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On the intrinsic geometric structure of extended irreversible thermodynamics

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Abstract

In this paper we reexamine the geometric structure of extended irreversible thermodynamics in the context of contact geometry. First, we consider the interplay between the contact manifold (M, ω) with thermodynamic state space B_N as its base, and the cotangent bundle T^*B_N equipped with a nondegenerate 2-form $\Omega = \mathrm{d}\omega$. We then show that the Legendre submanifold L of M and the Lagrangian submanifold of T^*B_N are intimately related to the entropy surface of the thermodynamic system. Second, we further generalize the symmetry transformations considered in our previous work that preserve the laws of thermodynamics as well as the pseudo-Riemannian metric in L. Finally, we consider some examples on coordinate transformations in M that illustrate the transformation between the entropy surface and the energy surface, and the relationship between Legendre involution and the submanifold of (T^*B_N, Ω).

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1. Introduction

It is well known that equilibrium thermodynamics (ET) has a geometric structure in terms of a contact manifold M equipped with a contact 1-form

$$\omega = \mathrm{d}u - \sum_{i=1}^{N} y_i \,\mathrm{d}x^i = \mathrm{d}u - y_i \,\mathrm{d}x^i$$

where $x = (x^1, \ldots, x^N)$, $y = (y_1, \ldots, y_N)$ and u form a coordinate cover of M [1]. Furthermore, the fundamental equation of states in ET is a Legendre submanifold of M. In 1975, Weinhold [2] suggested that the second derivative matrix elements of the internal energy might be employed to define a metric structure on the set of thermodynamic states. In 1983, Salamon *et al* [3] constructed a group of coordinate transformations that preserve the contact structure of M as well as the metric structure of Weinhold. The work of Salamon *et al* was later generalized to extended irreversible thermodynamics (EIT) by Chen [4]. In this paper we further examine the intrinsic geometric structure of EIT from statistical point of view. First, we introduce the generalized Gibbs 1-form based on the maximum entropy principle. Second, based on the generalized Gibbs 1-form we then formulate the geometric structure of thermodynamics in terms of a contact manifold. Finally, we consider the symmetry transformations that preserve the first law and the second law of thermodynamics as well as the metric structure defined by the second derivative matrix elements of the entropy density function. These symmetry transformations contain the coordinate transformations considered by Salamon *et al*.

Consider a system of molecules in r components contained in a region $\Omega \subset R^3$ with volume V, where no chemical reactions take place. Let f_a be the one-particle distribution function of molecular species a at spacetime $(\vec{r}, t)$ with molecular velocity $\vec{v}_a$. For simplicity, we adopt the notation $\langle A, B\rangle = \int AB\,\mathrm{d}\vec{v}_a$, and define the following field variables:

$$\text{density:}\quad \rho = \sum_a \rho_a = \sum_a \langle f_a, m_a\rangle \tag{1}$$

$$\text{mean velocity } \vec{u}:\quad \rho\vec{u} = \sum_a \langle f_a, m_a\vec{v}_a\rangle \tag{2}$$

$$\text{mass fraction:}\quad c_a = \rho_a\rho^{-1} = \rho_a v \tag{3}$$

$$\text{peculiar velocity:}\quad \vec{c}_a = \vec{v}_a - \vec{u} \tag{4}$$

$$\text{internal energy density } e:\quad \rho e = \sum_a \left\langle f_a, \frac{1}{2}m_a\vec{c}_a\cdot\vec{c}_a\right\rangle \tag{5}$$

$$\text{generalized fluxes } \hat{\phi}_a^{(i)}:\quad \rho\hat{\phi}_a^{(i)} = \left\langle f_a, h_{a,i}^{(m)}\right\rangle. \tag{6}$$

Here the subscript a refers to the molecular species a and $\left\{h_{a,i}^{(m)}\right\}$ is a set of tensor Hermite polynomials constructed by Eu [5]. Note that $h_{a,i}^{(m)}$, $i = (i_1, i_2, \ldots, i_m), 1 \leqslant i_k \leqslant 3$, is a tensor of order m as well as a polynomial in $\vec{c}_a$ of degree m. For example, $h_a^{(0)} = 1, h_{a,i}^{(1)} = m_a\vec{c}_a, h_{a,i}^{(2)} = m_a\vec{c}_a\vec{c}_a - 1/3T_r(\vec{c}\cdot\vec{c}_a)\hat{I}$ ($\hat{I}$: unit second-order tensor), etc. In order to simplify the notation, hereafter we drop the tensor index i and denote $h_{a,i}^{(m)} = h_a^{(m)}$ and $\hat{\phi}_{a,i}^{(m)} = \hat{\phi}_a^{(m)}$. Thus $\vec{J}_a = \hat{\phi}_a^{(1)}$ is the diffusion flux, $\vec{\vec{\pi}}_a = \hat{\phi}_a^{(2)}$ is the traceless symmetric stress tensor and $\vec{Q}_a = \langle f_a, 1/2m_a(\vec{c}_a\cdot\vec{c}_a - 5T)\vec{c}_a\rangle$ is the heat flux obtained by the contraction of the third-order tensor $\hat{\phi}_a^{(3)}$, etc.

