

A Review of Information in Nonequilibrium Thermodynamics

Adam Rupe

*Complexity Sciences Center
Department of Physics
University of California Davis*

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Abstract

While there have been some great advances in nonequilibrium thermodynamics in recent years, a lot of approaches seem to be coming at the problem from rather different directions. There is often little common ground over interpretation and importance of various nonequilibrium quantities, chief among them being entropy production. I will argue that information theory is an emerging thread that is beginning to tie a lot of these approaches together. The main focus will be information-theoretic formulations of entropy production.

Entropy is Information

John von Neumann was being more prescient than he realized when he suggested Claude Shannon name his new information measure *entropy*. It is no coincidence that the thermodynamic entropy of Boltzmann and Gibbs shares the same mathematical form of the information entropy of Nyquist, Hartley, and Shannon. *Thermodynamic entropy is a Shannon information entropy*. Historically, entropy has been one of the least understood concepts in natural science. If you look up entropy in any common thermodynamics or statistical mechanics text book it would most likely say that entropy is a measure of disorder, or something along those lines. This is just the latest in a long line of misinterpretations of thermodynamic entropy [1].

The true interpretation of thermodynamic entropy S is as a Shannon information measure H . Specifically,

$$S \propto H[\text{microstate}|\text{macrostate}] \quad (1)$$

In Shannon communication terms, it is this; say you know the macrostate of a thermodynamic system and a Maxwellian demon then tells you the actual microstate of the system. It has conveyed an amount of information to you equal to the thermodynamic

entropy (in units of nats times Boltzmann's constant). This statement is not just some technical point but, as we will see, rather fundamental.

That we distinguish between a microstate and a macrostate at all is not trivial. There may be "fundamental" physics happening on a scale that can not be directly resolved (microstate), yet at the same time we perceive some "effective" theory occurring on the human scale (macrostate) that is actually observable. The description of the system on the observable macroscopic scale is not independent from the hidden, microscopic description. Knowing something about the macrostate of the system tells you about what microstate it could possibly be in. This is why entropy is so often described as a measure of order. A more ordered state often (but not always [2]) coincides with a low entropy state. Order implies regularities and symmetries in the macrostate, and these put restrictions on what the possible microstate can be. Thus reducing the uncertainty in the microstate (low entropy).

Dichotomy of scales in effective theories is not limited to just human scale vs not humanly resolvable. New phenomena and effective theories seem to exist at all scales [3]. Philip Anderson championed the notion of a hierarchy of scale in the sciences while maintaining that each level of the hierarchy is fundamental in its own right, even though in principle behavior at one scale may be derived from a lower scale [4]. This also is not just some technical point, but gets right to the heart of complex systems theory. Understanding how one level emerges from another, as well as the dependencies and connections between layers of the hierarchy is of utmost importance. New roads being paved by information and computation theory offer a tantalizing glimpse of a revolution in how we understand this hierarchy and the scientific endeavor as a whole [5]. The longest studied and best understood interface between levels is equilibrium statistical mechanics.

Information in Equilibrium

Equilibrium statistical mechanics bridges two levels of description; the microscopic Hamiltonian (classical or quantum) dynamics of the particles of a system and macroscopic thermodynamics. The classical microstate of the system is given by all the position and momenta of the particles, in quantum mechanics it is an eigenstate of the many-body Hamiltonian. The macrostate, or thermodynamic state, is simply a list of thermodynamic state variables. This thermodynamic state is always defined in conjunction with external constraints placed upon the system. The most common constraints are the system being in contact with a heat bath (canonical ensemble), a heat bath and a particle reservoir (grand-canonical ensemble), or being completely isolated (microcanonical ensemble). Formally, constraints are specified through the thermodynamic variables of total internal energy, system volume, and particle number denoted U , V , and N respectively. In equilibrium, the constraints are time independent. Note this assumes the absence of any external fields, in which case more variables would be needed to fully specify the equilibrium state. As discussed below, these three variables (in the absence of external fields) have been traditionally used in thermodynamics as the constraints that

fully specify the equilibrium macrostate and define the three types of thermodynamic equilibrium. The main reason these three play such a big role in thermodynamics is that they are the quantities that exist on both the micro and macro scales, and are well defined in and out of equilibrium.

Consider a thermodynamic system and its environment. In the thermodynamics literature, there are three kinds of equilibrium; thermal, mechanical, and chemical. In thermal equilibrium the system and environment exchange internal energy U , but have the same temperature T . In mechanical equilibrium they exchange volume V , but have the same pressure P . In chemical equilibrium they exchange particles N , but have the same chemical potential μ . By definition, an equilibrium macrostate is always time independent. But if the system is not isolated and exchanges one or more of U, V , or N with its environment, the microscopic values may fluctuate. It is only their averages that are time independent.

As stated previously, statistical mechanics is a bridge between microscopic and macroscopic levels of hierarchy. U , V , and N on the macroscale are just averages of their counterparts on the microscale. But what about temperature, and chemical potential that don't have counterparts on the microscale? And what about the most important of thermodynamic variables, entropy? After all, the Gibbs principle states that the equilibrium distribution over microstates is that which maximizes the entropy. Why should this be the case? Realizing thermodynamic entropy is a Shannon information entropy Edwin Jaynes formulated the information-theoretic foundations of statistical mechanics and went about answering this question [6]. In the process, he uncovered some deep insights that are only recently being fully appreciated.

A typical thermodynamic system has of order 10^{23} particles, each with three components of position and three of momentum defining the microscopic phase space. The macrostate, which is the one directly accessible to us, is defined by a handful of state variables. Jaynes realized the problem of statistical mechanics is one of inference. What can those handful of variables tell us about the microscopic configuration of the system? We certainly can not ascertain the exact configuration, we don't have nearly enough information. What we can do however is use the macroscopic information to infer a distribution of possible microscopic configurations, as was first realized by Boltzmann when he first developed statistical mechanics.

Jaynes realized the Gibbs principle is just a specific application of a more general principle of logical inference, which he called the Principle of Maximum Entropy (PME). Stated in Bayesian terms, the PME is a way of using available information to construct a prior. Given the full set of possible outcomes of an event and some information about that event (most commonly in the form of expectation values), what is the most logical assignment of probabilities one can make for the outcomes? Laplace had realized with his principle of indifference that if all one knows are the possible outcomes and nothing else the most logical assignment of probabilities is a uniform distribution. Jaynes used information theory to generalize this notion to situations when one knows more than just the possible outcomes. The extra information amounts to a set of constraints the inferred distribution must obey. One must then find the distribution that is most uniform

yet still consistent with the constraints. Well Shannon's information entropy is exactly a measure of the flatness of a distribution. Thus the most logical distribution is that which maximizes the entropy subject to the constraints, hence Principle of Maximum Entropy.

