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► To cite this version:

Judy Najnudel, Thomas H  lie, David Roze, R  my Muller. From statistical physics to macroscopic port-Hamiltonian Systems: A roadmap. 7th IFAC Workshop on Lagrangian and Hamiltonian Methods for Nonlinear Control, Oct 2021, Berlin, Germany. <10.1016/j.ifacol.2021.11.057>. <hal-03327546>

HAL Id: hal-03327546

<https://hal.science/hal-03327546v1>

Submitted on 4 Oct 2021

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From statistical physics to macroscopic port-Hamiltonian Systems: A roadmap

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Abstract This paper addresses the power-balanced modeling of physical systems with numerous degrees of freedom. The proposed approach combines statistical physics and port-Hamiltonian formulation, to produce macroscopic power balanced systems with reduced complexity. Thermodynamic variables are explicitly taken into account in the modeling to ensure thermodynamic consistency. The method is illustrated on two applications: an ideal gas in a thermostat, and a ferromagnet in a thermostat.

Keywords: physical modeling; statistical physics; thermodynamics; port-Hamiltonian systems

1. INTRODUCTION

Physical modeling is concerned with the representation of a system governed by laws of physics. An accurate physical model provides insight into the system's behavior, beyond the conditions available to the experimenter.

Several physical modeling techniques have been developed over the years: see e.g. Ersal et al. (2008) for an overview. In this paper, we consider in particular the state-space form known as port-Hamiltonian systems (PHS) introduced in Maschke et al. (1992); van der Schaft et al. (2014). PHS are multi-physical (that is, mechanical, electrical, thermal ... or a combination as well), and modular (a power-conserving or dissipative interconnection assembly of PHS is still a PHS). Most importantly, the PH formalism structurally fulfills the physical power balance. Moreover, numerical methods that preserve this guarantee in the discrete-time domain are available for simulations: Falaize and H  lie (2016). Nevertheless, simulating PHS with numerous degrees of freedom can prove an issue, as it involves very large matrices.

On the other hand, statistical physics is especially designed to describe complex systems with a reduced number of variables. From a collection of interacting elementary particles subject to constraints, statistical physics predicts macroscopic thermodynamic phenomena, such as entropy creation and phase transitions: Stowe (2007); Landsberg (2014).

While thermodynamics has been broadly studied in the context of PHS modeling in e.g. Eberard and Maschke (2004); Eberard et al. (2007); Ramirez et al. (2013); Delvenne and Sandberg (2014); van der Schaft (2020), the proper derivation of thermodynamic variables through statistical physics is seldomly addressed. In this paper, we combine the two approaches and propose a series of steps to systematically construct a simplified yet physically-based, structured macroscopic PHS, from a complex system described by statistical physics.

This paper is structured as follows. Section 2 presents the key principles behind statistical physics, and details the derivation of a macroscopic PHS from a stochastic description. Section 3 applies the method to two illustrative examples: an ideal gas, and a ferromagnet. Finally, section 4 gives some conclusions and perspectives.

2. THEORETICAL FRAMEWORK

2.1 Micro-state of a system

Consider a system composed of particles of matter occupying a volume. Denote \mathbb{M} the set of all possible configurations of all (or subsets of) countable particles for all volume values. A particular configuration $\mathbf{m} \in \mathbb{M}$ is called a *micro-state* of a system. For instance, each micro-state of a gas can be described in classical mechanics by a particular set of positions and momenta.

Each micro-state is mapped to a number of particles, a volume, and an energy, corresponding to the following functions:

$$\begin{aligned} \mathcal{N} : \mathbb{M} &\mapsto \mathbb{N}^* \\ \mathbf{m} &\mapsto \mathcal{N}(\mathbf{m}) \quad \text{micro-state number of particles,} \\ \mathcal{V} : \mathbb{M} &\mapsto \mathbb{R}^{+*} \\ \mathbf{m} &\mapsto \mathcal{V}(\mathbf{m}) \quad \text{micro-state volume,} \\ \mathcal{E} : \mathbb{M} &\mapsto \mathbb{R} \\ \mathbf{m} &\mapsto \mathcal{E}(\mathbf{m}) \quad \text{micro-state energy,} \end{aligned} \tag{1}$$

where the energy function \mathcal{E} is assumed to have an inferior bound, i.e., $\mathcal{E}(\mathbf{m}) \geq c$ for some $c \in \mathbb{R}$.

