Nonequilibrium thermodynamics as a gauge theory

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Abstract – We assume that markovian dynamics on a finite graph enjoys a gauge symmetry under local scalings of the probability density, derive the transformation law for the transition rates and interpret the thermodynamic force as a gauge potential. A widely accepted expression for the total entropy production of a system arises as the simplest gauge-invariant completion of the time derivative of Gibbs’s entropy. We show that transition rates can be given a simple physical characterization in terms of locally-detailed-balanced heat reservoirs. It follows that Clausius’s measure of irreversibility along a cyclic transformation is a geometric phase. In this picture, the gauge symmetry arises as the arbitrariness in the choice of a prior probability. Thermostatics depends on the information that is disposable to an observer; thermodynamics does not.

Introduction. – Open systems subject to dissipation are usually modelled through markovian dynamics and further characterized by nonequilibrium thermodynamics \([1]\). The link between dynamics and thermodynamics is the concept of thermodynamic force. In this work we assume that dynamics enjoys a gauge symmetry and show that the thermodynamical sector of the theory arises very naturally from the requirement that physical observables, in particular the entropy production, are gauge invariant. The driving force plays the role of gauge potential.

A gauge theory has an internal symmetry whose action leaves all physical observables invariant \([2]\). Strictly speaking, any symmetry leaves observables invariant, there comprising the choice of units and reference frames \([3]\). However, conventionally one refers to gauge symmetries as to supplementary redundancies of the variables, which are not related to space-time symmetries: hence “internal”. One copy of the internal space \(Ψ\), where the gauge symmetry acts, is thought to be attached to each point \(i\) of space-time, or more generally of a base manifold. The peculiarity of gauge symmetries is that they act locally, that is, pointwise differently. The tool to compare nearby transformations is the connection, or gauge potential, \(A\). Its transformation properties are employed to adjust observables \(e.g.\) the Lagrangian in field theories) in order to guarantee the internal consistency of the theory.

Crucial gauge-invariant observables can be built by circulating the connection along closed paths \(γ\) over the manifold, obtaining the Wilson loops of the theory

\[
W(γ) = \text{tr} \{ P \exp \oint_γ A \}.
\]

(1)

The trace over internal group-representation indices and the path-ordering operator \(P\) will be inessential in our theory. Wilson loops are the finite version of the curvature of a connection, telling how different paths between two given points carry different transformations. They play an even more prominent role in our understanding of many phenomena besides field theories, from adiabatic phases in quantum mechanics \([4]\) and quantum computation schemes \([5]\) to a proposal of quantum gravity \([6]\).

According to a celebrated theory by J. Schnakenberg \([1]\), the macroscopic external forces (affinities) that maintain a nonequilibrium system into a dissipative steady state are defined as circulations of the thermodynamic force. Schnakenberg claimed that affinities are the fundamental observables which characterize nonequilibrium steady states, bringing as evidence that they satisfy Onsager’s reciprocity relations in the regime where forces and currents are linearly related. Andrieux and Gaspard \([7]\) complemented his insight with a Green-Kubo relation for the linear response coefficients; the author proved that affinities serve as constraints for a formulation of the minimum entropy production principle near equilibrium \([8]\).
Schnakenberg’s theory applies to markovian evolution of a normalized probability density over a discrete space, obeying the master equation
\[ \dot{\rho}_i(\tau) = \sum_j J_{ij}(\tau) \rho_j(\tau) - w_{ij}\rho_i(\tau) \] (2)
where \( w_{ij} \) is a positive transition rate from site \( j \) to site \( i \), and \( J_{ij} = w_{ij}\rho_j - w_{ji}\rho_i \) is the probability current. In spite of space-time, the base manifold \( V \) consists of a number \( |V| \) of sites. We define for later convenience an order relation \( i < j \). Sites are pairwise connected by a number \( |E| \) of edges \( ij \in E \), which are assigned a conventional orientation \( ij \leftrightarrow i \). We assume that the graph \( G = (V,E) \) is connected and that forward and backward rates are nonnull along all edges. The prominent role played by circulations in Schnakenberg’s theory is an indicator that it is a gauge theory, with the driving force
\[ A_{ij} = \log \frac{w_{ij}}{w_{ji}}. \] (3)

He then advised to replace Laplace’s with the maximum entropy principle. So doing, he swept the dirt under the carpet, as the Shannon-Khintchin’s set of axioms for the entropy include equiprobability [15], and Shannon’s monotonicity axiom [14, p. 630] makes reference to it.

