a)^2 + (d\tilde{I}^a)] = \delta_{ab}(\, d\tilde{E}^a\, d\tilde{E}^b + \, d\tilde{I}^a\, d\tilde{I}^b).
\end{aligned}$$

Thus $\varphi^* G^a = \tilde{G}^a$ as desired. //

Definition 3.15. Let $(\mathcal{T}, \Theta)$ and $(\tilde{\mathcal{T}}, \tilde{\Theta})$ be two thermodynamic phase spaces for a thermodynamic system. Suppose G is a metric on $(\mathcal{T}, \Theta)$. Construct the new metric $\tilde{G}$ on $(\tilde{\mathcal{T}}, \tilde{\Theta})$ by defining

$$\tilde{G}(\tilde{\Phi}, \tilde{E}^a, \tilde{I}^a) = G(\Phi = \tilde{\Phi}, E^a = \tilde{E}^a, I^a = \tilde{I}^a).$$

If the Legendre transform $\varphi : \tilde{\mathcal{T}} \to \mathcal{T}$ from Definition 3.9 induces the isometry $\varphi^* G = \tilde{G}$, then the metric G is said to be Legendre invariant [29].

The rationale behind considering this class of metrics is that standard thermodynamics is Legendre invariant; one can perform Legendre transformations to equivalent descriptions of the system. The metrics G^I and G^{II}, given by

$$\begin{aligned}
G^I &= \Theta \otimes \Theta + (\delta_{ij} E^i I^j)(\delta_{cd}\, dE^c\, dI^d) \quad \text{and} \\
G^{II} &= \Theta \otimes \Theta + (\delta_{ij} E^i I^j)(\eta_{cd}\, dE^c\, dI^d),
\end{aligned}$$

where η is the diagonal $n \times n$ matrix $\operatorname{diag}(-1, 1, ..., 1)$, are two such metrics which have been used for thermodynamics [31]. Pulling these back to the space of equilibrium states, we obtain the metrics

$$g^I = \left(E^c \frac{\partial \Phi}{\partial E^c} \right) \left(\frac{\partial^2 \Phi}{\partial E^a \partial E^b}\, dE^a\, dE^b \right) \quad \text{and} \tag{12}$$

$$g^{II} = \left(E^c \frac{\partial \Phi}{\partial E^c} \right) \left(\eta_{ab} \delta^{bc} \frac{\partial^2 \Phi}{\partial E^c \partial E^d}\, dE^a\, dE^d \right). \tag{13}$$

3.4 Metrics and Phase Transitions

The metrics of §3.3 have been used to study various thermodynamic systems. The methodology is to first find a fundamental equation for a thermodynamic system, secondly to construct the metric of interest in coordinates, and finally to compute its Ricci scalar [29]. The singularities of these scalars are then compared with the points where the *heat capacities* of a thermodynamic system diverge. Given a change in heat with corresponding change in temperature of a thermodynamic system, then the ratio of these two quantities is a specific heat. Heat capacities are often computed and measured with respect to a thermodynamic variable that is held constant. The points where a heat capacity diverges, indicates the existence of a *phase transition*. For example, the heat capacity at constant pressure diverges for the water-steam phase transition at standard temperature and pressure.

In standard thermodynamics, heat capacities C_x are computed with

$$C_x = T\frac{\partial S}{\partial T} \tag{14}$$

where U, T, and S are internal energy, temperature, and entropy [9]. Here x stands for thermodynamic variables that are held constant when differentiating. Heat capacities are functions of thermodynamic variables. If there are points where C_x diverges, then we say that the system has a phase transition at those points.

In geometric thermodynamics, it is argued that the singularities of the Ricci scalar of the metric under are exactly the phase transitions for a thermodynamic system [29, 32]. While this is the case for some systems, let us turn our attention where this is false; not all singularities are phase transitions.

4. Black Holes

4.1 A Fundamental Equation

One black hole which seems to have not been explored using thermodynamic metrics is the Euler-Heisenberg-AdS black hole. It is a charged, nonrotating black hole with cosmological constant, with an additional parameter called the *Euler-Heisenberg parameter* [25]. The Euler-Heisenberg parameter a appears as a nonlinear correction term to the standard Lagrangian for classical electrodynamics. Roughly speaking, a characterizes the pair production of virtual electron-positron pairs that exist in vacuum. For further discussion, see [16]. The Euler-Heisenberg-AdS black hole, being parameterized by its mass M, charge Q, cosmological constant Λ, and Euler-Heisenberg parameter a, is an extension of the Reissner-Nordström-AdS black hole, which is characterized by mass, charge, and cosmological constant.

