



# Dirac Structures in Open Thermodynamics

Hiroaki Yoshimura<sup>1(✉)</sup> and François Gay-Balmaz<sup>2</sup>

<sup>1</sup> Waseda University, 3-4-1, Okubo, Shinjuku, Tokyo 169-8555, Japan  
yoshimura@waseda.jp

<sup>2</sup> Ecole Normale Supérieure, Paris, France  
francois.gay-balmaz@lmd.ens.fr

**Abstract.** Dirac structures are geometric objects that generalize Poisson structures and presymplectic structures on manifolds. They naturally appear in the formulation of constrained mechanical systems and play an essential role in the understanding of the interrelations between system elements in implicit dynamical systems. In this paper, we show how nonequilibrium thermodynamic systems can be naturally understood in the context of Dirac structures, by mainly focusing on the case of open systems, i.e., thermodynamic systems exchanging heat and matter with the exterior.

**Keywords:** Dirac structures · Open systems · Dirac dynamical systems · Nonequilibrium thermodynamics

## 1 Introduction

Nonequilibrium thermodynamics is a phenomenological theory which aims to identify and describe the relations among the observed macroscopic properties of a physical system and to determine the macroscopic dynamics of this system with the help of fundamental laws, see [15]. A novel Lagrangian variational approach for nonequilibrium thermodynamic has been proposed by the authors [4, 5] for both finite dimensional (discrete) and infinite dimensional (continuum) systems. This variational formulation was extended to the case of open systems as in [6]. The authors have also shown that, in the case of adiabatically closed systems, the variational formulation leads to an associated geometric formulation in terms of Dirac structures [7]. Recall that Dirac structures are geometric objects that extend both Poisson structures and presymplectic structures on manifolds [2]. Such structures play an essential role in formulating constrained systems such as electric circuits and nonholonomic mechanical systems (e.g., [16, 17]). On the

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other hand, for *equilibrium thermodynamics*, the geometric formulations have been mainly given by using contact geometry, see [1, 8, 9, 11–13]. In this geometric setting, the thermodynamic properties are encoded by Legendre submanifolds of the thermodynamic phase space. It was shown by [3] that a geometric formulation of irreversible processes can be made by lifting port-Hamiltonian systems to the thermodynamic phase space. The underlying geometric structure is again given in the context of contact geometry.

In this paper, we show that the equations of evolutions for an *open system* exchanging matter with the exterior can be geometrically formulated by using Dirac structures. This geometric formulation is associated to the variational formulation given in [6]. To achieve this goal, we first recall below the first and second laws as they apply to an open system. Then, we develop a general Dirac formulation for a class of systems with time-dependent nonlinear nonholonomic constraints. In particular, we introduce a time-dependent Dirac structure on the covariant Pontryagin bundle over a thermodynamic configuration manifold. Finally, we apply our Dirac formulation of systems with nonlinear time-dependent constraints to the case of open thermodynamic systems and we show that the system of evolution equations of the open system can be directly formulated as a Dirac dynamical system.

## 2 A Fundamental Setting for Open Systems

### 2.1 The First Law for Open Thermodynamic Systems

The first law of thermodynamics, following [15], asserts that for every system there exists an extensive state function, the energy, which satisfies

$$\frac{d}{dt}E = P_W^{\text{ext}} + P_H^{\text{ext}} + P_M^{\text{ext}},$$

where  $t$  denotes time,  $P_W^{\text{ext}}$  is the power associated to the work done on the system,  $P_H^{\text{ext}}$  is the power associated to the transfer of heat into the system, and  $P_M^{\text{ext}}$  is the power associated to the transfer of matter into the system. In particular, a system in which  $P_M^{\text{ext}} \neq 0$  is called *open*. For such an open system, matter can flow into or out of the system through several ports,  $a = 1, \dots, A$ . We suppose, for simplicity, that the system involves only one chemical species and denote by  $N$  the number of moles of this species. In this case, the mole balance equation is

$$\frac{d}{dt}N = \sum_{a=1}^A \mathcal{J}^a,$$

where  $\mathcal{J}^a$  is the molar flow rate *into* the system through the  $a$ -th port, so that  $\mathcal{J}^a > 0$  for flow into the system and  $\mathcal{J}^a < 0$  for flow out of the system.