2.2 Accessible micro-states under constraints

According to experimental conditions, any quantity $\varphi \in \mathbb{F} = \{\mathcal{N}, \mathcal{V}\}$ can be fixed while \mathcal{E} and the remaining unfixed quantities in \mathbb{F} are left free to fluctuate¹. In this

¹ Note that \mathbb{F} is susceptible to contain other functions, depending on the physics (electric, magnetic, etc) of the considered system.

case, the experimental constraints determine the set of *accessible* micro-states \mathbb{M}_a . For instance, a *closed* system (no exchange of particles with the environment) has a fixed $\mathcal{N}(\mathbf{m}) = \mathcal{N}_0 \forall \mathbf{m}$, while \mathcal{V} and \mathcal{E} can fluctuate. However these fluctuations are coupled through the quantity $\mathcal{E}(\mathbf{m}) + P_0 \mathcal{V}(\mathbf{m})$, where P_0 is the (constant) external pressure². Similarly, an *isochoric* system has a fixed volume $\mathcal{V}(\mathbf{m}) = \mathcal{V}_0$, and the fluctuations of \mathcal{N} and \mathcal{E} are coupled through the quantity $\mathcal{E}(\mathbf{m}) - \mu_0 \mathcal{N}(\mathbf{m})$, where μ_0 is the (constant) external chemical potential. Denote $\mathbb{Q} = \{\mathcal{E}, \mathcal{E} + P_0 \mathcal{V}, \mathcal{E} - \mu_0 \mathcal{N}, \mathcal{E} + P_0 \mathcal{V} - \mu_0 \mathcal{N}\}$. If the system is thermally insulated, the constraint on $\Psi \in \mathbb{Q}$ is $\Psi(\mathbf{m}) = \Psi_0$ with a given $\Psi_0 \in \mathbb{R}$, hence :

$$\mathbb{M}_a = \{\mathbf{m} \in \mathbb{M} \mid \Psi(\mathbf{m}) = \Psi_0\}. \quad (2)$$

The case of a system in thermal contact with its environment is addressed in section 2.4.

2.3 Stochastic modeling and measure of uncertainty

The system may be in any accessible micro-state, and goes randomly from one accessible micro-state to another. As it is not possible to predict these fluctuations in a deterministic fashion, statistical physics adopts a stochastic description. This description assigns to each micro-state \mathbf{m} a probability $p(\mathbf{m})$ to be the actual state of the system.

Given a probability distribution p , a measure of the uncertainty on the fluctuating micro-state is the statistical entropy Gray (2011), defined as (for a discrete distribution³):

$$S : p \mapsto -k \sum_{\mathbf{m} \in \mathbb{M}_a} p(\mathbf{m}) \ln p(\mathbf{m}), \quad (3)$$

where k is a positive constant. The entropy is indeed a measure of lack of information. For instance, a probability distribution assigning 1 to some micro-state \mathbf{m}_0 and 0 to all others would mean that the system is in the micro-state \mathbf{m}_0 for certain. From (3), the system entropy would be zero for such a distribution. Conversely, an equiprobable distribution between all micro-states would maximize the uncertainty for an observer, as well as the entropy.

The entropy is a positive quantity, since $0 \leq p(\mathbf{m}) \leq 1 \forall \mathbf{m}$. Moreover, the total entropy of two independent systems is the sum of their entropies, since $p(\mathbf{m}, \mathbf{m}') = p(\mathbf{m})p(\mathbf{m}')$. It follows that the entropy is an extensive quantity.

2.4 Principle of maximum entropy at thermodynamic equilibrium

Thermodynamic equilibrium is reached when the constraints on the system are met. At that point, the system stops evolving and provides a minimal amount of information. Therefore, at equilibrium, the micro-state probability distribution maximizes the statistical entropy, given the constraints on the system. Moreover, at thermodynamic equilibrium, statistical physics assumes the *ergodic hypothesis* (see e.g. Patrascioiu (1987) for a discussion about its validity; here we will admit it as a working hypothesis).

² The derivation of such coupling quantities is not detailed here. However, they are listed in Table 1, see also Graben and Ray (1991).

³ It is similarly defined for a continuous distribution: the sum is replaced with an integral.