A formal statement of the PME is as follows [7]. Let $\{x_i\}$ be an exhaustive set of n mutually exclusive propositions. Assume information is interpretable as expectation values of a set of independent functions over the propositions $\{f_r(x)\}$, $r = 1, \dots, m < n$. The constraints on the distribution are thus

$$\sum_{i=1}^n P_i = 1 \quad , \quad P_i > 0 \quad (2)$$

$$\langle f_r(x) \rangle = \sum_{i=1}^n P_i f_r(x_i) \quad (3)$$

The PME distribution is that which maximizes the Shannon entropy $H(P) = -k \sum_i P_i \ln P_i$ subject to the above constraints. Using Lagrange multipliers, this yields

$$P_i = \frac{1}{Z} e^{-\lambda \cdot f(x_i)} \quad (4)$$

$$Z(\lambda_1, \dots, \lambda_m) = \sum_i e^{-\lambda \cdot f(x_i)} \quad (5)$$

where $\lambda \cdot f(x_i) \equiv \lambda_1 f_1(x_i) + \dots + \lambda_m f_m(x_i)$. The maximized Shannon entropy of the distribution, denoted S , is given by

$$S = k \ln Z + k \lambda \cdot \langle f \rangle \quad (6)$$

Jaynes showed that this construction uniquely provides the least biased distribution consistent with the given constraints. Any other distribution carries implicit information / bias other than the given constraints.

The current interest however is in the application of the PME to the foundations of traditional statistical mechanics where one wishes to infer a distribution over possible microstates subject to the information provided by macrostate constraints. For reasons that will be made explicit later when the PME is generalized to nonequilibrium settings we proceed using operator formalism, be it classical or quantum. Thus the set of possible microstates for which we wish to create a distribution over will be the eigenstates of the many-body Hamiltonian (up to basis choices in degenerate eigenspaces). The distribution is encapsulated in the spectrum of a statistical operator ρ . The thermodynamic constraints U , V , and N are given as expectation values of the Hamiltonian, volume, and particle number operators.

$$\langle H \rangle = \text{Tr} \rho H = U \quad (7)$$

$$\langle V \rangle = \text{Tr} \rho V = V \quad (8)$$

$$\langle N \rangle = \text{Tr} \rho N = N \quad (9)$$

Along with

$$\text{Tr} \rho = 1 \quad (10)$$

these are always the constraints used to create the equilibrium microstate distribution. If a system does not exchange one of these quantities with its environment, the corresponding constraint equation reduces to (10). Therefore, if the system is isolated the only constraint is (10) and the distribution is the microcanonical ensemble

$$P_i = \frac{1}{\Omega} \quad (11)$$

where Ω is the number of microstates. If the system is in contact with a heat bath (8) and (9) reduce to (10) since V and N are still fixed on the micro scale while the internal energy is no longer fixed. Thus (7) and (10) are the final constraints. This gives the canonical ensemble

$$\rho = \frac{1}{Z} e^{-\beta H} \quad (12)$$

with entropy

$$S = k \ln Z + \beta \langle H \rangle = k \ln Z + \beta U \quad (13)$$

Using $\frac{\partial S}{\partial U} = \frac{1}{T}$, we find that β is the inverse temperature, as is standard. As a Lagrange multiplier β enforces the constraint of $\langle H \rangle = U$ in the distribution. This matches our intuition of the physical picture of a system in contact with a heat bath. The system and heat bath can exchange internal energy, but only in a restricted way in equilibrium. Specifically, the expected value of the systems internal energy is fixed, which is enforced by both system and heat bath having the same temperature.

While not providing any new novel results for equilibrium statistical mechanics, Jaynes' PME puts the theory on a much more solid foundation of logical inference. It also allows for concepts from statistical mechanics to be generalized to other fields [8][9]. As we will see later, it also lays the foundations for generalizing statistical mechanics to nonequilibrium settings. The most important contribution, however, is to shed light on the role of statistical mechanics as an interface theory bridging microscopic and macroscopic levels of hierarchy, and the essential role that information theory and logical inference play at this interface.

Classical Irreversible Thermodynamics

The Gibbs principle of maximum entropy determines the equilibrium macrostate under given constraints. There have been many similar extremum principles proposed for determination of nonequilibrium steady-states. Chief among them are extremum principles of entropy production. By counterexample, we will see this is likely not the

case. Nonetheless, entropy production still seems to be a very important quantity for nonequilibrium situations. As with the many misinterpretations of equilibrium entropy over the years, there is still no clear consensus on just what exactly entropy production is. Thus the main focus of the remainder of this review will be to try and pin down entropy production and give its information-theoretic interpretation. If there are to be general principles for nonequilibrium thermodynamics, they are likely to be based on information theory. Entropy production and nonequilibrium steady-states are a good place to start.

We begin with the Classical Irreversible Thermodynamic treatment of entropy production, developed mainly by Onsager and Prigogine [10]. This formalism assumes a local equilibrium field theory in which the system is divided into a continuum of elementary volume cells. The Gibb's relation $dU = TdS - PdV + \sum_k \mu_k dN_k$ holds in each cell. Thus intensive thermodynamic variables become functions of space and time

$$T = T(\vec{x}, t) ; P = P(\vec{x}, t) ; \mu = \mu(\vec{x}, t) \quad (14)$$

and extensive variables (excluding volume) become densities

$$s(\vec{x}, t) = \text{entropy per unit volume} \quad (15)$$

$$u(\vec{x}, t) = \text{energy per unit volume} \quad (16)$$

$$n_k(\vec{x}, t) = \text{particle number per unit volume} \quad (17)$$

Changes in entropy have two contributions ;

$$dS = d_e S + d_i S \quad (18)$$

where $d_e S = \frac{dQ}{T}$ denotes changes due to exchange of energy and matter and $d_i S$ are changes due to irreversible processes.

$$d_i S \geq 0 \text{ is the entropy production} \quad (19)$$

The decomposition (18) nicely encapsulates many well-known properties of entropy. Namely, the Clausius inequality $dS \geq \frac{dQ}{T}$; entropy changes of reversible processes $d_i S = 0 \Rightarrow dS = \frac{dQ}{T}$; the 2nd Law (which applies for isolated systems) $d_e S = 0 \Rightarrow dS \geq 0$; and irreversible cycles $dS = 0 \Rightarrow d_e S = -d_i S < 0 \Rightarrow dQ < 0$ which means the system must dump waste heat during the cycle.