As matter enters or leaves the system, it carries its internal, potential, and kinetic energy. This energy flow rate at the  $a$ -th port is the product  $E^a \mathcal{J}^a$  of the energy per mole (or molar energy)  $E^a$  and the molar flow rate  $\mathcal{J}^a$  at the  $a$ -th port. In addition, as matter enters or leaves the system it also exerts work on

the system that is associated with pushing the species into or out of the system. The associated energy flow rate is given at the  $a$ -th port by  $p^a \mathbf{V}^a \mathcal{J}^a$ , where  $p^a$  and  $\mathbf{V}^a$  are the pressure and the molar volume of the substance flowing through the  $a$ -th port. In this case, the power exchange due to the mass transfer is

$$P_M^{\text{ext}} = \sum_{a=1}^A \mathcal{J}^a (\mathbf{E}^a + p^a \mathbf{V}^a).$$

A system is called adiabatically closed if  $P_H^{\text{ext}} = P_M^{\text{ext}} = 0$ .

## 2.2 The Second Law for Open Thermodynamic Systems

Following [15], the evolution part of the second law of thermodynamics asserts that for every adiabatically closed system, there exists an extensive state function, the entropy, which satisfies

$$\frac{d}{dt} S = I \geq 0,$$

where  $I$  is the entropy production of the system. Let us deduce the expression of the entropy production in an open system of one chemical component, with constant volume and an internal energy given by  $U = U(S, N)$ . The balance of mole and the balance energy, i.e., the first law, are respectively given by

$$\frac{d}{dt} N = \sum_{a=1}^A \mathcal{J}^a, \quad \frac{d}{dt} U = \sum_{a=1}^A \mathcal{J}^a (U^a + p^a \mathbf{V}^a) = \sum_{a=1}^A \mathcal{J}^a H^a,$$

where  $H^a = U^a + p^a \mathbf{V}^a$  is the molar enthalpy at the  $a$ -th port and where  $U^a$ ,  $p^a$ , and  $\mathbf{V}^a$  are respectively the molar internal energy, the pressure and the molar volume at the  $a$ -th port, see [10, 14]. From these equations and the second law, one obtains the equations for the rate of change of the entropy of the system as

$$\frac{d}{dt} S = I + \sum_{a=1}^A S^a \mathcal{J}^a,$$

where  $S^a$  is the molar entropy at the  $a$ -th port and  $I$  is the rate of internal entropy production of the system given by

$$I = \frac{1}{T} \sum_{a=1}^A [\mathcal{J}_S^a (T^a - T) + \mathcal{J}^a (\mu^a - \mu)],$$

where  $T = \frac{\partial U}{\partial S}$  denotes the temperature and  $\mu = \frac{\partial U}{\partial N}$  the chemical potential. The entropy flow rate is given by  $\mathcal{J}_S^a := S^a \mathcal{J}^a$  and we also have the relation  $H^a = U^a + p^a \mathbf{V}^a = \mu^a + T^a S^a$ . The thermodynamic quantities known at the ports are usually the pressure and the temperature  $p^a$ ,  $T^a$ , from which the other thermodynamic quantities, such as  $\mu^a = \mu^a(p^a, T^a)$  or  $S^a = S^a(p^a, T^a)$  are deduced from the state equations of the gas.

### 3 Dirac Formulation of Time-Dependent Nonlinear Nonholonomic Systems

#### 3.1 Variational and Kinematic Time Dependent Constraints

In order to formulate an open thermodynamic system in the context of Dirac structures, we first introduce two different constraints  $C_V$  and  $C_K$  which depend explicitly on time  $t$ . For a thermodynamic configuration manifold  $\mathcal{Q}$  which is the space of the thermodynamic variables as well as the mechanical variables, we define the *extended configuration manifold* as  $Y := \mathbb{R} \times \mathcal{Q} \ni (t, x)$ , which can be seen as a trivial vector bundle  $Y = \mathbb{R} \times \mathcal{Q} \rightarrow \mathbb{R}$ ,  $(t, x) \mapsto t$ , over the space of time  $\mathbb{R}$ . Consider the vector bundle  $(\mathbb{R} \times T\mathcal{Q}) \times_Y TY \rightarrow Y$  over  $Y$ , whose vector fiber at  $y = (t, x)$  is given by  $T_x\mathcal{Q} \times T_{(t,x)}Y = T_x\mathcal{Q} \times (\mathbb{R} \times T_x\mathcal{Q})$ . An element in the fiber at  $(t, x)$  is denoted  $(v, \delta t, \delta x)$ . In general, by definition a *variational constraint* is a subset  $C_V \subset (\mathbb{R} \times T\mathcal{Q}) \times_Y TY$ , such that  $C_V(t, x, v)$ , defined by  $C_V(t, x, v) := C_V \cap (\{(t, x, v)\} \times T_{(t,x)}Y)$ , is a vector subspace of  $T_{(t,x)}Y$ , for all  $(t, x, v) \in \mathbb{R} \times T\mathcal{Q}$ . In general, a *kinematic constraint* is a submanifold  $C_K \subset TY$ . More concretely, given functions  $A^r : \mathbb{R} \times T\mathcal{Q} \rightarrow T^*\mathcal{Q}$  and  $B^r : \mathbb{R} \times T\mathcal{Q} \rightarrow \mathbb{R}$ ,  $r = 1, \dots, m$ , the variational constraint  $C_V$  is given by