Moreover, alleged paradoxes are found in the continuous variables case, where the differential entropy [16, Ch.9]
\[ S(\rho) = -\int_X dx \rho(x) \log \rho(x) \] (5)
has been a source of dismay [17–19], for it is not invariant under a change of variables. In fact, letting \( x' \mapsto x(x') \) be invertible with Jacobian \( J(x') = \det(\partial x/\partial x') \), one has
\[ S(\rho) = S(\rho') + (\log J)_{\rho'} \] (6)
where the probability measure and its density transform respectively as a volume form and as a volume density,
\[ \rho'(x')dx' = \rho(x)dx, \quad \rho'(x') = J(x')\rho(x(x')). \] (7)

Related to this is the following riddle (from [20, Ch.8]): if we pick a number \( x \) between 1 and 10 at random, the probability that it is smaller than 5 is \( 1/2 \); but if we pick \( x' \) at random between 1 and 100, the probability that it is smaller than 25 is \( 1/4 \). How is it possible that picking either a number or its square aren’t equally likely? The solution to this puzzle is to recognize that the choice of an arbitrary prior is congenital. It hides in that “at random” which is the continuous counterpart of Laplace’s principle: in the first case we assume \( x \) is uniform, so that the prior is \( 1/10 \) dx; in the second we assume that \( x' = x^2 \) is uniform, with prior \( 1/100 \) dx' = \( 1/100 \) x dx. Formally, in order to make eq.(6) mathematically sound, one will interpret \( \rho(x) \) as the Radon-Nikodym derivative of the probability measure \( \rho(x)dx \) with respect to the arbitrary prior dx. A change of variables corresponds to a change of prior.

This is not, as Jaynes thought, an artifact of continuous variables. Think for example of a dice. Basing on visual impressions — which, by the way, are the result of a measure process — we might be tempted to assign equal probabilities \( 1/6 \) to each face. However, if we knew that an incredibly huge mass was hidden near one of its corners, due to friction with air and the inelastic impact with the gaming table, we would have sufficient reason
to believe that the three faces which are adjacent to the
loaded corner will have probability approximately ½, and the
others near zero. Our gambling strategy will depend
on this prior knowledge. As a way out, in spite of invok-
ing measure theory, up to additive constants we might just
regard (neg)entropy as a special case of relative entropy
\[ S(\rho \parallel \mu) = \sum_i p_i \log p_i / \rho_i^{(pr)} , \]
with respect to a uniform prior \( \rho_i^{(pr)} = |V|^{-1} \). We refer the
reader to Banavar and Maritan’s work [21] for some nice
physical implications of working with relative entropy.

The physical rationale is that the quantification of the
entropy of a system depends on the choice of the under-
lying degrees of freedom. If we assume that all configu-
5
rations of positions and momenta of a number of classical
particles are equiprobable, we implicitly coarse-grain the
atomic and subatomic structure. The question “how much
entropy.

Thermodynamics

manner, irregardless of our quantification of the system’s

comes the key point — if we put a gas in contact with

p-3

\[ \rho_i' = e^{-\phi_i} \rho_i \]

\[ J_{ij}' = J_{ij} \]

The following graph-theoretical analysis proves that
large than the number of the unknowns. The only universal

solution is \( \pi_{ij} = c, \forall i; j \); the constant can then be scaled
to unity with a redefinition of the time unit \( \tau \rightarrow \tau/c \).