In the classical theory of irreversible thermodynamics [6], the thermodynamic state is described by the conserved variables (e, v, c_a). In order to consider some non-equilibrium phenomena, such as, ultrasound propagation, light or neutron scattering, it is necessary to include the dissipative fluxes $\hat{\phi}_a^{(m)}$ in addition to the conserved variables e, v and c_a. Let $x = \left\{e, v, c_a, \hat{\phi}_a^{(i)}; 1 \leqslant a \leqslant r, 1 \leqslant i \leqslant n\right\} = (x^1, \ldots, x^N) \in B_N$. Depending on the particular problem under consideration, n can be taken as large as necessary. Henceforth, we consider x as the set of thermodynamic variables in EIT [7]. The dynamical behaviour of x^i can be obtained from the Boltzmann equation. Since we are only interested in the geometric aspects of EIT, in this paper we do not consider the evolution of the thermodynamic system.

2. Maximum entropy principle and the generalized Gibbs 1-form

In this section we consider $\vec{c}_a$ as a random variable with f_a as its (unnormalized) probability density function. By the definition of the thermodynamic variable x it is evident that x^i are the velocity moments of $\vec{c}_a$. We now construct f_a in terms of x^i. To this end, let w_a be a function of $(\vec{v}_a, \vec{r}, t)$ with the following properties:

$$\text{(i) } w_a \geqslant 0 \qquad \text{(ii) } \langle w_a, m_a \rangle = \rho_a.$$

In kinetic theory the entropy density function is defined by

$$\rho S = -\sum_a \langle f_a, \ln(f_a) - 1 \rangle \tag{7}$$

where we have set the Boltzmann constant $k = 1$. Thus,

$$\rho S \leqslant -\sum_a \langle f_a, \ln(w_a) - 1 \rangle.$$

We look for w_a that maximizes S subject to the constraints given by (1)–(6). Define

$$\begin{aligned} H(f_1, \ldots, f_a) = -\sum_{a=1}^{r} \Bigg\{ & \langle f_a, \ln(f_a) - 1 \rangle + \lambda_1[\rho_a - \langle f_a, m_a \rangle] + \vec{\lambda}_2 \cdot \left[\frac{1}{r}\rho\vec{u} - \langle f_a, m_a \vec{v}_a \rangle \right] \\ & + \lambda_3 \left[\frac{1}{r}\rho e - \left\langle f_a, \frac{1}{2} m_a \vec{c}_a \cdot \vec{c}_a \right\rangle \right] + \sum_{i=1} \lambda_a^{(i)} : \left[\rho \hat{\phi}_a^{(i)} - \left\langle f_a, h_a^{(i)} \right\rangle \right] \Bigg\} \end{aligned} \tag{8}$$

where A:B denotes scalar product of tensors A and B. Then $\frac{\partial H}{\partial f_a} = 0$ yields the following result:

$$w_a = \lim_{\substack{\varepsilon \to 0 \\ n \to \infty}} \exp \left\{ -\lambda_1 m_a - \vec{\lambda}_2 \cdot (m_a \vec{v}_a) - \lambda_3 \left(\frac{1}{2} m_a \vec{c}_a \cdot \vec{c}_a \right) - \sum_{i=1} \lambda_a^{(i)} : h_a^{(i)} - \varepsilon (\vec{c}_a \cdot \vec{c}_a)^n \right\}. \tag{9}$$

Here ε is an infinitesimal real number. The term $-\varepsilon(\vec{c}_a \cdot \vec{c}_a)^n$ is included in (9) to ensure that w_a can be normalized. The Lagrange multipliers λ_1, $\vec{\lambda}_2$ and λ_3 can be determined by setting $f_a = f_a^0$ in (1), (2) and (5) with f_a^0 as the Maxwell–Boltzmann distribution at local equilibrium. On the other hand, $\lambda_a^{(i)}$ can be determined by (6). Thus the one-particle distribution function f_a that maximizes the entropy density function S under the conditions (1)–(6) can be written as

$$w_a = \lim_{\substack{\varepsilon \to 0 \\ n \to \infty}} \exp \left\{ -T^{-1} \left[-m_a \mu_a + \frac{1}{2} m_a \vec{c}_a \cdot \vec{c}_a + \sum_{i=1} X_a^{(i)} : h_a^{(i)} + \varepsilon (\vec{c}_a \cdot \vec{c}_a)^n \right] \right\} \tag{10}$$

where we have denoted $X_a^{(i)} = \lambda_a^{(i)}$, T is the local thermodynamic temperature given by $\frac{3}{2} nT = \left\langle f_a^0, \frac{1}{2} m_a \vec{c}_a \cdot \vec{c}_a \right\rangle$, and μ_a is the chemical potential of molecular species a determined by the normalization condition of w_a.

In general, it is difficult to obtain exact solutions for $\lambda_a^{(i)}$. However, approximate solutions can be found in [7]. Particularly in the linear-order approximation, it is known that the Lagrange multiplier conjugated to the viscous pressure is given by $\overset{\leftrightarrow}{X}_a^{(t)} = -\tau_2 (2\rho\eta)^{-1} \overset{\leftrightarrow}{\pi}$, whereas the Largrange multiplier conjugated to the heat flux is $\overset{\leftrightarrow}{X}_a^{(h)} = -\tau_1 (\rho\lambda T)^{-1} \vec{Q}$, where τ_2 and τ_1 are the relaxation times of $\overset{\leftrightarrow}{\pi}$ and $\vec{Q}$ respectively, η is the shear viscosity and λ is the thermal conductivity. These results can easily be obtained from the work of Jou *et al*. Therefore, among the set of all f_a that satisfy the constraint conditions (1)–(6), w_a is the unique one-particle distribution function that maximizes the entropy density function. This is called the maximum entropy principle.