$$C_V = \left\{ (t, x, v, \delta t, \delta x) \in (\mathbb{R} \times T\mathcal{Q}) \times_Y TY \mid \right. \\ \left. A_i^r(t, x, v)\delta x^i + B^r(t, x, v)\delta t = 0, r = 1, \dots, m \right\} \tag{1}$$

and the associated kinematic constraint  $C_K$  of thermodynamic type is

$$C_K = \left\{ (t, x, \dot{t}, \dot{x}) \in TY \mid A_i^r(t, x, \dot{x})\dot{x}^i + B^r(t, x, \dot{x})\dot{t} = 0, r = 1, \dots, m \right\}. \tag{2}$$

We will see later how  $C_V$  and  $C_K$  are concretely given in thermodynamics.

#### 3.2 Covariant Pontryagin Bundles and the Generalized Energy

Associated to the extended configuration manifold  $Y = \mathbb{R} \times \mathcal{Q}$  for the time-dependent system, we define the *covariant Pontryagin bundle* by

$$\pi_{(\mathcal{P}, Y)} : \mathcal{P} = (\mathbb{R} \times T\mathcal{Q}) \times_Y T^*Y = (\mathbb{R} \times T\mathcal{Q}) \times_{\mathbb{R} \times \mathcal{Q}} T^*(\mathbb{R} \times \mathcal{Q}) \rightarrow Y = \mathbb{R} \times \mathcal{Q}.$$

An element in the fiber at  $(t, x)$  is denoted  $(v, \mathbf{p}, p)$ . Given the Lagrangian  $\mathcal{L} : \mathbb{R} \times T\mathcal{Q} \rightarrow \mathbb{R}$ , the *covariant generalized energy* is defined on  $\mathcal{P}$  as

$$\mathcal{E} : \mathcal{P} \rightarrow \mathbb{R}, \quad \mathcal{E}(t, x, v, \mathbf{p}, p) = \mathbf{p} + \langle p, v \rangle - \mathcal{L}(t, x, v). \tag{3}$$

#### 3.3 Dirac Structures on the Covariant Pontryagin Bundle

Given a variational constraint  $C_V \subset (\mathbb{R} \times T\mathcal{Q}) \times_Y TY$ , we consider the distribution  $\Delta_{\mathcal{P}}$  on the covariant Pontryagin bundle defined by

$$\Delta_{\mathcal{P}}(t, x, v, \mathbf{p}, p) := \left( T_{(t, x, v, \mathbf{p}, p)}\pi_{(\mathcal{P}, Y)} \right)^{-1}(C_V(t, x, v)) \subset T_{(t, x, v, \mathbf{p}, p)}\mathcal{P}.$$

From the expression of  $C_V$  in (1), we get

$$\Delta_{\mathcal{P}}(t, x, v, \mathbf{p}, p) = \{(\delta t, \delta x, \delta v, \delta \mathbf{p}, \delta p) \in T\mathcal{P} \mid A_i^r(t, x, v)\delta x^i + B^r(t, x, v)\delta t = 0, r = 1, \dots, m\}. \tag{4}$$

Consider the canonical symplectic form on  $T^*Y$  given by  $\Omega_{T^*Y} = -\mathbf{d}\Theta_{T^*Y}$ , where  $\Theta_{T^*Y}$  is the canonical one-form on  $T^*Y$ . In local coordinates, we have  $\Theta_{T^*Y} = p_i dx^i + \mathbf{p}dt$  and  $\Omega_{T^*Y} = dx^i \wedge dp_i + dt \wedge d\mathbf{p}$ . Using the projection  $\pi_{(\mathcal{P}, T^*Y)} : \mathcal{P} \rightarrow T^*Y, (t, x, v, \mathbf{p}, p) \mapsto (t, x, \mathbf{p}, p)$  onto  $T^*Y$ , we get the presymplectic form on the covariant Pontryagin bundle given by  $\Omega_{\mathcal{P}} = \pi_{(\mathcal{P}, T^*Y)}^* \Omega_{T^*Y}$ . The local expression is given by  $\Omega_{\mathcal{P}} = dx^i \wedge dp_i + dt \wedge d\mathbf{p}$ .