Regardless of whether we wish to treat this with standard thermodynamics or metrics, we need a fundamental equation. The nonlinear correction to the Lagrangian modifies the electromagnetic stress-energy tensor T in Einstein's field equations by adding higher order (in a) couplings of the Maxwell tensor F to T (see [25] for explicit formulas). The following metric

$$ds^2 = -f(r)\, dt^2 + \frac{1}{f(r)} dr^2 + r^2 d\Omega^2,$$

where

$$f(r) = 1 - \frac{2M}{r} + \frac{Q^2}{r^2} - \frac{\Lambda r^2}{3} - \frac{aQ^4}{20r^6}, \tag{15}$$

solves the modified Einstein's field equations with cosmological constant [25]. Due to the $1/f(r)$ in the metric, the largest root $r = r_+$ of $f(r)$ is the event horizon of the black hole (it is a null hypersurface, see [25, II.B]). We identify the mass of the black hole as

$$M = \frac{r_+}{2} - \frac{\Lambda r_+^3}{6} + \frac{Q^2}{2r_+} - \frac{aQ^4}{40r_+^5}\,.$$

Hawking's result shows that the entropy S of a black hole is $S = A/4$ in natural units, where $A = 4\pi r_+^2$ is the surface area of the event horizon [14]. Substitution provides a formula for the mass

$$M = \sqrt{\frac{S}{4\pi}} \left(1 - \frac{\Lambda S}{3\pi} + \frac{Q^2 \pi}{S} - \frac{aQ^4 \pi^3}{20S^3}\right). \tag{16}$$

As given, Λ and a are constants of the theory. However, there is a sense in which they should be allowed to vary. The mass of a black hole, being a function of dimensionful physical quantities, will satisfy Euler's homogenous function theorem, which states that if a smooth function $f(x, y)$ satisfies

$$f(\alpha^r x, \alpha^s y) = \alpha^q f(x, y)$$

for some real number α and integers r, s, and q, then

$$qf(x, y) = rx\frac{\partial f}{\partial x} + sy\frac{\partial f}{\partial y}\,.$$

This result holds in general for smooth functions of n variables. Our version of the theorem is obtained through the chain rule [cf. 39].

All the physical quantities defining our mass M must be summed and multiplied together so that the overall dimension matches that of mass, which leads us to this homogeneity argument. The resulting quadratic form for the mass is then a function of all the defining variables and their conjugates. This argument originated with Smarr [35].

Applying the theorem to M where α is an arbitrary constant, note that

$$M(\alpha^2 S, \alpha Q, \alpha^{-2}\Lambda, \alpha^2 a) = \alpha M(S, Q, \Lambda, a).$$

Therefore

$$M(S, Q, \Lambda, a) = 2S\left(\frac{\partial M}{\partial S}\right) + Q\left(\frac{\partial M}{\partial Q}\right) - 2\Lambda\left(\frac{\partial M}{\partial \Lambda}\right) + 2a\left(\frac{\partial M}{\partial a}\right).$$

Taking

$$T = \frac{\partial M}{\partial S}, \quad \Phi = \frac{\partial M}{\partial Q}, \quad \Psi = \frac{\partial M}{\partial \Lambda}, \quad \text{and} \quad A = \frac{\partial M}{\partial a},$$

we obtain the Smarr formula [25, eq. 26] for the Euler-Heisenberg-AdS black hole

$$M = 2TS + \Phi Q - 2\Lambda\Psi + 2aA\,.$$

By Euler's theorem, one can see that in the quadratic form for M, the defining parameters come paired with their conjugates. For some physical intuition, the cosmological constant behaves as a pressure term [20, 21], Ψ is a volume, Φ is an electric potential, a is a polarization, and A is an electric field. The Smarr formula being a quadratic form of these eight variables supports the choice of (S, Q, Λ, a) as being the set of defining parameters (i.e., coordinates for the space of equilibrium states, a Legendrian submanifold) for the mass.

Some authors [26, 30, 37] still consider the choice (S, Q) as being the set of defining parameters (for a Reissner-Nordström-AdS black hole), especially in regards to the use of Ruppeiner's metric (§3.3.2) to analyze thermodynamics. Let us compare these two choices by analyzing metrics defined using either this reduced phase space with parameters S, Q or the extended phase space with parameters S, Q, Λ, and a.