This hypothesis states that at equilibrium, the system visits all accessible micro-states, given a sufficiently long period of time. As a result, the temporal mean $\bar{\Psi}$ of a fluctuating quantity $\Psi \in \mathbb{Q}$ coincides with its expectation:

$$\mathbb{E}[\Psi] := \sum_{\mathbf{m} \in \mathbb{M}_a} p(\mathbf{m}) \Psi(\mathbf{m}) = \bar{\Psi}. \quad (4)$$

It follows that the micro-state probability distribution at equilibrium p^* is:

$$p^* = \arg \max_p S(p) \quad \text{subject to} \quad \begin{cases} \mathbb{E}[\Psi] = \bar{\Psi} \\ \sum_{\mathbf{m} \in \mathbb{M}_a} p(\mathbf{m}) = 1 \end{cases} \quad (5)$$

In the following, the constant k in (3) is taken as the Boltzmann constant $k_b = 1.38 \times 10^{-23} \text{ J.K}^{-1}$. This ensures that the statistical entropy coincides with the thermodynamic entropy at equilibrium.

To solve (5), we introduce and optimize the Lagrangian:

$$\mathcal{L} : (p, \lambda_\Psi, \lambda_0) \mapsto -k_b \sum_{\mathbf{m} \in \mathbb{M}_a} p(\mathbf{m}) \ln p(\mathbf{m}) + \lambda_\Psi (\mathbb{E}[\Psi] - \bar{\Psi}) + \lambda_0 \left(\sum_{\mathbf{m} \in \mathbb{M}_a} p(\mathbf{m}) - 1 \right), \quad (6)$$

where λ_Ψ and λ_0 are Lagrange multipliers.

Case 1: system thermally insulated. From (2), $\mathbb{E}[\Psi] = \Psi_0$. The Lagrangian simplifies, and solving $\partial \mathcal{L} = 0$ yields the equiprobable distribution:

$$p^*(\mathbf{m} \mid \Psi_0) = 1/\Omega, \quad \Omega = \text{card}(\mathbb{M}_a). \quad (7)$$

Case 2: system in thermal contact. Solving $\partial \mathcal{L} = 0$ yields:

$$p^*(\mathbf{m} \mid \bar{\Psi}) = \frac{\exp(\lambda_\Psi \Psi(\mathbf{m})/k_b)}{\mathcal{Z}(\lambda_\Psi)}, \quad \mathcal{Z}(\lambda_\Psi) = \sum_{\mathbf{m} \in \mathbb{M}_a} \exp(\lambda_\Psi \Psi(\mathbf{m})/k_b). \quad (8)$$

A more detailed derivation can be found in Jaynes (1982).

For systems in thermal contact with their environment, the Lagrange multiplier λ_Ψ has a direct physical interpretation. Indeed, from (4)-(8), we deduce :

$$\bar{\Psi} = \frac{\partial}{\partial \lambda_\Psi} k_b \ln \mathcal{Z}(\lambda_\Psi). \quad (9)$$

Moreover, reinjecting (8) in (3) yields the thermodynamic entropy S :

$$S = S(p^*) = k_b \ln \mathcal{Z}(\lambda_\Psi) - \lambda_\Psi \bar{\Psi} := \mathcal{S}(\bar{\Psi}). \quad (10)$$

It follows that \mathcal{S} is a Legendre transform of $k_b \ln \mathcal{Z}$ and that:

$$-\lambda_\Psi = \frac{\partial}{\partial \bar{\Psi}} \mathcal{S}(\bar{\Psi}) = -\frac{1}{T}, \quad (11)$$

where T is the temperature (both internal and external, at equilibrium).

By applying maximum entropy to each constraint, we systematically derive the micro-state probability and the entropy for the corresponding statistical ensemble (Table 1, see also Ray (2005)).

Table 1. Statistical ensembles and associated constraints.