Given the distribution  $\Delta_{\mathcal{P}}$  in (4) and the presymplectic form  $\Omega_{\mathcal{P}}$ , the Dirac structure  $D_{\Delta_{\mathcal{P}}}$  on  $\mathcal{P}$  is given by

$$D_{\Delta_{\mathcal{P}}}(x) = \{(\mathbf{u}_x, \mathbf{a}_x) \in T_x\mathcal{P} \times T_x^*\mathcal{P} \mid \mathbf{u}_x \in \Delta_{\mathcal{P}}(x), \langle \mathbf{a}_x, \mathbf{v}_x \rangle = \Omega_{\mathcal{P}}(x)(\mathbf{u}_x, \mathbf{v}_x), \forall \mathbf{v}_x \in \Delta_{\mathcal{P}}(x)\}, \tag{5}$$

for all  $x \in \mathcal{P}$ .

### 3.4 Dirac Dynamical Systems

Using the Dirac structure  $D_{\Delta_{\mathcal{P}}}$  on  $\mathcal{P}$  in (5), we can define a Dirac dynamical system for a curve  $x(t)$  in  $\mathcal{P}$  as follows:

$$(\dot{x}, \mathbf{d}\mathcal{E}(x)) \in D_{\Delta_{\mathcal{P}}}(x). \tag{6}$$

Equivalently, condition (6) gives the equations of motion

$$\mathbf{i}_{\dot{x}}\Omega_{\mathcal{P}} - \mathbf{d}\mathcal{E}(x) \in \Delta_{\mathcal{P}}(x)^\circ, \quad \dot{x} \in \Delta_{\mathcal{P}}(x). \tag{7}$$

Using coordinates, we can now explicitly express these equations as follows. The differential of  $\mathcal{E}$  is given by

$$\mathbf{d}\mathcal{E}(t, x, v, \mathbf{p}, p) = \left( -\frac{\partial \mathcal{L}}{\partial t}, -\frac{\partial \mathcal{L}}{\partial x}, p - \frac{\partial \mathcal{L}}{\partial v}, 1, v \right)$$

and the tangent vector  $\dot{x}$  to  $T_{x(t)}\mathcal{P}$  is given by  $(t, x, \dot{t}, \dot{x})$ . We deduce that the Dirac dynamical system (7) gives the following conditions on the curve  $x(t) \in \mathcal{P}$ ,

$$\begin{aligned} \dot{x} = v, \quad \dot{t} = 1, \quad p = \frac{\partial \mathcal{L}}{\partial v}, \\ (t, x, \dot{t}, \dot{x}) \in C_V(t, x, v), \quad \left( \dot{\mathbf{p}} - \frac{\partial \mathcal{L}}{\partial t}, \dot{p} - \frac{\partial \mathcal{L}}{\partial x} \right) \in C_V(t, x, v)^\circ. \end{aligned} \tag{8}$$

In local expressions, these evolution Eq. (8) read

$$\begin{cases} \dot{x}^i = v^i, & \dot{t} = 1, & p_i - \frac{\partial \mathcal{L}}{\partial v^i} = 0, & A_i^r(t, x, v)q^i + B^r(t, x, v) = 0, \\ \dot{p}_i - \frac{\partial \mathcal{L}}{\partial x^i} = \lambda_r A_i^r(t, x, v), & \dot{p} - \frac{\partial \mathcal{L}}{\partial t} = \lambda_r B^r(t, x, v). \end{cases} \tag{9}$$

### 3.5 Energy Balance Equations

One immediately notices that the covariant generalized energy  $\mathcal{E}(t, x, v, \mathbf{p}, p)$  defined in (3) is preserved along the solution curve  $\mathbf{x}(t) = (t, x(t), v(t), \mathbf{p}(t), p(t))$  of the Dirac dynamical system (9),

$$\frac{d}{dt}\mathcal{E}(t, x, v, \mathbf{p}, p) = 0. \tag{10}$$

Note that  $\mathcal{E}$  does not represent the total energy of the system. The total energy is represented by the generalized energy  $E : \mathbb{R} \times T\mathcal{Q} \times T^*\mathcal{Q} \rightarrow \mathbb{R}$  defined as

$$E(t, x, v, p) = \langle p, v \rangle - \mathcal{L}(t, x, v)$$

and Eq. (10) yields

$$\frac{d}{dt}E(t, x, v, p) = -\frac{d}{dt}\mathbf{p} = \frac{\partial \mathcal{L}}{\partial t}(t, x, v) - \lambda_r B^r(t, x, v).$$

This is the *balance of energy* for the Dirac system. Note that  $\frac{d}{dt}\mathbf{p}$  is interpreted as the power flowing out of the system. The first term on the right hand side is essentially due to the explicit dependence of the Lagrangian on time. The second term is due to the affine character of the constraint and will be interpreted later as the energy flowing in or out of the systems through its ports.