4.2 Curvature Scalars

Following the procedure, let us compute the heat capacity at constant charge C_Q (see Equation (14)):

$$C_Q = T\frac{\partial S}{\partial T} = \frac{\partial_S M}{\partial_{SS} M} = \frac{2S(4\Lambda S^4 - \pi^4 Q^4 a + 4\pi^2 Q^2 S^2 - 4\pi S^3)}{4\Lambda S^4 + 7\pi^4 Q^4 a - 12\pi^2 Q^2 S^2 + 4\pi S^3}\,. \tag{17}$$

The divergences in C_Q occur at zeroes of the denominator:

$$0 = 4\Lambda S^4 + 7\pi^4 Q^4 a - 12\pi^2 Q^2 S^2 + 4\pi S^3. \tag{18}$$

It is also useful to consider the denominator in terms of r_+ (see (15)) instead. Using $S = \pi r_+^2$, (18) becomes

$$4\Lambda r_+^8 + 4r_+^6 - 12Q^2 r_+^4 + 7Q^4 a.$$

Another interesting feature of C_Q are the zeroes of the numerator that come from the polynomial (in S) term

$$0 = 4\Lambda S^4 - \pi^4 Q^4 a + 4\pi^2 Q^2 S^2 - 4\pi S^3.$$

These zeroes indicate sign changes of C_Q. In terms of r_+, this becomes

$$4\Lambda r_+^8 - 4r_+^6 + 4Q^2 r_+^4 - Q^4 a.$$

Black holes can have negative heat capacities. Physically speaking, a negative heat capacity indicates that as the black hole emits Hawking radiation, its temperature increases. A positive heat capacity is the opposite; for an everyday example, a mug of coffee cools down by emitting infrared radiation and its temperature decreases asymptotically to room temperature. A black hole with a positive C_Q is said to be *stable* and a negative C_Q is said to be *unstable* [15, 25].

Let us now compute the scalar curvatures of the metrics g (10), g^I (12), and g^{II} (13) and see if their singularities correspond the points where C_Q diverges. We use SageMath to express the curvature scalars in the form N/D, where N and D are factored polynomials over the integers. Possible curvature singularities are thus given by zeroes of D; we will numerically check the behavior of the curvature scalar around the zeroes to see if it is a genuine singularity.

In the reduced phase space, Table 1 shows that g^{II} recovers the divergence in the heat capacity whereas g and g^I do not. However, the metric

Table 1: Denominators of scalar curvature D for metrics g, g^I, and g^{II}, in the reduced phase space with $M = M(S, Q)$, and comparison with C_Q

Metric	D	Agreement
g	$(\pi^6 Q^6 a^2 - 26\pi^4 Q^4 S^2 a + 12\pi^2 \Lambda Q^2 S^4 a$ $+12\pi^3 Q^2 S^3 a + 40\pi^2 Q^2 S^4 - 40\Lambda S^6 - 40\pi S^5)^2$	no
g^I	$(\pi^6 Q^6 a^2 - 26\pi^4 Q^4 S^2 a + 12\pi^2 \Lambda Q^2 S^4 a$ $+12\pi^3 Q^2 S^3 a + 40\pi^2 Q^2 S^4 - 40\Lambda S^6 - 40\pi S^5)^2$ $\times\left(3\pi^4 Q^4 a - 60\pi^2 Q^2 S^2 + 20\Lambda S^4 - 20\pi S^3\right)^3$	no
g^{II}	$\left(7\pi^4 Q^4 a - 12\pi^2 Q^2 S^2 + 4\Lambda S^4 + 4\pi S^3\right)^2$ $\times\left(3\pi^4 Q^4 a - 60\pi^2 Q^2 S^2 + 20\Lambda S^4 - 20\pi S^3\right)^3$ $\times\left(3\pi^2 Q^2 a - 10S^2\right)^2$	partial

Table 2: Denominators of scalar curvature D for metrics g, g^I, and g^{II}, in the extended phase space with $M = M(S, Q, \Lambda, a)$ and comparison with C_Q

Metric	D	Agreement
g	1	no
g^I	$Q^2\left(3\pi^4 Q^4 a - 36\pi^2 Q^2 S^2 + 20\Lambda S^4 - 12\pi S^3\right)^3$	no

g^{II} potentially has additional singularities; let us check the behavior of the Ricci scalar around the zeroes of these other polynomials.