According to (7) and (10) the entropy density function can be written as

$$S = T^{-1} e + (pT^{-1}) v - \sum_a (\mu_a T^{-1}) \vec{c}_a + \sum_{a,i} \left(X_a^{(i)} T^{-1} \right) : \phi_a^{(i)} + 0(\varepsilon). \tag{11}$$

Since $-\varepsilon(\vec{c}_a \cdot \vec{c}_a)^n$ carries no physical significance, hereafter we drop the terms $-\varepsilon(\vec{c}_a \cdot \vec{c}_a)^n$ in (10) and $0(\varepsilon)$ in (11). Denote $y = \left(T^{-1}, pT^{-1}, -\mu_a T^{-1}, X_a^{(i)} T^{-1}\right) = (y_1, y_2, \ldots, y_N)$. Then the entropy density function S can be expressed as $S = \sum_i y_i x^i = y_i x^i$. It should be borne in mind that y_i are differentiable functions of the Lagrange multipliers. Now that S attains its maximum value when λ_i are determined by the constraints (1)–(6), the variation of S with respect to λ_i vanishes. Thus

$$\mathrm{d}S = \sum_{i,j} \frac{\partial S}{\partial y_i} \frac{\partial y_i}{\partial \lambda_j} \,\mathrm{d}\lambda_j = \sum_i x^i \,\mathrm{d}y_i = 0.$$

This is the generalized Gibbs–Duhem relation. Consequently we have the generalized Gibbs relation (Gibbs 1-form)

$$\mathrm{d}S = T^{-1}\,\mathrm{d}e + pT^{-1}\,\mathrm{d}v - \sum_a (\mu_a T^{-1})\,\mathrm{d}c_a + \sum_{a,i} \left(X_a^{(i)} T^{-1}\right) : \mathrm{d}\hat{\phi}_a^{(i)} = y_i\,\mathrm{d}x^i. \tag{12}$$

The microscopic derivation of the generalized Gibbs 1-form has been carried out by various authors in the past [8]. Here we present a different derivation of (12) to serve as an introduction to the concept of contact manifold. Next we define the graph space G_f by

$$G_f = \left\{(x, u, y) | u = S = f(x), y_i = \frac{\partial f}{\partial x_i} = \partial_i f\right\}. \tag{13}$$

In the following section we show that G_f is the foundation of the geometric structure of thermodynamics.

3. Geometric structure of thermodynamics

In order to discuss the geometric structure of thermodynamics, we first consider the local formulations of the first law and the second law. Let w be the work 1-form defined by

$$w = -p\,\mathrm{d}v + \sum_a \mu_a\,\mathrm{d}c_a - \sum_{a,i} X_a^{(i)} : \mathrm{d}\hat{\phi}_a^{(i)}.$$

The local formulation of the first law can be written as

$$\Delta e = w + \Delta q_c + \Delta q_d \tag{14}$$

while the local formulation of the second law can be expressed as [9]

$$\xi \wedge \mathrm{d}\xi = 0 \qquad \xi = \mathrm{d}e - w \tag{15a}$$

$$\Delta q_d \geqslant 0. \tag{15b}$$

Here Δq_c is the exchange of heat between the local system and its surroundings (reservoir), and Δq_d represents the dissipative energy, which cannot be converted into any form of energy available to the system. The expressions in (14) represent infinitesimal changes in (e, w, q_c, q_d) from a state specified by x to its neighbouring state $x + \Delta x$. However, it should be noted that Δq_d is a function of x and its spatial gradients. It cannot be expressed as a 1-form in the vector space $\Lambda(B_n)$ of differential forms defined on B_N. By the inaccessibility condition (integrability condition) (15a) we can prove the existence of a local thermodynamic temperature T and the entropy density function S, such that $\xi = T\,\mathrm{d}S$. Thus $\mathrm{d}S = y_i\,\mathrm{d}x^i$ with $y_i = \partial_i S$ [9].

In 1973, Hermann suggested that equilibrium thermodynamics (ET) might be formulated in the context of a contact manifold M [1]. Recently Mrugala *et al* further investigated the applications of contact geometry to ET [10], where thermodynamics processes were considered as flows of vector fields in the tangent space of the contact manifold. This geometric structure has also been extended to EIT by the present author [11]. In the following discussions we first consider the interplay between the contact manifold M with base space B_N and the associated symplectic bundle T^*B_N. Second, we show that the Legendre submanifold L of M and the Lagrangian submanifold L_a of T^*B_N are intimately related to the entropy surface in EIT. In section 4 we further generalize our previous work on symmetry transformations on M that preserve the thermodynamic laws as well as the pseudometric on L. These symmetry transformations include the special example of coordinate transformations considered by Salamon *et al*. In addition, the relationship between Legendre involutions and the Lagrangian submanifold L_a can also be exhibited.