## 4 Dirac Formulation of Open Thermodynamics

### 4.1 Geometric Setting

Consider a simple open finite dimensional system with a single entropy  $S$  and a single chemical species with number of moles  $N$  in a single compartment. The system has a constant volume  $V = V_0$ , it has  $A$  external ports, through which matter can flow into or out of the system as well as  $B$  ports, through which heat can flow in or out of the system. Let  $U(S, N)$  be the internal energy of the system. Let  $\mathcal{J}^a(t), \mathcal{S}^a(t), T^a(t), \mu^a(t)$  be given functions of time associated to the external flow of matter into the system through the  $a$ -port and define  $\mathcal{J}_S^a(t) = \mathcal{J}^a(t)\mathcal{S}^a(t)$ . We assume that there exist external heat sources at the  $b$ -port with entropy flow rate  $\mathcal{J}^b(t)$ , molar entropy  $S^b(t)$  and temperature  $T^b(t)$ .

The thermodynamic configuration space is  $\mathcal{Q} = \mathbb{R}^5 \ni x = (S, N, \Gamma, W, \Sigma)$ , with  $\Gamma, W, \Sigma$  the thermodynamic displacements, see [6]. As in Sect. 3.1, let  $Y = \mathbb{R} \times \mathcal{Q}$  be the trivial bundle over  $\mathbb{R}$  and consider the thermodynamic phase space  $\mathbb{R} \times T\mathcal{Q}$  over  $Y$  with coordinates  $(t, x, v) \in \mathbb{R} \times T\mathcal{Q}$ , where  $v = (v_S, v_N, v_\Gamma, v_W, v_\Sigma) \in T_q\mathcal{Q}$ . Let us employ the local coordinates for  $(t, x, \delta t, \delta x) \in TY$  and  $(t, x, \mathbf{p}, p) \in T^*Y$ , where  $\delta x = (\delta S, \delta N, \delta \Gamma, \delta W, \delta \Sigma) \in T_q\mathcal{Q}$  and  $p = (p_S, p_N, p_\Gamma, p_W, p_\Sigma) \in T_x^*\mathcal{Q}$ .

## 4.2 Nonholonomic Constraints in Thermodynamics

For open thermodynamic systems, the constraint (1) reads

$$C_V = \left\{ (t, x, v, \delta t, \delta x) \in (\mathbb{R} \times TQ) \times_Y TY \mid \right. \\ \left. - \frac{\partial U}{\partial S} \delta \Sigma = \sum_{a=1}^A [\mathcal{J}^a \delta W + \mathcal{J}_S^a \delta \Gamma - (\mu^a \mathcal{J}^a + T^a \mathcal{J}_S^a) \delta t] + \sum_{b=1}^B \mathcal{J}_S^b (\delta \Gamma - T^b \delta t) \right\}.$$

Hence the nonlinear kinematic constraint (2) becomes

$$C_K = \left\{ (t, x, \dot{t}, \dot{x}) \in TY \mid \right. \\ \left. - \frac{\partial U}{\partial S} \dot{\Sigma} = \sum_{a=1}^A [\mathcal{J}^a \dot{W} + \mathcal{J}_S^a \dot{\Gamma} - (\mu^a \mathcal{J}^a + T^a \mathcal{J}_S^a) \dot{t}] + \sum_{b=1}^B \mathcal{J}_S^b (\dot{\Gamma} - T^b \dot{t}) \right\},$$

where we have denoted  $\dot{x} = (\dot{S}, \dot{N}, \dot{\Gamma}, \dot{W}, \dot{\Sigma})$ .

## 4.3 Dirac Structures on $\mathcal{P}$ for Open Thermodynamic Systems

As in Sect. 3.2, let  $\mathcal{P} = (\mathbb{R} \times TQ) \times_Y T^*Y$  be the covariant Pontryagin bundle over  $Y$ , whose coordinates are given by  $x = (t, x, v, \mathbf{p}, p) \in \mathcal{P}$ . The canonical one form  $\Theta_{T^*Y}$  and the canonical symplectic form  $\Omega_{T^*Y} = -\mathbf{d}\Theta_{T^*Y}$  are expressed as

$$\Theta_{T^*Y} = p_i dx^i + \mathbf{p} dt \\ = p_S dS + p_N dN + p_\Gamma d\Gamma + p_W dW + p_\Sigma d\Sigma + \mathbf{p} dt,$$

$$\Omega_{T^*Y} = dx^i \wedge dp_i + dt \wedge dp \\ = dS \wedge dp_S + dW \wedge dp_W + dN \wedge dp_N + d\Gamma \wedge dp_\Gamma + d\Sigma \wedge dp_\Sigma + dt \wedge dp.$$

Recall that the presymplectic form on  $\mathcal{P}$  is defined by  $\Omega_{\mathcal{P}} = \pi_{(\mathcal{P}, T^*Y)}^* \Omega_{T^*Y}$ .