We now face a seeming paradox. In fact, considering the
transformed master equation \( \dot{\rho}_i' = \sum_j J_{ij}' \) and keeping into
account eq.(9) and eq.(11), we obtain an equation which
is not equivalent to the starting master equation, eq.(2)!

The solution delves into the geometrical interpretation of
summation symbols. We introduce the incidence matrix

\[ \delta_{jk}^{ij} = \begin{cases} +1, & \text{if } j < k, \ k = i \\ -1, & \text{if } j < k, \ j = i \\ 0, & \text{elsewhere} \end{cases} \]

and rewrite the master equation as a continuity equation

\[ \dot{\rho}_i + \partial J = 0. \]

Technically speaking, the incidence matrix is a boundary
operator which maps edges into their boundary sites. Nor-
malization of the probability can be written as

\[ \sum_{i \in V} \rho_i = \partial \rho = 1 \]
where we introduced one further boundary operator \( \partial^0 = (1, 1, \ldots, 1) \), which maps sites to the connected component of the graph they belong to. Although this latter definition is rather trite, it gets more interesting when the graph has several disconnected components. Notice that \( \partial^0 \partial = 0 \), from which conservation of probability follows. Therefore “summation over \( i \)” has different geometrical meanings according to the context.

Strictly speaking, \( \rho_i \) should not be considered as a number, but rather as a one-component vector which lives in the internal vector space \( \Psi_i \cong \mathbb{R} \) which is attached to site \( i \). The gauge transformation eq.(9) is interpreted as a linear change of basis in \( \Psi_i \). It follows that we should consider the boundary operator’s entries as linear maps on \( \Psi_i \), which therefore transform according to

\[
\partial_i^0 e^{-\varphi_i} \partial_i^0 = e^{-\varphi_i} \partial_i^0,
\]

With this prescription, eq.s (15) and (16) are covariant. To simplify the notation a bit, we introduce a modified sum symbol \( \tilde{\sum} \) such that

\[
\tilde{\sum}_i \equiv \sum_i e^{\varphi_i}.
\]

This modified symbol is crucial for the up-coming result, so let us further linger on it. Consider the average of a gauge-invariant site function \( f = f(\chi) \) (a scalar field),

\[
(f)_\rho = \sum_i \rho_i f_i = \tilde{\sum}_i \rho_i f_i.
\]

Requiring gauge invariance \( \forall f \) yields the transformation law for the summation symbol. In other words, while the probability measure \( (\cdotp)_\rho \) is gauge invariant, the probability density \( \rho_i \) is, in analogy with the continuous variables case, see eq.(7).

We now focus on the Gibbs-Shannon entropy, which transforms according to

\[
\delta S = S'(\rho(\tau)) - S(\rho(\tau)) = \langle \varphi \rangle_\rho = -S(\rho' || \rho)
\]

where \( S' \) is calculated using \( \tilde{\sum}' \). On the r.h.s., the transformation law is succinctly expressed in terms of relative entropy. Remarkably, while relative entropy is not a difference of entropies, in this context it is naturally interpreted as (minus) the entropy change after a gauge transformation. The rate at which the entropy of the system changes is subject to

\[
\delta \dot{S} = \sum_{i<j} J_{ij}(\varphi_i - \varphi_j).
\]

In gauge theories, non-gauge invariant terms are adjusted with the introduction of a connection, which is an antisymmetric edge variable \( A_{ij} = -A_{ji} \) such that

\[
\delta A_{ij} = \varphi_j - \varphi_i.
\]