	Ensemble	Constraint	$p^*(\mathbf{m})$	Entropy	Example
No thermal contact	Micro-canonical	$\mathcal{E}(\mathbf{m}) = \mathcal{E}_0$	$1/\Omega$	$k_b \ln \Omega$	Gas in an isolated tank
	Isoenthalpic-isobaric	$\mathcal{E}(\mathbf{m}) + P_0 \mathcal{V}(\mathbf{m}) = \mathcal{H}_0$	$1/\Omega$	$k_b \ln \Omega$	Gas in a closed tank with a piston, thermally insulated
	Unnamed	$\mathcal{E}(\mathbf{m}) - \mu_0 \mathcal{N}(\mathbf{m}) = L_0$	$1/\Omega$	$k_b \ln \Omega$	Gas in a porous tank, thermally insulated
	Unnamed	$\mathcal{E}(\mathbf{m}) + P_0 \mathcal{V}(\mathbf{m}) - \mu_0 \mathcal{N}(\mathbf{m}) = \mathcal{R}_0$	$1/\Omega$	$k_b \ln \Omega$	Gas in a porous tank with a piston, thermally insulated
Thermal contact	Canonical	$\mathbb{E}[\mathcal{E}] = \bar{\mathcal{E}}$	$\frac{\exp(-\mathcal{E}(\mathbf{m})/k_b T)}{\mathcal{Z}(T)}$	$k_b \ln \mathcal{Z}(T) + \bar{\mathcal{E}}/T$	Gas in a closed tank, in contact with a thermostat
	Isothermal-isobaric	$\mathbb{E}[\mathcal{E} + P_0 \mathcal{V}] = \bar{\mathcal{H}}$	$\frac{\exp(-\mathcal{H}(\mathbf{m})/k_b T)}{\mathcal{Z}(T, P_0)}$	$k_b \ln \mathcal{Z}(T, P_0) + \bar{\mathcal{H}}/T$	Gas in a closed tank with a piston, in contact with a thermostat
	Grand-canonical	$\mathbb{E}[\mathcal{E} - \mu_0 \mathcal{N}] = \bar{L}$	$\frac{\exp(-L(\mathbf{m})/k_b T)}{\mathcal{Z}(T, \mu_0)}$	$k_b \ln \mathcal{Z}(T, \mu_0) + \bar{L}/T$	Gas in a porous tank, in contact with a thermostat
	Unnamed	$\mathbb{E}[\mathcal{E} + P_0 \mathcal{V} - \mu_0 \mathcal{N}] = \bar{\mathcal{R}}$	$\exp(-\mathcal{R}(\mathbf{m})/k_b T)$	$\bar{\mathcal{R}}/T$	Gas in a porous tank with a piston, in contact with a thermostat

2.5 Macro-state of a system and PHS formulation

Following the ergodic hypothesis, the macroscopic number of particles at equilibrium is $N = \mathbb{E}[\mathcal{N}]$. Similarly, the macroscopic volume at equilibrium is $V = \mathbb{E}[\mathcal{V}]$. A third macroscopic variable is the thermodynamic entropy S . If all external efforts constraining the system (that is, T, μ_0, P_0 , or a combination of them depending on the experimental conditions) are kept constant in time, there is no dynamics since all macroscopic variables become constant in time. However if these quantities are allowed to vary (slowly, so that the ergodic hypothesis is still verified), one can study the system dynamics between successive equilibrium states.

In order to do that, we rely on port-Hamiltonian systems: Duindam et al. (2009); van der Schaft et al. (2014), under a differential-algebraic formulation Beattie et al. (2017). This formulation allows the representation of a dynamical system as a network of:

- (1) storage components of state \mathbf{x} and energy $E(\mathbf{x})$, storing the power $P_{\text{stored}} = \nabla E(\mathbf{x})^\top \dot{\mathbf{x}}$;
- (2) dissipative components of flow \mathbf{w} and effort $z(\mathbf{w})$, such as the dissipated power $P_{\text{diss}} = z(\mathbf{w})^\top \mathbf{w}$ is non-negative for all \mathbf{w} ;
- (3) connection ports conveying the *outgoing* power $P_{\text{ext}} = \mathbf{u}^\top \mathbf{y}$ where \mathbf{u} are inputs and \mathbf{y} are outputs.

The flows \mathbf{f} and efforts \mathbf{e} of all components are coupled through a skew-symmetric interconnection matrix $\mathbf{J} = -\mathbf{J}^\top$ (possibly dependent on \mathbf{x}):

$$\underbrace{\begin{bmatrix} \dot{\mathbf{x}} \\ \mathbf{w} \\ \mathbf{y} \end{bmatrix}}_{\mathbf{f}} = \mathbf{J} \underbrace{\begin{bmatrix} \nabla E(\mathbf{x}) \\ z(\mathbf{w}) \\ \mathbf{u} \end{bmatrix}}_{\mathbf{e}}. \quad (12)$$

For instance, an open system in a thermostat is governed by the conservative PHS in Fig. 1, where $\delta_e S/\text{dt}$ denotes the outgoing entropy flow, _{int} indexes internal flows and efforts, _{ext} indexes external flows and efforts.