Let us examine the graph space defined in (13). The thermodynamic states in EIT can be considered as a smooth manifold B_N with coordinate cover $x = (x^1, \dots, x^N)$. Define the map $\phi : B_N \to G = B_N \times R$ by $\phi(x) = (x, u), u = f(x)$, such that $\phi^*(\mathrm{d}x^1 \wedge \cdots \wedge \mathrm{d}x^N) \neq 0$, where ϕ^* is the pull back of ϕ. The coordinate cover of G is (x, u). Let $K = G \times R^N$ be a $(2N + 1)$-dimensional smooth manifold with coordinate cover $(x, u, y),\ y = (y_1, \dots, y_N)$. Now the Gibbs 1-form $\mathrm{d}u = y_i\, \mathrm{d}x^i$ can be employed to define the 1-form $\omega = \mathrm{d}u - y_i\, \mathrm{d}x$, where (x, u, y) are independent coordinates in K. Since $\omega \wedge (\mathrm{d}\omega)^N$ is a nonzero volume element in K, and $\omega \wedge (\mathrm{d}\omega)^{N+1} = 0$, ω is a nondegenerate 1-form. Next we extend the map ϕ to the map $\bar{\phi} : B_N \to K$ by the requirement $\bar{\phi}^*\omega = 0$. Then $\bar{\phi}^*\omega = \bar{\phi}^*(\mathrm{d}u) - \bar{\phi}^*(y_i\, \mathrm{d}x^i) = \mathrm{d}u - \bar{\phi}^*(y_i)\, \mathrm{d}x^i = 0$. Thus $\bar{\phi}^*(y_i) = \partial_i u$. This implies that the graph space G_f in (13) is the integral manifold of the Pfaffian equation $\omega = 0$, i.e., $\omega\big|_{G_f} = 0$. Let x_0 be a fixed point in B_N, and let v be a tangent vector in $T_{x_0}B_N$. The differential of f at x_0, denoted by $\mathrm{d}f$, is defined by $\langle v, \mathrm{d}f\rangle = v^i \partial_i f$, where $v = (v^1, \dots, v^N)$. Here $\mathrm{d}f$ is called a covector, which is a linear form on $T_{x_0}B_N$. The tangent hyperplanes (THP) to the level surface of f at x_0 is given by $\langle v, \mathrm{d}f\rangle = 0$. In general, a THP to a smooth manifold M at x_0 is a subspace of dimension 1 less than the tangent space to M at x_0. This THP is a zero level set of a linear function which is not identically zero.

Consider the cotangent space T^*B_N. A symplectic structure of T^*B_N is defined by the choice of a 2-form Ω, such that, (i) Ω is nondegenerate ($\Omega^N \neq 0, \mathrm{d}(\Omega)^{N+1} = 0$), (ii) Ω is closed ($\mathrm{d}\Omega = 0$). According to Darboux theorem, there exists a local coordinate system $(x^1, \dots, x^N, y_1, \dots, y_N)$ such that $\Omega = \mathrm{d}y_i \wedge \mathrm{d}x^i$. In other words, Ω is nondegenerate if the rank of Ω is $2N$, the dimension of T^*B_N. Thus (T^*B_N, Ω) is a symplectic manifold, which is a vector bundle with base B_N and with $T^*_xB_N$ as the fibre of $x \in B_N$. Define $\alpha = y_i\, \mathrm{d}x^i$ in T^*B_N, such that $(\mathrm{d}\alpha)^N \neq 0$, $(\mathrm{d}\alpha)^{N+1} = 0$. Then $\Omega = \mathrm{d}\alpha$ defines the symplectic structure of T^*B_N. Next we consider $M = T^*B_N \times R$ with coordinate cover (x, u, y). Let $\omega = \mathrm{d}u - \alpha$. Then ω is a nondegenerate 1-form. It is interesting to note that $T^*B_N \times R$ can be identified with a 1-jet space $J^1(B_N, R)$ from B_N to R. This is a vector bundle with base B_N, and the fibre at x is $T^*_xB_N \times R$. For every real-valued function g defined in a neighbourhood of $x \in B_N$, the jet j^1g is a mapping j^1g: $j^1_xg = (g(x), \mathrm{d}g(x))$, and the canonical projection $\pi : J^1(B_N, R) \to B_N$ is the mapping $j^1_xg \to x$. A local section of $J^1(B_N, R)$ is a mapping $\sigma : B_N \to J^1(B_N, R)$ such that $\pi \circ \sigma = i_d$ is an identity. Hence j^1g defines a local section of $J^1(B_N, R)$. On the other hand, a section of $T^*B_N \times R$ can be expressed as $\sigma = (u, \xi)$, where u is a real number and ξ is a 1-form. Now $\sigma = j^1g$ if and only if $u = f$ (a real-valued function) and $\xi = \mathrm{d}f$. Hence $\sigma^*\omega = \sigma^*(\mathrm{d}u - y_i\, \mathrm{d}x^i) = \mathrm{d}u - \sigma^*(y_i)\, \mathrm{d}x^i = 0$ if and only if $\sigma^*(y_i) = \partial_i f$. A local section of $J^1(B_N, R)$ is called a Legendre submanifold of M. Let U be a neighbourhood of $x \in B_N$. The image of U under j^1f is the graph space G_f. Therefore the entropy surface $u = f(x)$ is a Legendre submanifold of $J^1(B_N, R)$.