Associated with  $\mathcal{P}$ , we have the natural projection  $\pi_{(\mathcal{P}, Y)} : \mathcal{P} \rightarrow Y$ , given by  $(t, x, v, \mathbf{p}, p) \mapsto (t, x)$ , and we can lift the constraint subspace  $C_V(t, x, v) \subset TY$  to get the constraint distribution  $\Delta_{\mathcal{P}}$  on  $\mathcal{P}$  defined as

$$\Delta_{\mathcal{P}} = (T\pi_{(\mathcal{P}, Y)})^{-1}(C_V(t, x, v)) \subset T\mathcal{P}.$$

As shown in (5), from the distribution  $\Delta_{\mathcal{P}}$  and the presymplectic form  $\Omega_{\mathcal{P}}$ , we can define the induced Dirac structure  $D_{\Delta_{\mathcal{P}}} \subset T\mathcal{P} \oplus T^*\mathcal{P}$  on  $\mathcal{P}$ .

## 4.4 Dirac Thermodynamic Systems on $\mathcal{P} = (\mathbb{R} \times TQ) \times_Y T^*Y$

For each  $x = (t, x, v, \mathbf{p}, p) \in \mathcal{P}$ , we write the vector and the covector in (5) as

$$u_x = (\dot{t}, \dot{x}, \dot{v}, \dot{\mathbf{p}}, \dot{p}) \in T_x\mathcal{P} \quad \text{and} \quad \alpha_x = (\pi, \alpha, \beta, u, w) \in T_x^*\mathcal{P},$$

where  $\dot{v} = (\dot{v}_S, \dot{v}_N, \dot{v}_\Gamma, \dot{v}_W, \dot{v}_\Sigma), \dot{p} = (\dot{p}_S, \dot{p}_N, \dot{p}_\Gamma, \dot{p}_W, \dot{p}_\Sigma), \alpha = (\alpha_S, \alpha_N, \alpha_\Gamma, \alpha_W, \alpha_\Sigma), \beta = (\beta_S, \beta_N, \beta_\Gamma, \beta_W, \beta_\Sigma),$  and  $w = (w_S, w_N, w_\Gamma, w_W, w_\Sigma).$  From (6) the Dirac system reads

$$((\dot{t}, \dot{x}, \dot{v}, \dot{p}, \dot{p}), (\pi, \alpha, \beta, u, w)) \in D_{\Delta_{\mathcal{P}}}(t, x, v, \mathbf{p}, p).$$

Using the definition of the Dirac structure in terms of  $C_V,$  we get

$$\dot{x} = w, \quad \dot{t} = u, \quad \beta = 0, \quad (t, x, \dot{t}, \dot{x}) \in C_V(t, x, v), \quad (\dot{p} + \pi, \dot{p} + \alpha) \in C_V(t, x, v)^\circ.$$

Following [6], the Lagrangian is given by  $\mathcal{L}(t, x, v) = -U(S, N) + v_W N + v_\Gamma(S - \Sigma).$  The covariant generalized energy is here given by

$$\begin{aligned} \mathcal{E}(t, x, v, \mathbf{p}, p) &= \mathbf{p} + \langle p, v \rangle - \mathcal{L}(t, x, v) \\ &= \mathbf{p} + p_S v_S + p_N v_N + (p_\Gamma + \Sigma - S)v_\Gamma + (p_W - N)v_W + p_\Sigma v_\Sigma + U(S, N). \end{aligned}$$

The differential of  $\mathbf{d}\mathcal{E}$  is obtained as

$$\mathbf{d}\mathcal{E}(t, x, v, \mathbf{p}, p) = \left( -\frac{\partial \mathcal{L}}{\partial t}, -\frac{\partial \mathcal{L}}{\partial x}, p - \frac{\partial \mathcal{L}}{\partial v}, 1, v \right) = (\pi, \alpha, \beta, \gamma, w),$$

where  $\pi = -\frac{\partial \mathcal{L}}{\partial t} = 0, \alpha = -\frac{\partial \mathcal{L}}{\partial x} = (-v_\Gamma + \frac{\partial U}{\partial S}, -v_W + \frac{\partial U}{\partial N}, 0, 0, v_\Gamma), \beta = p - \frac{\partial \mathcal{L}}{\partial v} = (p_S, p_N, p_\Gamma + \Sigma - S, p_W - N, p_\Sigma), w = v = (v_S, v_N, v_\Gamma, v_W, v_\Sigma).$