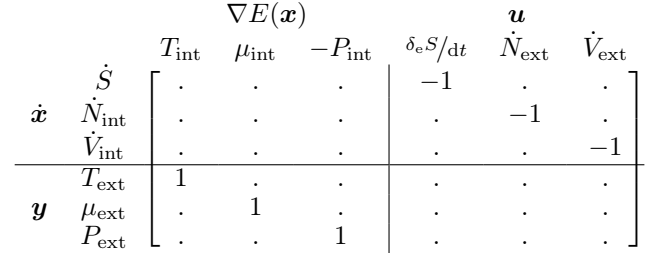


Figure 1. Conservative PHS of an open system in a thermostat (dots represent zeros).

2.6 Method recap

To sum up, the derivation of a macroscopic PHS from a stochastic description is performed in 5 steps:

- Step 1** Express micro-state \mathbf{m} and laws $\mathcal{N}, \mathcal{V}, \mathcal{E}$.
- Step 2** Pick a statistical ensemble of interest, according to experimental hypotheses.
- Step 3** Compute the corresponding micro-state probability distribution at equilibrium.
- Step 4** Compute the internal energy $\bar{\mathcal{E}}$ and the macroscopic state $\mathbf{x} = [S, N, V]^\top$.
- Step 5** Express the internal energy $\bar{\mathcal{E}}$ as a function of the macroscopic state to obtain $E(S, N, V)$.

A PHS is finally derived by adding ports accounting for the environment, as shown for each example in the next section.

2.7 Remark on thermodynamic potentials

If only some external efforts constraining the system are kept constant, it is possible to work with an appropriate Legendre transform of the internal energy, in order to reduce the PHS formulation. For instance, the (conservative) PHS of an open system in a *constant* thermostat, becomes that of Fig. 2, with $F(T, N, V) = E(S, N, V) - TS$.

Table 2 recaps usual Legendre transforms of the internal energy, also called *thermodynamic potentials*.

Table 2. Thermodynamic potentials.

Constant	Potential
	Internal energy $E(S, N, V)$
T	Helmholtz free energy $F(T, N, V) = E(S, N, V) - TS$
P	Enthalpy $H(S, N, P) = E(S, N, V) + PV$
T, P	Gibbs free energy $G(T, N, P) = H(S, N, P) - TS$
μ	Hill energy $L(S, \mu, V) = E(S, N, V) - \mu N$
T, μ	Grand potential $J(T, \mu, V) = L(S, \mu, V) - TS$
P, μ	Ray energy $R(S, \mu, P) = E(S, N, V) + PV - \mu N$
T, P, μ	Guggenheim energy $R(S, \mu, P) - TS = 0$

$$\begin{array}{c}
 \nabla F(\mathbf{x}) \quad \mathbf{u} \\
 \begin{array}{c} \dot{\mathbf{x}} \quad \dot{\mathbf{y}} \end{array} \begin{array}{c} \dot{N}_{\text{int}} \quad \dot{V}_{\text{int}} \\ \mu_{\text{ext}} \quad P_{\text{ext}} \end{array} \left[\begin{array}{cc|cc} \mu_{\text{int}} & -P_{\text{int}} & \dot{N}_{\text{ext}} & \dot{V}_{\text{ext}} \\ \cdot & \cdot & -1 & \cdot \\ \cdot & \cdot & \cdot & -1 \\ 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot \end{array} \right]
 \end{array}$$

Figure 2. Conservative PHS of an open system in a constant thermostat (dots represent zeros).

3. APPLICATIONS

3.1 Ideal gas in a thermostat

Consider N indiscernible, non-interacting atoms in a closed, rigid cube (constant volume V) in contact with a thermostat at temperature T .

Step 1. A micro-state of an atom is a vector $\mathbf{m} = [n_x, n_y, n_z] \in \mathbb{N}^{*3}$, where n_i is the energy quantization along axis i . Denoting by m the atom mass, a the cube edge length, and h the Planck constant, the Hamiltonian of the atom is given by Davies (1998):

$$\mathcal{E}(\mathbf{m}) = \left(n_x^2 + n_y^2 + n_z^2 \right) h^2 / 8ma^2. \quad (13)$$

Step 2. From the hypotheses, the statistical ensemble of interest is the canonical ensemble (see Table 1).