In the local equilibrium field theory, the entropy density also obeys the decomposition (18)

$$ds = d_e s + d_i s \quad (20)$$

It is further assumed that (19) holds for all possible subsystems ($d_i s \geq 0$), and that the entropy density obeys the balance equation

$$\frac{\partial s}{\partial t} + \nabla \cdot \vec{J}_s = \sigma \quad (21)$$

| Table of thermodynamic forces and flows | | |
|---|---|--|
| | Force F_α | Flow (Current) J_α |
| Heat conduction | $\nabla \frac{1}{T}$ | Energy flow \mathbf{J}_u |
| Diffusion | $-\nabla \frac{\mu_k}{T}$ | Diffusion current \mathbf{J}_k |
| Electrical conduction | $\frac{-\nabla \phi}{T} = \frac{\mathbf{E}}{T}$ | Ion current \mathbf{I}_k |
| Chemical reactions | $\frac{A_j}{T}$ | Velocity of reaction $v_j = \frac{1}{V} \frac{d\xi_j}{dt}$ |

Figure 1: Table of Thermodynamic forces and fluxes

where

$$\sigma(\vec{x}, t) = \frac{ds_i}{dt} \geq 0 \text{ is the local entropy production} \quad (22)$$

Both (19) and (22) are referred to as entropy production in the literature and it is sometimes not made explicit which one the author has in mind, though this conflation is usually innocuous. A much more troubling ambiguity often encountered is referring to any general change in entropy (the full dS in (18)) as entropy production.

Before moving on, we pause to reflect on the presumed extensivity of entropy, $dS = \int_V s dV$, as well as the balance equation (21). With the insight that thermodynamic entropy is a Shannon information entropy, neither of these equations seem appropriate for general nonequilibrium systems. Consider a system that is composed of two subsystems. The joint entropy of the total system is given as $H[1, 2] = H[1] + H[2] - I[1; 2]$ where $I[1; 2]$ is the mutual information between the subsystems. Extensivity implies independent subsystems with no mutual information. Spatial extensivity of thermodynamic entropy implies no spatial correlation in the system. Just looking at a BZ reaction or Rayleigh-Benard convection cells quickly convinces one that this is not the case, certainly for interesting patterning forming nonequilibrium systems. As for the balance equation, that implies entropy is a locally conserved quantity. This as well does not seem to be an appropriate statement for information. What exactly should replace (21) in taking into consideration non-local effects on spatial information is still, to my knowledge, an open question.

In the Classical Irreversible Thermodynamics literature, local entropy production is given as the production of thermodynamic forces and fluxes

$$\sigma = \sum_{\alpha} F_{\alpha} J_{\alpha} \quad (23)$$

A table of example forces and fluxes is given in figure 1 [10]. In near-equilibrium situations, the fluxes are linearly related to the forces as

$$J_k = \sum_j L_{kj} F_j \quad (24)$$

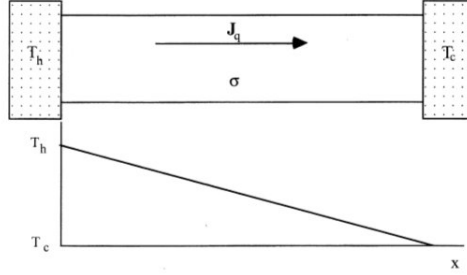


Figure 2: Above: a physical picture of heat conduction. Below: a plot of the steady-state temperature distribution over space

L is the matrix of phenomenological coefficients. It is positive definite, so that insertion into (23) guarantees the local entropy production is non-negative.

$$\sigma = \sum_{jk} L_{jk} F_j F_k \geq 0 \quad (25)$$

Furthermore, L is symmetric from the so-called Onsager Reciprocal Relations $L_{ij} = L_{ji}$. This is a non-trivial consequence of microscopic reversibility in the form of detailed balance. Equation (24) generalizes known phenomenological laws such as Fourier's heat law, Fick's law of diffusion, and Ohm's law. It also encompasses cross-coupling effects, such as the thermoelectric effect

$$\vec{J}_q = L_{qq} \nabla \frac{1}{T} + L_{qe} \vec{E} \quad (26)$$

$$\vec{I}_e = L_{ee} \vec{E} + L_{eq} \nabla \frac{1}{T} \quad (27)$$

We now use this formalism to analyze the familiar nonequilibrium scenario of heat conduction. Using the force and flux from Figure 1, the local entropy production is given as

$$\sigma = \vec{J}_q \cdot \nabla \frac{1}{T} \quad (28)$$

The total entropy production is then

$$\frac{d_i S}{dt} = \int_0^L J_q \left(\frac{\partial}{\partial x} \frac{1}{T} \right) dx = \frac{J_q}{T_c} - \frac{J_q}{T_h} > 0 \quad (29)$$

In steady-state, $dS = 0 \Rightarrow d_i S = -d_e S$. This matches our physical intuition that the system's desire to return to equilibrium ($d_i S$) is balanced by external driving keeping the system out of equilibrium ($d_e S$). We can also see equation (29) is consistent with this. In steady-state the entropy entering the system is $\frac{J_q}{T_h}$ and the entropy leaving is $\frac{J_q}{T_c}$, and so $\frac{d_e S}{dt} = \frac{J_q}{T_h} - \frac{J_q}{T_c} = -\frac{d_i S}{dt}$.

We now turn to the question of whether an extremum of the local entropy production determines the well-known steady-state. Using (24), we have

$$\frac{d_i S}{dt} = \int_0^L L_{qq} \left(\frac{\partial}{\partial x} \frac{1}{T} \right)^2 dx \quad (30)$$

L_{qq} is given as $L_{qq} = \kappa T^2(x) \approx \kappa T_{\text{avg}}^2$. To analyze the extremum of (30), we use the Euler-Lagrange equation. Using L_{qq} as approximately constant,

$$\kappa \frac{\partial T}{\partial x} = \text{constant} \quad (31)$$

and the correct steady-state is indeed recovered. However, using the full spatially dependent L_{qq} , the Euler-Lagrange equation gives

$$T \frac{\partial^2 T}{\partial x^2} = \left(\frac{\partial T}{\partial x} \right)^2 \quad (32)$$

which yields an exponential steady-state that has not been experimentally observed. Since we never see this distribution we must either believe that it is impossible to create a large enough steady-state temperature gradient such that the constant L_{qq} approximation fails, or that this steady-state is just not an extremum of the entropy production. The former is almost certainly not true, and we are inclined to conclude, as many have, that nonequilibrium steady-states are in general not given by an extremum of the entropy production.