Alternatively we can consider the vector bundle M from a different point of view. Let G be a smooth manifold of dimension $N + 1$ with coordinate cover (x, u). Let T^*G be equipped with a nondegenerate symplectic structure specified by a 2-form Ω. In local coordinates (u, x, y_0, y), $x = (x^1, \ldots, x^N)$, $y = (y_1, \ldots, y_N)$, Ω can be written as $\Omega = \mathrm{d}y_0 \wedge \mathrm{d}u + \mathrm{d}y_i \wedge \mathrm{d}x^i$. Let PT^*G be the projective space of T^*G. The points of PT^*G are nonzero 1-forms of T^*G defined up to a nonzero multiplicative factor, $\eta = y_0\,\mathrm{d}u + y_i\,\mathrm{d}x^i$. Suppose $y_0 \neq 0$. We can set $y_0 = -1$. Then the points in PT^*G can be written as $\eta = -\mathrm{d}u + y_i\,\mathrm{d}x^i$ (determined up to a nonzero multiplicative factor). Therefore PT^*G is a vector bundle of dimension $2N + 1$, whose base is G and the fibre at any point x of G is the projective space PT^*_xG. Furthermore, PT^*G is equipped with a distinguished 1-form $\omega = \mathrm{d}u - y_i\,\mathrm{d}x^i$ satisfying the nondegenerate condition $\omega \wedge (\mathrm{d}\omega)^N \neq 0$, $\omega \wedge (\mathrm{d}\omega)^{N+1} = 0$. In general, a smooth manifold of dimension $(2N + 1)$ equipped with a nondegenerate 1-form ω is called a contact manifold [12], where ω is called the contact 1-form. Let z be a fixed point on M. A THP to M at z is given by $\langle X, \omega\rangle(z) = (v^i\omega_i)(z) = 0$, $X = v^i(z)\partial_i \in T_zM$. Thus ω generates a nondegenerate distribution (field) of THPs called the contact structure of M. If λ is a nowhere vanishing real-valued function defined on M, then $\lambda\omega$ generates the same contact structure of M. A Legendre submanifold L of dimension N is an integral manifold of the fields of THPs, where $\omega|_L = 0$. By Darboux theorem, there exist local coordinates (x, u, y) in M such that $\omega = \mathrm{d}u - y_i\,\mathrm{d}x^i$. Note that $\mathrm{d}\omega = -\mathrm{d}y_i \wedge \mathrm{d}x^i$ and $(\mathrm{d}\omega)^N \neq 0$. Thus $\mathrm{d}\omega$ induces a 2-form $\Omega = \mathrm{d}y_i \wedge \mathrm{d}x^i$, which generates a nondegenerate symplectic structure of a $2N$-dimensional symplectic manifold (P, Ω). The contactification of (P, Ω) is the bundle M with fibre R over the base space P, i.e., $M = P \times R$. The contact structure of M is given by the 1-form $\omega = \mathrm{d}t - \Omega$, where t is the canonical coordinate of R. It is well known that the symplectic manifold (P, Ω) has an N-dimensional submanifold L_a (called the Lagrangian submanifold), which is the integral manifold of $\Omega = 0$. Now, $\Omega = \mathrm{d}(y_i\,\mathrm{d}x^i) = 0$, there exists a real-valued function g such that $\mathrm{d}g = y_i\,\mathrm{d}x^i$, i.e., $\Omega|_{L_a} = 0$. On the other hand, the Legendre submanifold L of (M, ω) is the N-dimensional integral manifold of $\omega = 0$. Thus L_a of (P, Ω) is the same as L of (M, ω).

From the discussions above it is clear that the geometric structure of EIT can be formulated as a vector bundle M of dimension $(2N + 1)$ equipped with a nondegenerate 1-form $\omega = \mathrm{d}u - y_i\,\mathrm{d}x^i$, where (x, u, y) is the coordinate cover of M. The thermodynamic state space B_N is the base of M, while the fibre at $x \in B_N$ is $T^*_xB_N \times R$. The intensive thermodynamic variables $\left(T, p, -\mu_a, X_a^{(i)}\right)$ can be used to define the normal coordinates $y = \left(T^{-1}, pT^{-1}, -\mu_aT^{-1}, X_a^{(i)}T^{-1}\right) = (y_1, \ldots, y_N)$ conjugate to x. The fundamental equation of the thermodynamic system is the entropy surface $u = f(x)$, i.e., the Legendre submanifold L of M, which is tangent to the contact structure THPs at every point of L. Therefore y_i are components of the contact element to L. Alternatively if we consider the canonical projection of $M = T^*B_N \times R$ onto T^*B_N equipped with the 2-form $\Omega = \mathrm{d}y_i \wedge \mathrm{d}x^i$, then the entropy surface (or the graph space G_f in (13)) can also be viewed as a Lagrangian submanifold of (T^*B_N, Ω).

In the following section we consider symmetry transformations that preserve the laws of thermodynamics.

4. Symmetry transformations in EIT

According to the local theory of EIT, the change of dissipative energy Δq_d cannot be expressed as a function of $x = \left(e, v, c_a, \hat{\phi}_a^{(i)}\right)$ alone in B_N. From a physical point of view the semipositive definite property of Δq_d must be invariant under symmetry transformations that preserve the Pfaffian equation $\xi = 0$ in (15a) together with the integrability condition $\xi \wedge \mathrm{d}\xi = 0$;