Let us fix values for a, Λ, and Q^2, plot the denominator of the heat capacity (18) as a polynomial in S (or r_+), and check if the other polynomials vanish at some S before the heat capacity diverges. Taking $a = 1$, $\Lambda = -3$, and $Q = 0.8$ [25], the heat capacity diverges at approximately $S \approx 1.75$, but the other polynomial has a zero at $S \approx 0.53$. Numerically, the curvature scalar of g^{II} at $S \approx 0.53$ does diverge, so this is an additional singularity that does not come from the divergence of the heat capacity. Thus g^{II} only has "partial" agreement with the divergence of C_Q; it recovers the divergence of C_Q but introduces additional singularities. The metrics g and g^I disagree because they do not recover the divergence of C_Q at all.

In the extended phase space, g^{II} is degenerate and therefore not a metric on the space of equilirium states. Table 2 shows that g has 1 as its denominator of scalar curvature, but it turns out that the Ricci scalar vanishes. Both g and g^I fail to reproduce the phase transition structure in the extended phase space.

Table 3: Denominators of scalar curvature D for the metric g, in the reduced phase space with variable potentials $F(T, Q)$ and $\Omega(T, \Phi)$, and comparison with C_Q

Potential	D	Agreement
F	$Q^6\left(4\Lambda r^8 + 4Q^2r^4 - 4r^6 - Q^4a\right)$ $\times\left(4\Lambda r^8 - 12Q^2r^4 + 4r^6 + 7Q^4a\right)^4$ $\times\left(10r^4 - Q^2a\right)^6$	partial
Ω	$P_{25}^5 P_{20}^2 \left(4\,\Lambda r^8 - 12\,Q^2r^4 + 4\,r^6 + 7\,Q^4a\right)$ $\times\left(10\,r^4 - Q^2a\right)^2\left(2\,r^4 - Q^2a\right)^3 r^{12}$	partial

Note: Here, P_{25} and P_{20} are polynomials with 25 and 20 terms respectively. The denominators are expressed in terms of $r = r_+$ instead of S due to the chain ruling used when computing metric coefficients.

Since G is not Legendre invariant, the curvature scalar of g is not necessarily preserved by Legendre transformations. On the reduced phase space, we can transform $M(S, Q)$ into three other potentials

$$F(T, Q) = M - TS,\ H(S, \Phi) = M - \Phi Q,\ \text{and}\ \Omega(T, \Phi) = M - TS - \Phi Q.$$

Table 3 gives the denominators of scalar curvature in these different thermodynamic representations. The potential H induces a degenerate matrix and thus does not provide a metric on the space of equilibrium states.

The potentials F and Ω induce metrics that are singular at the divergence of C_Q, but they also introduce additional divergences. For example, the metric derived from F has an additional singularity at $r_+ \approx 0.5$ (taking $a = 1, \Lambda = -3$, and $Q = 0.8$ again) due to the $(10r^4 - Q^2a)$ term, which occurs before the heat capacity divergence at $r_+ \approx 0.85$. Numerically, $r_+ \approx 0.5$ is a genuine singularity. The numerator of the heat capacity also appears, although it does not vanish in this case. In other cases though, the numerator of a black hole's heat capacity may not vanish [30, p. 978] and induce singularities.

5. Discussion

Metrics may not be the right objects to consider when describing thermodynamic interactions. These thermodynamic metrics might produce exactly the divergences of the heat capacity as curvature sinularities for less "pathological" black holes like the Kerr or Reissner-Nordström black holes [26, 30, 37], but this is not always the case. As we have seen, any singularities in the metrics could either correspond to points where the heat capacity diverges, the zeroes of the heat capacity, or neither, and the only way to figure this out is to have already computed the heat capacity, which defeats the purpose of using metrics in the first place. As such, one cannot assign these singularities a singular interpretation, of being phase transitions or otherwise.

Furthermore, the computational difficulty increases significantly. To check which polynomials in the denominators of the scalar curvatures are vanishing or nonvanishing, we must calculate and factor the Ricci scalar, which can take a lot more time than computing heat capacities. For example, calculating D for Ω in Table 3 took about four hours on a CPU running at roughly 3.5 GHz; the heat capacity calculation to obtain (17) finished in under a second. Treating thermodynamics with metrics is a computationally intensive task that is not guaranteed to produce the phase transitions of standard thermodynamics.

However, contact geometry still captures interesting thermodynamic information. For example, the Legendrian submanifolds of a thermodynamic phase space already contain information about *critical points*. At the level of Legendrian submanifolds, critical points are points where certain derivatives of equations of state vanish in the submanifold. Critical points are interesting in their own right, though they are also related to phase transitions. Despite these metric shortcomings, contact geometry naturally describes equilibrium thermodynamics.

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