Step 3. The micro-state probability distribution at equilibrium is $p^*(\mathbf{m}) = \exp(-\mathcal{E}(\mathbf{m})/k_b T) / \mathcal{Z}(T)$.

Step 4. From (8), the partition function for one atom is:

$$\mathcal{Z}_0(T) = (2\pi T/T_0)^{3/2}, \quad \text{with } T_0 = h^2/ma^2 k_b \quad (14)$$

(proof in Appendix A). For N atoms, the partition function becomes:

$$\mathcal{Z}(T) = \mathcal{Z}_0(T)^N / N! = (2\pi T/T_0)^{3N/2} / N!. \quad (15)$$

For the canonical ensemble, (9) can be rewritten as:

$$\bar{\mathcal{E}} = k_b T^2 \frac{\partial \ln \mathcal{Z}}{\partial T}(T), \quad (16)$$

so that:

$$\bar{\mathcal{E}} = 3/2 N k_b T. \quad (17)$$

From (10), we deduce:

$$\begin{aligned}
 S &= k_b \ln \mathcal{Z}(T) + \bar{\mathcal{E}}/T = S_0 + 3/2 N k_b \ln(T/T_0), \\
 S_0 &= 3/2 N k_b \ln \left(2\pi e / (N!^{2/3N}) \right).
 \end{aligned} \quad (18)$$

Step 5. From (18), we deduce:

$$T = T_0 \exp \left(2(S - S_0) / 3N k_b \right). \quad (19)$$

Reinjecting in (17), we obtain:

$$E(S) = 3/2 N k_b T_0 \exp \left(2(S - S_0) / 3N k_b \right). \quad (20)$$

It is immediately verified that, as expected, $\partial E / \partial S = T$. As N and V are constant, they are removed from the state of the PHS and the only state variable is the entropy S . The constraint due to the thermostat is expressed at the ports of the PHS. Finally, we obtain the following PHS:

$$\begin{array}{c}
 \nabla E(\mathbf{x}) \quad \mathbf{u} \\
 \begin{array}{c} \dot{\mathbf{x}} \quad \dot{\mathbf{y}} \end{array} \begin{array}{c} \dot{T}_{\text{int}} \quad \delta_e S / dt \\ T_{\text{ext}} \end{array} \left[\begin{array}{c|c} T_{\text{int}} & \delta_e S / dt \\ \cdot & -1 \\ 1 & \cdot \end{array} \right].
 \end{array}$$

3.2 Ferromagnetic core in a thermostat

Here, we sum up results of Najnudel et al. (2020). The goal is to illustrate the modeling of a more complex system exhibiting phase transitions and dissipation.

Consider a ferromagnetic core with constant number of atoms N , constant volume V , in contact with a thermostat at temperature T .

Step 1. Following the model of Ising (1925) (see also Newell and Montroll (1953); Strecka and Jascur (2015)), the core is represented as a set of N adimensional magnetic moments, interacting with one another. A micro-state of the core is a particular configuration $\mathbf{m} \in \mathbb{M} = \{-1, 1\}^N$. The corresponding energy is the Heisenberg Hamiltonian:

$$\mathcal{E}(\mathbf{m}) = -1/2 \mathbf{m}^\top \mathcal{J}_{\text{ex}} \mathbf{m}, \quad (21)$$

where each coefficient $\mathcal{J}_{\text{ex}, i, j}$ is the *exchange energy* between moment i and moment j Liechtenstein et al. (1984). Assuming isotropic interactions affecting nearest neighbours only, this exchange energy simplifies to:

$$\mathcal{J}_{\text{ex}, i, j} = \begin{cases} J & i, j \text{ nearest neighbours, } i \neq j, \\ 0 & \text{otherwise,} \end{cases} \quad (22)$$

where J is a constant energy characterizing the material.

Step 2. From the hypotheses, the statistical ensemble of interest is the canonical ensemble (see Table 1).

Step 3. The micro-state probability distribution at equilibrium is $p^*(\mathbf{m}) = \exp(-\mathcal{E}(\mathbf{m})/k_b T) / \mathcal{Z}(T)$.