There are other similar classical (not information-theoretic) approaches to entropy production and nonequilibrium thermodynamics [11]. The authors of [11] have laid out a challenge to find a general nonequilibrium theory that encompasses all of the classical approaches. A nonequilibrium generalization of the Principle of Maximum Entropy was developed by Jaynes and expanded by Walter T. Grandy Jr. which appears to be the closest theory yet of achieving this goal [7]. We give a brief outline of the theory, again focusing on entropy production.

Nonequilibrium Statistical Mechanics

We begin with the PME construction of a dynamical probability distribution for a general nonequilibrium system. As in equilibrium we will use operator formalism. Begin with an initial constraint given as the expectation of an operator corresponding to some observable $\langle F_0 \rangle$. This gives an initial distribution ρ_0 with standard use of the PME. Now introduce an additional constraint $\langle F_1 \rangle$. The distribution is updated to incorporate this new constraint by remaximizing the entropy subject to both constraints

$$\rho_1 = \frac{1}{Z_1} e^{-\lambda_0 F_0 - \lambda_1 F_1} \quad (33)$$

$$Z_1 = \text{Tr} e^{-\lambda_0 F_0 - \lambda_1 F_1} \quad (34)$$

This is where we see the necessity of operator formalism. If F_0 and F_1 were functions rather than operators, ρ_1 (rather, its distribution equivalent) would always be separable. For clarity, let the system be divided into two subsystems A and B with corresponding constraints be $\langle F_A \rangle$ and $\langle F_B \rangle$. Using functions, ρ_1 could always be written as $\rho_1 = \frac{1}{Z_A} e^{-\lambda_A F_A} \frac{1}{Z_B} e^{-\lambda_B F_B} = \rho_A \rho_B$. This will completely miss any possible correlations between subsystems A and B, unless put in by hand. In information theory terms, this will always miss any mutual information between A and B. Using operator formalism takes care of this automatically since the non-commutative algebra of the operators takes into account possible correlations. For two operators A and B that do not commute, we have the identity

$$e^{A+B} = e^A \left[1 + \int_0^1 e^{x^A} B e^{x(A+B)} dx \right] \quad (35)$$

which will be used later for perturbative expansions.

Continuing on with construction of the dynamical state distribution, we now consider a collection of constraints $\{\langle F_0 \rangle, \langle F_1 \rangle, \dots, \langle F_m \rangle\}$. Again, the distribution is updated by maximizing the entropy subject to all constraints.

$$\rho_n = \frac{1}{Z_n} \exp \left[- \sum_{i=1}^n \lambda_i F_i \right] \quad (36)$$

$$Z_n = \text{Tr} \exp \left[- \sum_{i=1}^n \lambda_i F_i \right] \quad (37)$$

You can think of these constraints as experimental measurements, in the spirit of inference. You measure the dynamical evolution of a system on the macroscale, what can you then infer about microscopic evolution? The sequence of constraints $\{\langle F_0 \rangle, \langle F_1 \rangle, \dots, \langle F_m \rangle\}$ could correspond to evolution over time, space, or both. Assume experimental measurements are made over a space-time region $R(\vec{x}, t)$. Let $\{\langle F_0 \rangle, \langle F_1 \rangle, \dots, \langle F_m \rangle\}$ vary over $R(\vec{x}, t)$ and take the continuum limit. This gives the dynamical statistical operator

$$\rho(\vec{x}, t) = \frac{1}{Z} \exp \left[- \int_R \lambda(\vec{x}, t) F(\vec{x}, t) d^3 \vec{x} dt \right] \quad (38)$$

with partition functional

$$Z[\lambda(\vec{x}, t)] = \text{Tr} \exp \left[- \int_R \lambda(\vec{x}, t) F(\vec{x}, t) d^3 \vec{x} dt \right] \quad (39)$$

If one just started with a continuous constraint $\langle F(\vec{x}, t) \rangle$, (38) would be the proper dynamical statistical operator that is the least biased distribution consistent with the space-time constraints.

We now discuss linear approximations in near-equilibrium situations. Consider a system that was in equilibrium in the past, with a corresponding Hamiltonian H . It is found to be out of equilibrium via the space-time constraint $\langle F(\vec{x}, t) \rangle$. The statistical

operator is

$$\rho = \frac{1}{Z} \exp \left[-\beta H - \int_R \lambda(\vec{x}, t) F(\vec{x}, t) d^3 \vec{x} dt \right] \quad (40)$$

To first order, the expected deviation from equilibrium of some other operator $C(\vec{x}, t)$ is

$$\langle \Delta C(\vec{x}, t) \rangle = - \int_R K_{CF}^0(\vec{x}, t; \vec{x}', t') \lambda(\vec{x}', t') d^3 x' dt' \quad (41)$$

where

$$K_{CF}^0(\vec{x}, t; \vec{x}', t') = \overline{\langle F(\vec{x}', t') C(\vec{x}, t) \rangle_0} - \langle F(\vec{x}') \rangle_0 \langle C(\vec{x}) \rangle_0 \quad (42)$$

The 0 subscripts indicate expectation values are to be taken from the non-perturbed equilibrium statistical operator, and $\overline{\langle F(\vec{x}', t') \rangle}$ denotes the Kubo transformation of F .

$$\overline{\langle F(\vec{x}, t) \rangle} \equiv \int_0^1 e^{-u \ln \rho_t} F(\vec{x}, t) e^{u \ln \rho_t} du \quad (43)$$

From this groundwork, most of Classical Irreversible Thermodynamics can be derived, as well as the other similar formalisms discussed in [11], and the Green-Kubo formalism for transport coefficients. For much more detail on this and nonequilibrium PME in general, see [7][12][13].

It is illuminating to replace C by F in (41) and omit variations over space so that $R(\vec{x}, t) \rightarrow R(t) = [-T, 0]$. This gives

$$\langle F(t) \rangle - \langle F \rangle_0 = - \int K_{FF}^0(t - t') \lambda(t') dt' \quad (44)$$

Running the integral over $t' \in R$ yields a Fredholm integral equation determining $\lambda(t)$, and this captures the behavior of $F(t)$ from observations during the interval R . We can then use this to infer the behavior of $F(t)$ in times outside the interval of observation. $t' > 0$ gives the predicted future of $F(t)$, and $t' < -T$ gives the retrodicted past of $F(t)$. Physical influence must propagate forward in time, but logical inference done in the present can affect our knowledge of the past as well as the future.