otherwise it leads to violation of the second law. Thus we consider symmetry transformations $(x, u, y) \to (x^*, u^*, y^*)$ such that $\{\Delta q_d \geqslant 0, \xi, \xi \wedge \mathrm{d}\xi = 0\} \to \{\Delta q_d^* \geqslant 0, \xi^*, \xi^* \wedge \mathrm{d}\xi^* = 0\}$. This implies the invariance of the integral surface of the entropy function $u = f(x)$ with the contact condition $\mathrm{d}u = y_i\,\mathrm{d}x^i$. Now the second derivative matrix D^2u of the entropy function $u = f(x)$ is symmetric and nondegenerate. However, it is not positive definite. Following Ruppeiner [13] we define a pseudometric D^2u on the Legendre submanifold L by $D^2u = (\partial_i\partial_j u)\,\mathrm{d}x^i\,\mathrm{d}x^j = g_{ij}\,\mathrm{d}x^i\,\mathrm{d}x^j = \mathrm{d}x^i\,\mathrm{d}y_i = \langle \mathrm{d}x, \mathrm{d}y\rangle$, where $\mathrm{d}y_i = g_{ij}\,\mathrm{d}x^j$, and $\langle\,,\,\rangle$ denotes scalar product of vectors in R^N. We generalize these results to the contact manifold M with coordinate cover (x, u, y), and equipped with contact 1-form $\omega = \mathrm{d}u - y_i\,\mathrm{d}x^i$. Let (M^*, ω^*) be another contact manifold with coordinate cover (x^*, u^*, y^*), which is endowed with the nondegenerate contact 1-form $\omega^* = \mathrm{d}u^* - y_i^*\,\mathrm{d}(x^*)^i$. Consider the transformation $\Psi : M \to M^*$ defined by $(x, u, y) \to (x^*, u^*, y^*)$ satisfying the conditions (i) $\omega^* = \lambda\omega$, (ii) $\langle \mathrm{d}x^*, \mathrm{d}y^*\rangle = B\langle \mathrm{d}x, \mathrm{d}y\rangle$, where λ and B are functions of (x, u, y) that do not vanish on M. Since $u = f(x)$ is an integral manifold of $\omega = 0$, there exists a function g with $\mathrm{d}u^* = \mathrm{d}g = y_i^*\,\mathrm{d}(x^*)^i$ such that ω^* vanishes on the surface of g. In other words, the Legendre submanifold L of M is mapped onto the Legendre submanifold L^* of M^* under these transformations. Consequently the laws of thermodynamics as well as the pseudo-Riemannian metric $\langle \mathrm{d}x, \mathrm{d}y\rangle|_L$ are invariant. In the following discussions we further elaborate on conditions (i) and (ii) in detail.

(I) Suppose $x^* = F(x, u, y), u^* = G(x, u, y)$ and $y^* = H(x, u, y)$, where $F = (F^1, F^2, \dots, F^N)$ and $H = (H_1, H_2, \dots, H_N)$. Then

$$\omega^* = [\partial_u G - (\partial_u F^i)y_i^*]\omega + [D_j G - (D_j F^i)y_i^*]\,\mathrm{d}x^j + [\partial^j G - (\partial^j F^i)y_i^*]\,\mathrm{d}y_j. \tag{16}$$

Hence $\omega^* = \lambda\omega$ if and only if

$$\lambda = \partial_u G - (\partial_u F^i)y_i^* \tag{17a}$$

and

$$(D_j F^i)y_i^* = D_j G \tag{17b}$$

$$(\partial^j F^i)y_i^* = \partial^j G \tag{17c}$$

where $\partial^j = \frac{\partial}{\partial y_j}$, and $D_j = \partial_j + y_j\partial_u$.

On the other hand, $\langle \mathrm{d}x^*, \mathrm{d}y^*\rangle = B(x, u, y)\langle \mathrm{d}x, \mathrm{d}y\rangle$ if and only if the following conditions are satisfied [4]:

$$\langle \partial_j F, \partial_k H\rangle = 0 \qquad \langle \partial_j F, \partial_u H\rangle = 0 \tag{18a}$$

$$\langle \partial_u F, \partial_k H\rangle = 0 \qquad \langle \partial_u F, \partial_u H\rangle = 0 \qquad \langle \partial_u F, \partial^k H\rangle = 0 \tag{18b}$$

$$\langle \partial^j F, \partial^k H\rangle = 0 \qquad \langle \partial^j F, \partial_u H\rangle = 0 \tag{18c}$$

$$B(x, u, y) = \delta_{jk}[\langle \partial_j F, \partial^k H\rangle + \langle \partial^j F, \partial_k H\rangle]. \tag{18d}$$

First we note that (17*b*) and (17*c*) are complementary conditions. Second, by (18*a*)–(18*c*), both F and H are independent of u. Next we examine the conditions $\langle \partial_j F, \partial_k H\rangle = 0$ and $\langle \partial^j F, \partial^k H\rangle = 0$. For simplicity we introduce the following notation $I = \{1, 2, \dots, m\}$, $II = \{m+1, \dots, N\}$. For example, $x_I = (x^1, \dots, x^m)$, $y_{II} = (y_{m+1}, \dots, y_N)$, $F_I = (F^1, \dots, F^m)$ and $H_{II} = (H_{m+1}, \dots, H_N)$. In order to satisfy the conditions $\langle \partial_j F, \partial_k H\rangle = 0$ and $\langle \partial^j F, \partial^k H\rangle = 0$, we set

$$F = (F_I(y_I), F_{II}(x_{II})) \qquad \text{and} \qquad H = (H_I(x_I), H_{II}(y_{II})).$$

Furthermore, we assume

$$G = au + c_1 x_I^i (y_I)_i + c_2 x_{II}^j (y_{II})_j \qquad a, c_1, c_2 \in R.$$

From (17*b*) and (17*c*) we obtain the following results:

$$\sum_{i=1}^{m} \partial^j F_I^{(i)}(y_I) y_i^* = c_1 x_I^j + c_2 x_{II}^j \tag{19a}$$

$$\sum_{i=m+1}^{N} \partial_j F_{II}^{(i)}(x_{II}) y_i^* = (a + c_2)(y_{II})_j + (a + c_1)(y_I)_j. \tag{19b}$$