Step 4. Above dimension 2 in space, there is no analytic expression for $\mathcal{Z}(T)$. Assuming small micro-state fluctuations, we rely on the mean-field approximation: Utermohlen (2018), which yields

$$\mathcal{Z}_{MF}(m, T) = \exp \left(-N J q m^2 / 2 k_b T \right) \left(2 \cosh \left(J q m / k_b T \right) \right)^N. \quad (23)$$

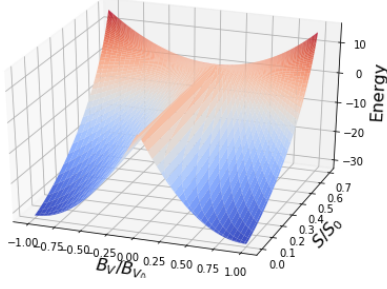


Figure 3. Energy function of the ferromagnetic core.

In (23), the auxiliary variable $m \in [-1, 1]$ can be interpreted as a mean magnetic moment, while q is the (constant) number of nearest neighbours of each moment. Reinjecting (23) in (16), the mean-field internal energy is found to be:

$$\bar{\mathcal{E}} \approx \mathcal{E}_{MF}(m, T) = E_0 \left(m^2/2 - m \tanh(mT_c/T) \right), \quad (24)$$

where $E_0 = NJq$, and $T_c = Jq/k_b$ is the critical temperature, above which the core becomes paramagnetic. Reinjecting (23) in (10), we obtain the thermodynamic entropy:

$$S \approx S_{MF}(m, T) = S_0 f(mT_c/T), \quad (25)$$

where $S_0 = Nk_b$ and $f(\chi) = \ln(2 \cosh(\chi)) - \chi \tanh(\chi)$. **Step 5.** Finally, introducing the total magnetic flux $B_{V_{\text{core}}} = m \mu_0 M_s V$, where $\mu_0 = 4\pi \times 10^{-7} \text{ H.m}^{-1}$ is the vacuum magnetic permeability and M_s is the core saturation magnetization, we obtain:

$$E_{\text{core}}(S, B_{V_{\text{core}}}) = E_0 \left(1/2 (B_{V_{\text{core}}}/B_{V_s})^2 - |B_{V_{\text{core}}}/B_{V_s}| g(S) \right), \quad (26)$$

where $B_{V_s} = \mu_0 M_s V$ and $g(S) = \tanh(f^{-1}(S/S_0))$.

The internal effort is $\nabla E_{\text{core}}(S, B_{V_{\text{core}}}) = [T_{\text{core}}, H_{\text{core}}]^T$, where T_{core} and H_{core} denote the core temperature and the internal magnetic field, respectively. Figure 3 shows the core going from two meta-stable equilibrium states to one stable equilibrium state, as the entropy increases. This corresponds to a phase transition from ferromagnetic to paramagnetic.

Dissipation. When the core is constrained by an exterior magnetic field H_{in} (created by a coil for instance), jumps between meta-stable states, called Barkhausen jumps, occur: Bertotti (1998). These jumps are damped (Fig. 4) due to domain structure and non-homogeneities (see Kittel (1949)). This damping can be modeled with a linear magnetic resistor r_{core} connected in series with the core (Fig. 5a). As the difference of energy before and after a jump is entirely dissipated as heat Bertotti (1998), Barkhausen jumps are also responsible for the variation of entropy creation $\delta_i S$ in the core. The associated thermal power is equal to the magnetic power dissipated through r_{core} , so that:

$$r_{\text{core}} H_{r_{\text{core}}}^2 - T_{\text{core}} \delta_i S / dt = 0, \quad (27)$$

where dt stands for an infinitesimal increment of time. We deduce the dissipative flow and effort:

$$\begin{aligned} \mathbf{w} &= [-T_{\text{core}}, H_{r_{\text{core}}}]^T \\ z(\mathbf{w}) &= [r_{\text{core}} H_{r_{\text{core}}}^2 / T_{\text{core}}, r_{\text{core}} H_{r_{\text{core}}}]^T = [\delta_i S / dt, \dot{B}_{V_{r_{\text{core}}}}]^T. \end{aligned} \quad (28)$$

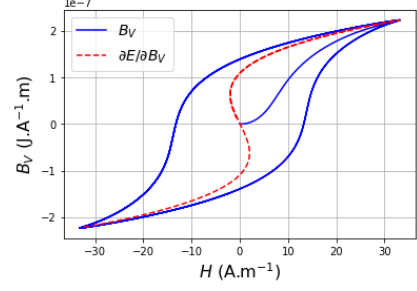


Figure 4. Damped Barkhausen jumps and resulting hysteresis during a cycle. The red curve is the theoretical core internal magnetic field, the blue curve is the real trajectory followed by the total magnetic flux of the core constrained by an external magnetic field.