Now we turn to the time-dependent entropy. First we must discuss briefly the concept of thermal driving. In short, thermal driving refers to macroscopic sources whose effects on the system are known on the macro scale, but details of the driving on the micro scale are unknown. This is in contrast to dynamical response theory, where the system is driven by an explicit time-dependent term in the Hamiltonian. We have essentially already laid the ground work for this, as thermal driving is just a type of dynamical external constraint imposed on the system. For simplicity we will again omit spatial variation. Consider a system initially in equilibrium with Hamiltonian H that is thermally driven by the constraint $\langle F(t) \rangle$. The statistical operator is

$$\rho_t = \frac{1}{Z_t} \exp \left[-\beta H - \int_0^t \lambda(t') F(t') dt' \right] \quad (45)$$

We introduce a source term

$$\sigma_F(t) \equiv \frac{d}{dt} \langle F(t) \rangle_t - \langle \dot{F}(t) \rangle_t = -\lambda(t) K_{FF}^t(t, t) \quad (46)$$

where K_{FF}^t is the full nonlinear covariance function. It is similar to (42), except that expectation values are taken with respect to ρ_t as indicated by the superscript t . Since thermal driving is entirely macroscopic driving, $\sigma_F(t)$ factors out the effects of microscopic dynamics of F from $\langle F(t) \rangle$, and so captures the full macroscopic effects of the thermal source. This will be useful shortly.

Time-dependent entropy during the driving is given by the Shannon entropy of ρ_t .

$$\frac{1}{k} S_t = \ln Z_t + \beta \langle H \rangle_t + \int_0^t \lambda(t') \langle F(t') \rangle_t dt' \quad (47)$$

It's time derivative is

$$\begin{aligned} \frac{1}{k} \frac{dS_t}{dt} &= \beta \frac{d\langle H \rangle_t}{dt} - \lambda(t) \int_0^t \lambda(t') K_{FF}^t(t, t') dt' \\ &= -\beta \lambda(t) K_{HF}^t(t, 0) - \lambda(t) \int_0^t \lambda(t') K_{FF}^t(t, t') dt' \\ &= \gamma_F(t) \sigma_F(t) \end{aligned} \quad (48)$$

Now use the expression for $\sigma_F(t)$ in (46) to write this is as

$$\frac{1}{k} \dot{S}_t = \gamma_F(t) \left(\frac{d}{dt} \langle F(t) \rangle_t - \langle \dot{F}(t) \rangle_t \right) \quad (49)$$

which gives us a familiar expression

$$\dot{S}_{tot}(t) = \dot{S}_t + \dot{S}_{int}(t) \quad (50)$$

This is the nonequilibrium stat-mech derivation of $dS = d_e S + d_i S$.

To illustrate some of the subtleties of the difference between \dot{S}_t and \dot{S}_{int} we go through a heat conduction example of starting in equilibrium, driving the energy density to an arbitrary nonequilibrium state, then letting the system relax to a new equilibrium. Since we are not interested in doing linear expansions near equilibrium we simply write the statistical operator for the driving phase as

$$\rho_t = \frac{1}{Z_t} \exp \left[\int_0^t dt' \int_V d^3x [-\beta(\vec{x}, t') h(\vec{x}, t')] \right] \quad (51)$$

with the assumption that the system was in equilibrium at time $t = 0$. The time-dependent entropy for the driving is

$$\frac{1}{k} S_t = \ln Z_t + \int_0^t dt' \int_V d^3x [\beta(\vec{x}, t') \langle h(\vec{x}, t') \rangle_t] \quad (52)$$

The time derivative of (52) will give $\dot{S}_t = \frac{d_e S}{dt}$, analogous to (48). The tendency to return to equilibrium, as described by the entropy production $\frac{d_i S}{dt}$, during the driving process is implicitly included in the time derivative of (52) as seen by (49). To analyze \dot{S}_{int} explicitly, we turn off the driving at $t = t_1$. For all $t_2 > t_1$ the system relaxes towards equilibrium. But what “drives” it to the new equilibrium? As we know from Classical Irreversible Thermodynamics, gradients in the system (thermodynamic forces) drive currents (fluxes) that try to smooth out the gradients and restore the system to equilibrium. This is the basis for the phenomenological constitutive relations (24). Thus the macro scale constraints during the relaxation process are solutions to the appropriate macroscopic effective theory, usually constitutive relations such as (24) in conjunction with appropriate conservation laws. Incidentally, the constitutive relations of (24) such as Fourier’s law, and Fick’s laws can be rigorously derived in this nonequilibrium PME formalism [7][13].

In our heat conduction example, the macro constraint is then the solution to Fourier’s law $\langle h(\vec{x}, t) \rangle$ with initial conditions given by the expectation value of $h(\vec{x}, t)$ evaluated with respect to ρ_t at $t = t_1$ when the driving is turned off and relaxation begins. The statistical operator for $t_2 > t_1$ is

$$\rho(t_2) = \frac{1}{Z(t_2)} \exp \left[- \int_V \beta(\vec{x}, t_2) h(\vec{x}, t_2) d^3 x \right] \quad (53)$$

Notice there is no time integral in (53). In contrast to the driving phase (51) in which the driving constraint can vary arbitrarily over time, the constraint governing relaxation is deterministic. Thus the a time-integral that takes memory effects into account is redundant. All that is needed is the initial condition given by ρ_t at $t = t_1$.

The corresponding time-dependent entropy during relaxation is given as

$$S_{int}(t) = \ln Z(t) + \int_V \beta(\vec{x}, t) \langle h(\vec{x}, t) \rangle_t d^3 x \quad (54)$$

It is perhaps misleading to label this $S_{int}(t)$, incorrectly suggesting $S_{tot}(t) = S_t(t) + S_{int}(t)$. Changes in the time-dependent entropy can have two different contributions, as in (18) and (50). But the time-dependent entropy itself does not have two components like $S_{tot}(t) = S_t(t) + S_{int}(t)$. The label S_{int} in (54) is just meant to distinguish how this entropy is calculated using deterministic constraints, in distinction from (52) which is calculated from arbitrary driving that must take memory of the driving process into account.