Equations (19*a*)–(19*b*) can be solved for y_i^* under appropriate choices of a_1, c_1 and c_2. For example, consider the linear case

$$\partial^j F_I^{(i)}(y_I) = b_{ji} \qquad b_{ji} \in R \qquad i, j \leqslant m$$

$$\partial_j F_{II}^{(i)}(x_{II}) = a_{ji} \qquad a_{ji} \in R \qquad i, j \geqslant m + 1.$$

By examining (19*a*) and (19*b*), we note that $c_2 = 0$ and $c_1 = -a$. Hence we have the following equations:

$$x^* = F(x, y) = (By_I, Ax_{II}) \tag{20a}$$

$$u^* = G(x, u, y) = au - \sum_{i=1}^{m} a x^i y_i \tag{20b}$$

$$y^* = H(x, y) = (-aB^{-1}x_I, aA^{-1}y_{II}) \tag{20c}$$

where B is an $m \times m$ nonsingular matrix with matrix elements $(B)_{ji} = b_{ji}$ and A is an $(N - m) \times (N - m)$ nonsingular matrix with matrix elements $(A)_{ji} = a_{ji}$. Finally, from (20*a*)–(20*b*) we obtain

$$\omega^* = [\partial_u G - (\partial_u F^i) y_i^*]\omega = a\omega$$

$$\langle \mathrm{d}x^*, \mathrm{d}y^* \rangle = \sum_j \{\langle \partial_j F, \partial^j H \rangle + \langle \partial^j F, \partial_j H \rangle\} \, \mathrm{d}x^j \, \mathrm{d}y_j = -a\big[\mathrm{d}x_I^i \, \mathrm{d}(y_I)_i - \mathrm{d}x_{II}^j \, \mathrm{d}(y_{II})_j\big]$$

and

$$(\omega^*)^* = a^2\omega \qquad \langle \mathrm{d}(x^*)^*, \mathrm{d}(y^*)^* \rangle = a^2 \left[\sum_{i=1}^{m} \mathrm{d}x^i \, \mathrm{d}y_i - \sum_{i=m+1}^{N} \mathrm{d}x^i \, \mathrm{d}y_i\right].$$

Set $a = -1$. Then $\langle \mathrm{d}x^*, \mathrm{d}y^* \rangle|_{L*}$ becomes a pseudo-Riemannian metric with signature $(m, N - m)$. To summarize, the following transformations,

$$x^* = F(x, y) = (By_I, \; Ax_{II}) + b \qquad b \in R^N \tag{21a}$$

$$u^* = G(x, u, y) = -u + \sum_{i=1}^{m} x^i y_i + c \qquad c \in R \tag{21b}$$

$$y^* = H(x, y) = \big(B^{-1}x_I, -A^{-1}y_{II}\big) + d \qquad d \in R^N \tag{21c}$$

preserve the contact structure as well as the pseudo-Riemannian metric in L. It is interesting to note that the Legendre involution $x^* = (y_I, x_{II})$, $u^* = -u + x_I^i (y_I)_i$ and $y^* = (x_I, -y_{II})$

is a special example of (21a)–(21c). It is well known that the Legendre involution plays an important role in ET [14]. Let $(P, \Omega = \mathrm{d}\omega)$ be the canonical projection of (M, ω). We can rewrite Ω as $\Omega = \mathrm{d}x_I^i \wedge \mathrm{d}(y_I)_i - \mathrm{d}(y_{II})_j \wedge \mathrm{d}x_{II}^j = \mathrm{d}\{x_I^i\,\mathrm{d}(y_I)_i - (y_{II})_j\,\mathrm{d}x_{II}^j\}$. Thus there exists a function $t = g(y_I, x_{II})$ such that Ω vanishes on the surface of g. We can easily check that the Lagrangian submanifold L_a of (P, Ω) is generated by the function $t = -u + x_I y_I$. Hence the Legendre involution $\{x_I, x_{II}, u, y_I, y_{II}\} \to \{y_I, x_{II}, t = -u + x_I y_I, x_I, -y_I\}$ gives rise to the Lagrangian submanifold L_a.

(II) We can relax the condition $\langle \mathrm{d}x^*, \mathrm{d}y^*\rangle = B(x, u, y)\langle \mathrm{d}x, \mathrm{d}y\rangle$ by the weaker condition $\langle \mathrm{d}x^*, \mathrm{d}y^*\rangle|_{L*} = \mu\langle \mathrm{d}x, \mathrm{d}y\rangle|_L$. Together with the requirement of the invariance of the contact structure $\omega^* = \lambda\omega$, the laws of thermodynamics and the pseudo-Riemannian metric are preserved. Hence we consider the transformations $x^* = F(x, u, y)$, $u^* = G(x, u, y)$, $y^* = H(x, u, y)$ such that $\omega^* = \lambda\omega$ and $\langle \mathrm{d}x^*, \mathrm{d}y^*\rangle_{L*} = \mu\langle \mathrm{d}x, \mathrm{d}y\rangle|_L$. Except for (18$b$) where $\langle \partial_u F, \partial^k H\rangle \neq 0$, the rest of the conditions in (17a)–(18d) remain the same. In order to simplify the notation, we set $\partial_j G = b_j(x, u, y)$, $\partial_u G = b(x, u, y)$, $\partial_j F^i = a_{ji}(x, u, y)$, $\partial_u F^i = a^i(x, u, y)$, $\partial^i F^i = b_{ji}(x, u, y)$ and $\partial^j G = c^j(x, u, y)$. Then (17$b$) and (17$c$) yield the following results:

$$b_j + by_j = \sum_i (a_{ji} + y_j a^i) y_i^* \tag{22a}$$

$$c^j = \sum_i b_{ji} y_i^*. \tag{22b}$$

Let B be a nonsingular $N \times N$ matrix with elements $(B)_{ij} = b_{ij}$. Then (22b) yields $y_i^* = (B^{-1})_{ij} c_j$. This result must be consistent with (22a). Again for simplicity we assume that G is a linear function of (x, u, y), $G(x, u, y) = bu + b_j x^j + c^j y_j, b, b_j, c^j \in R$. Now the conditions $\langle \partial^j F, \partial^k H\rangle = \langle \partial^j F, \partial_u H\rangle = 0$ imply that F is independent of y. On the other hand, the conditions $\langle \partial_j F, \partial_k H\rangle = \langle \partial_j F, \partial_u H\rangle = \langle \partial_u F, \partial_k H\rangle = \langle \partial_u F, \partial_u H\rangle = 0$ imply that H is a function of y only. Hence a_{ji} and a^i are functions of (x, u) and $b_{ji} = c^j = 0$. Therefore

$$G(x, u, y) = bu + b_j x^j \tag{23}$$

$$b_j + by_j = \sum_i [a_{ji}(x, u) + y_j a^i(x, u)] y_i^*. \tag{24}$$

Let D be a nonsingular $N \times N$ matrix with elements $(D)_{ij} = a_{ij} + y_j a^i$. Then (24) can be solved with $y_i^* = H_i(x, u, y) = (D^{-1})_{ij}(b_j + by_j)$. Since H is a function of y only, a_{ji} and a^i must be constants. Consequently, the following transformations

$$(x^*)^i = F^i(x, u) = a^i u + a_{ji} x^j + \alpha^i \tag{25a}$$

$$u^* = G(x, u, y) = bu + b_j x^j + c \tag{25b}$$

$$y_i^* = H_i(x, u, y) = (D^{-1})_{ij}(b_j + by_j) \tag{25c}$$

preserve the contact structure as well as the pseudo-Riemannian metric. Here a^i, a_{ij}, α^i, b, b_j, c are all constants.

Finally we consider two special examples of (25a)–(25c).

(i) Fix k. Let

$$a_{ij} = \begin{cases} \delta_{ij} & \text{if} \quad i \neq k \\ 0 & \text{if} \quad i = k \end{cases} \qquad a^i = \delta_{ik} \qquad b = 0 \qquad b_j = \hat{b}\delta_{jk}.$$

Then $x^* = (x^1, \ldots, x^{k-1}, u, x^{k+1}, \ldots, x^N)$, $u^* = (0, \ldots, \hat{b}x^k, 0, \ldots, 0)$ and $y^* = \left(-\hat{b}y_k^{-1}y_1, \ldots, -\hat{b}y_k^{-1}, \ldots, -\hat{b}y_k^{-1}y_N\right)$. Furthermore, we have $\omega^* = -\hat{b}y_k^{-1}\omega$, and $\langle \mathrm{d}x^*, \mathrm{d}y^* \rangle_{L*} = -\hat{b}y_k^{-1}\langle \mathrm{d}x, \mathrm{d}y \rangle|_L$. When $k = 1$, these transformations represent transitions from entropy surface to the energy surface.

(ii) The transformations in (25*a*)–(25*c*) have a special class of solutions with interesting mathematical structure. Let $a^i = 0$ for all i. Then (25*a*)–(25*c*) become

$$x^* = F(x, u) = A(x + \alpha) \qquad \alpha \in R^N$$
$$u^* = G(x, u) = bu + \langle \hat{b}, x \rangle + c \qquad \hat{b} \in R^N \quad c \in R$$
$$y^* = H(y) = A^{-1}(by + r) \qquad r \in R^N.$$

Here A is a nonsingular $N \times N$ matrix with $(A)_{ij} = a_{ij}$. These transformations are the coordinate transformations considered by Salamon *et al*.

5. Conclusion

In this paper we consider the geometric structure of EIT in the context of contact manifold from statistical point of view. This geometric structure is based on the generalized Gibbs 1-form (generalized Gibbs formula) which can be obtained from the maximum entropy principle. A simple extension of the entropy surface naturally leads to the concept of 1-jet space and its Legendre submanifold. We further elaborate on the relationship between the contact manifold (M, ω) with thermodynamic state space B_N as its base, and the associated symplectic manifold $(T^*B_N, \Omega = \mathrm{d}\omega)$. We then show that the Legendre submanifold L of M and the Lagrangian submanifold L_a of T^*B_N are intimately related to the entropy surface of the thermodynamic system. Next we generalize our previous work on symmetry transformations that preserve the thermodynamic laws as well as the pseudo-Riemannian metric in L. As a special result of these contact transformations, it can be shown that the Legendre involution gives rise to the Lagrangian submanifold L_a, the integral manifold of $\Omega = 0$. Finally we construct two special homogeneous linear coordinate transformations. The first example shows the transformation between the entropy surface and the energy surface. This transformation cannot be obtained from the work by Salamon *et al*. The second example is the coordinate transformation considered by Salamon *et al*.

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