Finally, the second law of thermodynamics Landsberg (2014) states:

$$\dot{S} = \delta_i S / dt - \delta_e S / dt. \quad (29)$$

Kirchoff's laws in receptor convention, as well as (26)-(28)-(29), yield the PHS formulation in Fig. 5b. Note that in addition to the power balance, the entropy balance is made explicit in this formulation.

This model has been successfully implemented in several applications simulating audio circuits (see Najnudel et al. (2020)).

4. CONCLUSION

In this paper, we presented a method for deriving an ad hoc macroscopic port-Hamiltonian formulation for a constrained system described by statistical physics.

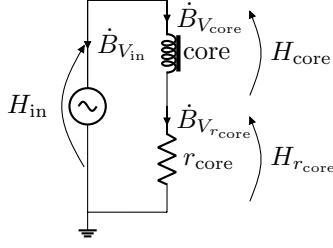
This method is based on two key principles of statistical physics (that is, maximum entropy and the ergodic hypothesis), and expresses the internal energy of the system as a function of extensive thermodynamic variables. The exchanges of energy and entropy are made explicit through the PH formulation. Constraints are modeled in ports as inputs, and entropy creation is modeled as dissipation. Alternative formulations based on thermodynamic potentials are also possible, under certain conditions.

The method is applied to model two systems: an ideal gas in a thermostat, and a ferromagnet in a thermostat. In the case of the ferromagnet, the method successfully captures complex phenomena such as phase transitions, meta-stability, dissipation and entropy creation, with only two state variables and one dissipative component.

A perspective of this work is to extend the method to other microscopic quantities and constraints, not restricted to the system number of atoms and volume. Another perspective is to generalize the mean-field approximation (for systems composed of particles interacting with one another), and introduce appropriate auxiliary variables in order to obtain approximations of the partition function with an arbitrary degree of accuracy. This shall be the object of future work.

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(a) Core with dissipation constrained by an external magnetic field.

		$\nabla E(\mathbf{x})$		$z(\mathbf{w})$		\mathbf{u}	
		T_{core}	H_{core}	$\delta_1 S/\text{dt}$	$\dot{B}_{V_{\text{rcore}}}$	$\delta_e S/\text{dt}$	H_{in}
$\dot{\mathbf{x}}$	\dot{S}	.	.	1	.	-1	.
	$\dot{B}_{V_{\text{core}}}$.	.	.	1	.	.
\mathbf{w}	$-T_{\text{core}}$	-1
	H_{rcore}	.	-1	.	.	.	1
\mathbf{y}	T_{ext}	1
	$\dot{B}_{V_{\text{in}}}$.	.	.	-1	.	.

(b) Corresponding PHS (dots represent zeros).

Figure 5. Equivalent circuit and PHS for the core constrained by an external magnetic field with dissipation.

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Appendix A. PARTITION FUNCTION OF AN ATOM IN A BOX

Denoting $\epsilon_0 = h^2/(8ma^2)$, we have

$$\begin{aligned}
 Z_0(T) &= \sum_{\mathbf{m}} \exp(-\mathcal{E}(\mathbf{m})/k_b T) \\
 &= \sum_{n_x=1}^{+\infty} \sum_{n_y=1}^{+\infty} \sum_{n_z=1}^{+\infty} \exp\left(-\left(n_x^2 + n_y^2 + n_z^2\right) \epsilon_0/k_b T\right) \\
 &= \left(\sum_{n=1}^{+\infty} \exp\left(-n^2 \epsilon_0/k_b T\right)\right)^3 \\
 &\approx \left(\int_0^{+\infty} \exp\left(-x^2 \epsilon_0/k_b T\right) dx\right)^3 \\
 &= \left(1/2\sqrt{\pi k_b T/\epsilon_0}\right)^3 = (2\pi T/T_0)^{3/2}, \quad T_0 = h^2/ma^2 k_b.
 \end{aligned} \tag{A.1}$$