By using this, the Dirac dynamical system

$$((\dot{t}, \dot{q}, \dot{v}, \dot{p}, \dot{p}), \mathbf{d}\mathcal{E}(t, q, v, \mathbf{p}, p)) \in D_{\Delta_{\mathcal{P}}}(t, q, v, \mathbf{p}, p)$$

is equivalent to the following evolution equations:

$$\left\{ \begin{aligned} \dot{p} &= -\sum_{a=1}^A (\mu^a \mathcal{J}^a + T^a \mathcal{J}_S^a) - \sum_{b=1}^B \mathcal{J}_S^b T^b, & \dot{I} &= \frac{\partial U}{\partial S}, & \dot{W} &= \frac{\partial U}{\partial N}, \\ \dot{t} &= 1, & \dot{N} &= \sum_{a=1}^A \mathcal{J}^a, & \dot{S} &= \dot{S} + \sum_{a=1}^A \mathcal{J}_S^a + \sum_{b=1}^B \mathcal{J}_S^b, \\ -\frac{\partial U}{\partial S} \dot{S} &= \sum_{a=1}^A [\mathcal{J}^a (\dot{W} - \mu^a) + \mathcal{J}_S^a (\dot{I} - T^a)] + \sum_{b=1}^B \mathcal{J}_S^b (\dot{I} - T^b). \end{aligned} \right.$$

Making arrangements, this system yields the equations of evolution as

$$\left\{ \begin{aligned} \dot{N} &= \sum_{a=1}^A \mathcal{J}^a, \\ \dot{S} &= I + \sum_{a=1}^A \mathcal{J}_S^a + \sum_{b=1}^B \mathcal{J}_S^b = \frac{d_i S}{dt} + \frac{d_e S}{dt}, \end{aligned} \right. \tag{11}$$

where  $I = \frac{1}{T} \sum_{a=1}^A [\mathcal{J}^a (\mu^a - \mu) + \mathcal{J}_S^a (T^a - T)] + \frac{1}{T} \sum_{b=1}^B \mathcal{J}_S^b (T^b - T)$  and  $\frac{d_i S}{dt} := I \geq 0$  denotes the internal entropy production due to the mixing of matter



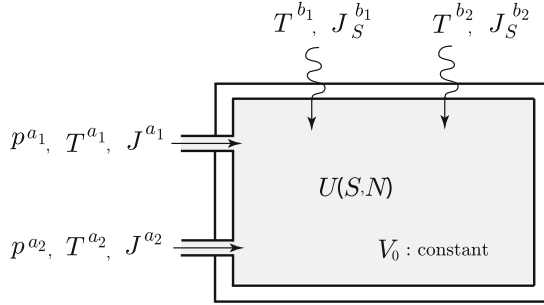
flowing into the system and  $\frac{d_e S}{dt}$  is the entropy flow. The system of equation also gives the definition of the thermodynamic displacement as  $\dot{I} = T$ ,  $\dot{W} = \mu$ , and  $\dot{\Sigma} = I$ . The momentum  $\mathbf{p}$  represents the part of the energy associated to the interaction of the system with exterior through its ports. In fact, it follows

$$-\frac{d}{dt}E = \frac{d}{dt}\mathbf{p} = -\sum_{a=1}^A (\mathcal{J}^a \mu^a + \mathcal{J}_S^a T^a) - \sum_{b=1}^B \mathcal{J}_S^b T^b = -P_M^{\text{ext}} - P_H^{\text{ext}},$$

where  $E$  is the total energy of the system, defined by

$$E(t, x, v) = \frac{\partial \mathcal{L}}{\partial v^i} v^i - \mathcal{L}(t, x, v).$$

**Example: A Piston Device with Ports and Heat Sources.** As illustrated in Fig. 1, we consider an open chamber containing a species with internal energy  $U(S, N)$ , where we assume that the cylinder has two external heat sources with entropy flow rates  $\mathcal{J}^{b_i}$ ,  $i = 1, 2$ , the volume of the chamber is constant  $V_0$  and two ports through which the species is injected into or flows out of the cylinder with molar flow rates  $\mathcal{J}^{a_i}$ ,  $i = 1, 2$ . The entropy flow rates at the ports are given by  $\mathcal{J}_S^{a_i} = \mathcal{J}^{a_i} S^{a_i}$ .