Since we can readily solve Fourier’s law for the relaxation constraints $\langle h(\vec{x}, t) \rangle$ we can take the $t_2 \rightarrow \infty$ limit. This yields the expected equilibrium results

$$\rho_{eq} = \frac{1}{Z} e^{-\beta H} \quad (55)$$

$$S_{eq} = \ln Z + \beta \langle H \rangle_0 \quad (56)$$

Note that the equilibrium constraint $\langle H \rangle_0 = \int_V \langle h(\vec{x}, \infty) \rangle$ is already determined at $t = t_1$ since this is when the driving is turned off and the system is isolated. From this point

on the total energy, and thus $\langle H \rangle_0$ is fixed. So the statistical operator during the relaxation phase (53) is always determined by at least as many constraints as the eventual equilibrium distribution (55). Thus the entropy during relaxation (54) is maximized subject to more (or the same) number of constraints as the equilibrium entropy (56), and thus over a more restricted class of variations. This means $S_{int}(t) \leq S_{eq}$, and so $\dot{S}_{int} \geq 0$, in agreement with the thermodynamic postulate (19).

To conclude the discussion of entropy production in the nonequilibrium PME formalism, we once again look at a heat conduction example. This time we look at a near-equilibrium steady-state distribution

$$\rho_{st} = \frac{1}{Z_{st}} \exp \left[-\beta H + \int_R \nabla \lambda(\vec{x}) \cdot \vec{q}(\vec{x}) d^3 x \right] \quad (57)$$

where $\vec{q}(\vec{x})$ is the energy current operator conjugate to the energy density $h(\vec{x})$ and $\lambda(\vec{x})$ is the Lagrange multiplier of $h(\vec{x})$. The linear approximation of the deviation of entropy from the equilibrium state is

$$S_{st} - S_0 \approx -\frac{1}{2} \int_R \int_R \nabla \lambda(\vec{x}) K_{qq}^0(\vec{x} - \vec{x}') \nabla' \lambda(\vec{x}') d^3 x d^3 x' \quad (58)$$

Evaluation of the linear covariance function $K_{qq}^0 = 2k\kappa T^2(\vec{x})\delta(\vec{x} - \vec{x}')$ and $\lambda(\vec{x}) = \frac{1}{T(\vec{x})}$ gives thermodynamic result for entropy production (30).

Dynamical Systems Perspective

In an approach similar to the nonequilibrium PME formalism, we next consider a nonequilibrium process as a symbolic dynamics problem [14]. The micro scale is the deterministic dynamical system with phase space Γ and evolution $\Phi : \Gamma \rightarrow \Gamma$. As discussed above, the microstates are generally not observable, and we thus have the notion of a macro scale in which the macrostates $\omega \in \Omega$ form a finite disjoint partition of the micro scale phase-space Γ ,

$$\Gamma = \bigcup_{\omega=1}^N C_\omega \quad (59)$$

where C_ω are the phase-space cells of Γ that correspond to the macrostate $\omega \in \Omega$. Consistent with the notions of microstates and macrostates in statistical mechanics, each measurement observable is a many-to-one mapping, with each microstate mapping uniquely to a single macrostate, but each macrostate can have many distinct microstates that map to that macrostate. Formally, a measurement observable is the mapping $M : x \in \Gamma \rightarrow \omega \in \Omega$, and the phase-space cells are given as $C_\omega = M^{-1}[\{\omega\}] = \{x \in \Gamma : M[x] = \omega\}$.

On the micro scale, the nonequilibrium process is simply the dynamical evolution $x(t = k) = \Phi^k x_0$, using discrete time for simplicity. The macroscopic time-series $\omega(t = k) = M\Phi^k x_0$ is then a course-grained description of the process. However, the

microstates are not observable and so the initial conditions for the nonequilibrium process can not be a single microstate $x_0 \in \Gamma$, but rather a distribution of microstates $\varrho_0 : \Gamma \rightarrow \mathbb{R}$. This can be from either using a single macrostate or a distribution of macrostates as the initial condition for the nonequilibrium process. The macro scale evolution can either be deterministic (hydrodynamics, Fourier's law, etc.) or stochastic (Langevin equation, etc.).

For generality, let's start with an initial macrostate distribution $\bar{p}^{(0)}$. We then use the PME to generate the appropriate distribution over microstates $\varrho^{(0)}$ consistent with the macroscopic constraints $M[\{x \in \varrho^{(0)}\}] = \{\omega \in \bar{p}^{(0)}\}$. Now propagate forward in time on both the micro and macro scales. The micro scale evolution Φ evolves single microstates $x \in \Gamma$ forward in time. To evolve the distribution $\varrho^{(0)}$ of microstates forward, the Perron-Frobenius operator is used. This yields the fine-grained time evolved distribution

$$\varrho_{\text{fg}}^{(\tau)}(x) = \frac{\varrho^{(0)}(\Phi^{-1}(x))}{J^{(\tau)}(\Phi^{-1}(x))} \quad (60)$$

where $J^{(\tau)} = \prod_{k=1}^{\tau} J(\Phi^k(x))$, and J is the Jacobian determinant of Φ .

Macro scale time evolution $\bar{p}^{(\tau)}$ of $\bar{p}^{(0)}$ is done via an appropriate effective theory (like Fourier's Law, Langevin equation, etc) or simply another measurement is made after time τ . This represents the time evolved (observable) macro scale constraints on the underlying dynamical system. Thus we again use the PME to infer the appropriate distribution over Γ subject to these new constraints $M[\{x \in \varrho_{\text{cg}}^{(\tau)}\}] = \{\omega \in \bar{p}^{(\tau)}\}$ to get the course-grained distribution $\varrho_{\text{cg}}^{(\tau)}$.

We must assume a mutual consistency between scales.

$$\int_{C_\omega} \varrho_{\text{fg}}^{(\tau)} dx = \bar{p}^{(\tau)} \quad (61)$$

That is to say, the description on each scale is describing the same physical process and everything is properly accounted for. We don't want, for example, the distribution over macrostates that is experimentally observed actually being influenced by an external field that is not included in Φ .