**Fig. 1.** An open chamber with ports and heat sources.

Recall that the Lagrangian is given by

$$\mathcal{L}(t, x, v) = -U(S, N) + v_W N + v_I (S - \Sigma).$$

The equations of evolution of the Dirac open thermodynamic system (11) read

$$\dot{N} = \sum_{a=1}^A \mathcal{J}^a, \quad \dot{S} = I + \sum_{i=1}^2 \mathcal{J}_S^{a_i} + \sum_{j=1}^2 \mathcal{J}_S^{b_j},$$

where  $I = \dot{\Sigma}$  is the internal entropy production given by

$$I = \frac{1}{T} \sum_{i=1}^2 [(\mu^{a_i} - \mu) + S^{a_i} (T^{a_i} - T)] \mathcal{J}^{a_i} + \frac{1}{T} \sum_{j=1}^2 \mathcal{J}_S^{b_j} (T^{b_j} - T).$$

The first term represents the entropy production associated to the mixing of gas flowing into the cylinder at the two ports  $a_1$ ,  $a_2$ , and the third term denotes the entropy production due to the external heating. The second law requires that each of these terms is positive. The first law, i.e., the energy balance holds as

$$\frac{d}{dt}E = \underbrace{\sum_{j=1}^2 \mathcal{J}_S^{b_j} T^{b_j}}_{=P_H^{\text{ext}}} + \underbrace{\sum_{i=1}^2 (\mathcal{J}^{a_i} \mu^{a_i} + \mathcal{J}_S^{a_i} T^{a_i})}_{=P_M^{\text{ext}}}.$$

## References

1. Carathéodory, C.: Untersuchungen über die Grundlagen der Thermodynamik. *Math. Ann.* **67**, 355–386 (1909)
2. Courant, T.J.: Dirac manifolds. *Trans. Am. Math. Soc.* **319**, 631–661 (1990)
3. Eberard, D., Maschke, B.M., van der Schaft, A.J.: An extension of Hamiltonian systems to the thermodynamic phase space: towards a geometry of nonreversible processes. *Rep. Math. Phys.* **60**(2), 175–198 (2007)
4. Gay-Balmaz, F., Yoshimura, H.: A Lagrangian variational formulation for nonequilibrium thermodynamics. Part I: discrete systems. *J. Geom. Phys.* **111**, 169–193 (2017a)
5. Gay-Balmaz, F., Yoshimura, H.: A Lagrangian variational formulation for nonequilibrium thermodynamics. Part II: continuum systems. *J. Geom. Phys.* **111**, 194–212 (2017b)
6. Gay-Balmaz, F., Yoshimura, H.: A variational formulation of nonequilibrium thermodynamics for discrete open systems with mass and heat transfer. *Entropy* **20**(3), 1–26 (2018a). <https://doi.org/10.3390/e20030163>
7. Gay-Balmaz, F., Yoshimura, H.: Dirac structures in nonequilibrium thermodynamics. *J. Math. Phys.* **59**, 012701–29 (2018b)
8. Gibbs, J.W.: Graphical methods in the thermodynamics of fluids. *Trans. Connecticut Acad.* **2**, 309–342 (1873)
9. Hermann, R.: *Geometry, Physics and Systems*. Dekker, New York (1973)
10. Klein, S., Nellis, G.: *Thermodynamics*. Cambridge University Press, Cambridge (2011)
11. Mrugala, R.: Geometrical formulation of equilibrium phenomenological thermodynamics. *Rep. Math. Phys.* **14**, 419–427 (1978)
12. Mrugala, R.: A new representation of thermodynamic phase space. *Bull. Polish Acad. Sci.* **28**, 13–18 (1980)
13. Mrugala, R., Nulton, J.D., Schon, J.C., Salamon, P.: Contact structure in thermodynamic theory. *Rep. Math. Phys.* **29**, 109–121 (1991)
14. Sandler, S.I.: *Chemical, Biochemical, and Engineering Thermodynamics*. Wiley, Hoboken (2006)
15. Stueckelberg, E.C.G., Scheurer, P.B.: *Thermocinétique Phénoménologique Galiléenne*. Birkhäuser (1974)
16. Yoshimura, H., Marsden, J.E.: Dirac structures in Lagrangian mechanics. Part I: Implicit Lagrangian systems. *J. Geom. Phys.* **57**, 133–156 (2006a)
17. Yoshimura, H., Marsden, J.E.: Dirac structures in Lagrangian mechanics. Part II: Variational structures. *J. Geom. Phys.* **57**, 209–250 (2006b)