Since $\varrho_{\text{fg}}^{(\tau)}$ takes all microscopic correlations into account during the evolution Φ , it is generally true that $\varrho_{\text{fg}}^{(\tau)} \neq \varrho_{\text{cg}}^{(\tau)}$, while (by definition) $\varrho_{\text{fg}}^{(0)} = \varrho_{\text{cg}}^{(0)}$. We therefore define the relative entropy as

$$S_{\text{rel}}^{(t)} = \mathcal{D}_{\text{KL}}[\varrho_{\text{fg}}^{(t)} || \varrho_{\text{cg}}^{(t)}] \quad (62)$$

where $\mathcal{D}_{\text{KL}}[\varrho || \varrho'] = \int \varrho \ln \frac{\varrho}{\varrho'} dx$ is the Kullback-Liebler divergence of ϱ' from ϱ . It measures the amount of information lost when assuming the distribution ϱ' when the actual distribution being sampled from is ϱ . Thus $S_{\text{rel}}^{(t)}$ measures the information lost when using assuming $\varrho_{\text{cg}}^{(t)}$ upon observation of $\bar{p}^{(t)}$ when it is actually being sampled from $\varrho_{\text{fg}}^{(t)}$. This wonderfully quantifies the intuition that has been around since Jaynes that entropy

production is a loss of information that is dynamically written to inaccessible degrees of freedom. In fact, in the context of stochastic thermodynamics, the authors of [14] show that this is indeed the case.

$$\Delta S_{\text{tot}}^{(t)} = \Delta S_{\text{sys}}^{(t)} + \Delta S_{\text{env}}^{(t)} = d_i S_{\text{tot}}^{(t)} = S_{\text{rel}}^{(t)} \quad (63)$$

The Kullback-Liebler divergence is non-negative, and therefore (63) is consistent with $d_i S \geq 0$.

Before moving on, we point out the similarity with nonequilibrium PME. Again start with some initial macroscopic constraint $\vec{p}^{(0)}$ and infer an initial microscopic distribution in the form of a statistical operator $\rho^{(0)}$. Use the time evolution of the macroscopic constraints, via an effective theory or measurement/observation, to produce the course-grained distribution $\rho_{\text{cg}}^{(t)}$, similar to (53). The fine-grained statistical operator is produced via unitary time evolution with the appropriate many-body Hamiltonian. That is, $\rho_{\text{fg}}^{(t)}$ is the solution to $i\hbar\dot{\rho}_{\text{fg}}^{(t)} = [H, \rho_{\text{fg}}^{(t)}]$. Since the nonequilibrium PME has been used (as shown above) in the context of Classical Irreversible Thermodynamics, this could open the door for testing (63) in more traditional settings, in addition to stochastic thermodynamics.

Entropy Production as Correlation Between System and Reservoir

Another result bolstering the information-theoretic notion of entropy production as a loss of information to inaccessible degrees of freedom is developed in [15]. Consider a quantum system in contact with r finite reservoirs. By nature of being a reservoir, the corresponding Hamiltonian of each is time-independent and denoted as H_r . Being initially in thermal equilibrium, the associated density matrices for the reservoirs are $\rho_r(0) = \rho_r^{\text{eq}} = \exp(-\beta_r H_r)/Z_r$. At time $t=0$ the quantum system, with Hamiltonian $H_s(t)$, is connected to the reservoirs by switching on an interaction term $V(t)$. The total Hamiltonian is then

$$H(t) = H_s(t) + V(t) + \sum_r H_r \quad (64)$$

Initially the system and all reservoirs are independent and uncorrelated. The initial density matrix for the full set up is then

$$\rho(0) = \rho_s(0) \prod_r \rho_r \quad (65)$$

Since the evolution of the full system is unitary, the total entropy is time-translation invariant. This can be used to analyze the time-dependent entropy of the system that is in contact with the reservoirs

$$S(t) = -\text{Tr} \rho_s(t) \ln \rho_s(t) \quad (66)$$

$\rho_s(t)$ is the trace of $\rho(t)$ over the reservoir degrees of freedom and its time evolution is non-unitary. Hence the system entropy in (66) is in general a function of time. Using $-\text{Tr}\rho(t) \ln \rho(t) = -\text{Tr}\rho(0) \ln \rho(0) = -\text{Tr}\rho_s(0) \ln \rho_s(0) - \sum_r \text{Tr}\rho_r(0) \ln \rho_r(0)$ we find the entropy change for the system to be

$$\begin{aligned} \Delta S &= S(t) - S(0) \\ &= -\text{Tr}\rho(t) \ln \left[\rho_s(t) \prod_r \rho_r^{\text{eq}} \right] + \text{Tr}\rho(t) \ln \rho(t) \\ &\quad + \sum_r \text{Tr} [\rho_r(t) - \rho_r^{\text{eq}}] \ln \rho_r^{\text{eq}} \end{aligned} \tag{67}$$

This is of the familiar form $\Delta S(t) = \Delta_e S(t) + \Delta_i S(t)$, and after some algebra we find

$$\Delta_e S(t) = - \sum_r \beta_r (\langle H_r \rangle_t - \langle H_r \rangle_0) \tag{68}$$

where $\langle H_r \rangle_t = \text{Tr}[H_r \rho(t)]$ and $\langle H_r \rangle_0 = \text{Tr}[H_r \rho(0)]$. This is essentially just $d_e S = \frac{dQ}{T}$ for each reservoir. The entropy production again takes the form of a Kullback-Liebler divergence,

$$\Delta_i S(t) = \mathcal{D}[\rho(t) || \rho_s(t) \prod_r \rho_r^{\text{eq}}] \tag{69}$$

\mathcal{D} is the quantum equivalent of the Kullback-Liebler divergence and is given by

$$\mathcal{D}[\rho || \rho'] \equiv \text{Tr}\rho \ln \rho - \text{Tr}\rho \ln \rho' \tag{70}$$

The information-theoretic interpretation of entropy production here is the information lost by assuming the system never becomes correlated with the reservoirs. That is, the entropy production is the amount of information about the system flowing into the reservoirs, and thus becoming inaccessible.

Concluding Remarks and Discussion of Irreversibility

Through some recent work in nonequilibrium thermodynamics we have come to see that entropy production is the loss of information that is written to inaccessible degrees of freedom. This effect can be seen indirectly through macroscopic effects (58) (62), or directly via correlations with external reservoirs (69), and is nicely quantified using information theory. This is the fundamental difference between $d_e S$ and $d_i S$, which both contribution changes in the entropy $S = H[\text{micro}|\text{macro}]$. $d_e S$ moves information around in degrees of freedom that are macroscopically accessible, while $d_i S$ quantifies information being irreversibly lost to inaccessible degrees of freedom.

To give some more insight into this notion, consider the classic thermodynamics problem of the expansion of gas in a box. The box is partitioned in two via a movable wall with the gas on one side. Expansion or contraction occurs from motion of the wall.

If the expansion happens quasi-statically then there is no entropy production and the process is reversible. The gas can be compressed back to the original state and the information lost during expansion can be recovered. Otherwise there is a non-negative entropy production and the expansion produces irreversible changes.

How is information not irreversibly lost during quasi-static expansion? The answer comes from a combination of insights provided by Boltzmann and Jaynes. Boltzmann developed statistical mechanics and was the first to think of entropy as being related to the number of microstates associated with a macrostate (this number is called the multiplicity of the macrostate). He saw the 2nd Law as a consequence of increasing multiplicity. The equilibrium macrostate is the one that can be realized in the most number of ways. Jaynes thought of thermodynamics as an inference problem. Given the macroscopic constraints, what is the best inference that can be made about the microstate of the system? (These two views are completely equivalent. Information theory had not been formulated in Boltzmann's time, so while he was thinking in these terms he did not have the formal context of information theory that we have now). The key to why quasi-static processes have no irreversible losses of information is in the nature of how the constraints change in quasi-static processes. By definition, the constraints change so slowly that the system always remains in equilibrium and the process is a locus of equilibrium states. The fundamental nature of the constraints are the same at all points in the process, and thus the inferences we make are of the same nature. In Boltzmann terms, the multiplicity always remains at a maximum during the process. As the constraints slowly change so do the maximum value of the multiplicity, but the maximum is always maintained. This is why information flow only occurs through macroscopic degrees of freedom in quasi-static processes, and hence why that information can be recovered. One of the most visually stunning examples of information flowing through macroscopic degrees of freedom and then being recovered is the reversibility of low Reynolds number flow. There are plenty of fun videos of dye being mixed around in a clear cylinder, and then the cylinder is turned in the other direction and the dye perfectly de-mixes. Information certainly changes during the mixing, as $d_e S$ does change the information/entropy, it just does so in a reversible manner. This is why that information is recovered after de-mixing.

Contrast this to an irreversible process like completely removing the barrier from the box of gas rather than slowly sliding it along. Now the nature of the macroscopic constraints fundamentally change. In this example it has a jump discontinuity but there can be irreversible processes where this is not the case, like rapid compression of the gas etc. The sudden removal of the barrier creates thermodynamic forces and fluxes on the macro scale that are new types of constraints. Inference is now memory-dependent and complex micro scale interactions and correlations are occurring that can not be fully accounted for. We have seen some in-depth mathematical analysis of how this produces an irreversible loss of information. In Boltzmann terms, the multiplicity is no longer held at the maximum possible value at all times. Think of the standard Gaussian curve for multiplicity seen in introductory statistical mechanics textbooks for simple problems, like the gas in a box. The single Gaussian curve of multiplicities is for a fixed set of

constraints. In a quasi-static process, the system is always at the center of the Gaussian as the Gaussian slowly changes in response to the slow changes of constraints. While in a non quasi-static process the system is suddenly pulled off the center of the Gaussian. For the gas in a box, when it is in equilibrium in one half of the box with the wall in place it is sitting at the top of the multiplicity Gaussian corresponding to that constraint. Once the wall is removed, the multiplicity Gaussian for the eventual equilibrium state of being evenly distributed in the whole box is completely shifted. Where the system was at the center of the old Gaussian, it is now way off to the side somewhere on the new Gaussian. The march towards the new center is where the irreversibility occurs.

To close, we look at another interesting notion of entropy production that is known as the Crooks relation [16]

$$\sigma[x(t)] = \ln \frac{P[x(t)]}{\tilde{P}[\tilde{x}(t)]} \quad (71)$$

where $P[x(t)]$ is the probability of the forward process happening, while $\tilde{P}[\tilde{x}(t)]$ is the probability of the reverse process under reverse protocol. While (71) does not immediately seem information-theoretic in nature it certainly is a natural way to think about entropy production, which quantifies the irreversibility of a process. However, [14] and [15] both have shown (71) to be consistent with (62) and (69). That is, the loss of information to inaccessible degrees of freedom during the forward process is related to the difference in likelihood of the reverse process occurring. It is interesting to note that Bennett had this notion in mind when he was thinking of the entropy production in RNA transcription [17]. He was directly concerned with the relation between information transduction (computation) and thermodynamics, and intuitively made use of (71) before Crooks had formulated it. Bennett was thinking of energy dissipation via the entropy production as given by the Crooks relation (71) while at the same time thinking about the loss of information during the transcription process.

References

- [1] Ben-Naim, Arieh. *A Farewell to Entropy: Statistical Thermodynamics Based on Information*: S. World Scientific, 2008.
- [2] Onsager, Lars. "The effects of shape on the interaction of colloidal particles." *Annals of the New York Academy of Sciences* 51.4 (1949): 627-659.
- [3] Georgi, Howard. "Effective field theory." *Annual review of nuclear and particle science* 43.1 (1993): 209-252.
- [4] More Is Different P. W. Anderson *Science New Series*, Vol. 177, No. 4047 (Aug. 4, 1972), pp. 393-396
- [5] Crutchfield, James P. "Between order and chaos." *Nature Physics* 8.1 (2012): 17-24.

- [6] Jaynes, Edwin T. "Information theory and statistical mechanics." *Physical review* 106.4 (1957): 620.
- [7] Grandy, Jr Walter T. *Entropy and the time evolution of macroscopic systems*. Vol. 141. OUP Oxford, 2008.
- [8] Strong, Steven P., et al. "Entropy and information in neural spike trains." *Physical review letters* 80.1 (1998): 197.
- [9] Bialek, William, et al. "Statistical mechanics for natural flocks of birds." *Proceedings of the National Academy of Sciences* 109.13 (2012): 4786-4791.
- [10] Kondepudi, Dilip, and Ilya Prigogine. *Modern thermodynamics: from heat engines to dissipative structures*. John Wiley & Sons, 2014.
- [11] Cimmelli, Vito Antonio, et al. "Entropy principle and recent results in non-equilibrium theories." *Entropy* 16.3 (2014): 1756-1807.
- [12] Grandy Jr, Walter T. *Foundations of Statistical Mechanics: Volume I: Equilibrium Theory*. Vol. 1. Springer Science & Business Media, 1987.
- [13] Grandy Jr, Walter T. *Foundations of Statistical Mechanics: Volume II: Nonequilibrium Phenomena*. Vol. 2. Springer Science & Business Media, 1987.
- [14] Altaner, Bernhard; Vollmer, Jürgen A microscopic perspective on stochastic thermodynamics 2012arXiv1212.4728A
- [15] Esposito, Massimiliano, Katja Lindenberg, and Christian Van den Broeck. "Entropy production as correlation between system and reservoir." *New journal of physics* 12.1 (2010): 013013.
- [16] Crooks, Gavin E. "Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences." *Physical Review E* 60.3 (1999): 2721.
- [17] Bennett, Charles H. "The thermodynamics of computation—a review." *International Journal of Theoretical Physics* 21.12 (1982): 905-940.