Once a connection is given, the term\(^1\)

\[
\sigma = \sum_{i<j} J_{ij} A_{ij}
\]

has a transformation law which balances eq.(21), making \( S + \sigma \) invariant. In principle, connections can be constructed as convex linear combinations of terms such as

\[
\log \frac{\rho_j^*}{\rho_j}, \quad \frac{\omega_j}{\omega_i}
\]

where \( \omega_i = \sum_k w_{ki} \) is the average frequency of a jump out of site \( i \). So, for example, adding \( \sum_{i<j} J_{ij} \log \frac{\rho_j^*}{\rho_j} \) yields the relative entropy with respect to the steady state. The latter plays an important role in the theory of Markov processes as a Lyapunov functional [1, Sec. V]; fitly, it is gauge invariant, while entropy \( \text{per se} \) is not. However, the options listed above are, technically speaking, exact: they are differences of site functions, so that their circuitations vanish, thus making the graph’s geometry rather dull. As a further consequence, gauge invariant terms obtained this way vanish at the steady state.

A good candidate as a “truly edge” connection variable is given by the driving force, defined in eq.(3). Although it is not the only antisymmetric edge variable that one could engineer which transforms according to eq.(22), it is certainly the simplest. Then \( S + \sigma \) coincides with Schnakenberg’s total entropy production [1, eq.(7.6)],

\[
\sigma_{\text{tot}} = \dot{S} + \sigma = \sum_{i<j} J_{ij} \log \frac{w_{ij}}{w_{ji}} \frac{\rho_j^*}{\rho_i}
\]

which is widely accepted as the entropy production rate of a Markov process [24, 25]. In this setting \( \sigma \) arises as the simplest term which completes \( \dot{S} \) into a gauge invariant quantity and which does not vanish at the steady state.

A gauge transformation will result in a shift of a total time derivative from \( \sigma \) to \( \dot{S} \), with a consequent redefinition of the internal entropy and of the entropy flow towards the environment. For example, letting \( \varphi_i = \log \rho_i^* \), we obtain

\[
\dot{S}' = -S(\rho || \rho^*), \quad \sigma' = \sum_{i<j} J_{ij} \log \frac{w_{ij}}{w_{ji}} \frac{\rho_j^*}{\rho_i},
\]

whose microscopic analogues along single stochastic trajectories have been interpreted by Esposito and Van den Broeck as non-adiabatic and adiabatic terms, obeying detailed fluctuation theorems [26]. Gauge transformations of fluctuation theorems will be discussed in a later work.

**Wilson loops.** – From a geometrical viewpoint [27], not only \( A \) provides a connection over the manifold, but it also constitutes a measure of the oriented length of paths along chains of edges \( \eta = (i_1, i_2, \ldots, i_n) \),

\[
\Sigma(\eta) = \sum_{k=1}^n A_{i_ki_{k+1}} = \int_\eta A.
\]

Since the length is additive upon composition of paths, the real positive numbers obtained by exponentiating \( \Sigma(\eta) \) can be thought of as elements in the multiplicative group of real positive numbers (\( \mathbb{R}^+ \), \( \times \)), which is the gauge group of the theory. In the representation theory of groups,
group elements are not seen as “static” objects, but rather as “active” linear maps; they act on vectors $\psi_i$ which live in the internal vector spaces $\Psi_i$. Such vectors acquire phases as they are parallel transported along paths, thus connecting far-apart sites,

$$\bar{\psi}_{i_n} = \exp \Sigma(\eta) \psi_{i_0},$$  \hspace{1cm} (28)

where $\bar{\psi}_{i_n}$ represents the result of parallel transport along path $\eta$. In our case, due to the very simple gauge group, the displaced vector is just a real number and parallel transport produces a scaling factor. The interpretation of group elements as linear maps further entails that new equivalent representations can be obtained by performing basis transformations in $\Psi_i$, one per each site: this yields a gauge transformation. In the case at hand, such a basis change amounts to an orientation-preserving rescaling $\psi_i^\prime = e^{\varphi_i} \psi_i$. Transformed vectors are parallel transported according to $\bar{\psi}_{i_n} = \exp \Sigma'_i \psi_i^\prime$, where $\Sigma'$ is a new representation of the group element, defined in terms of a transformed connection $A'$. Requiring equivalence with eq.(28) for any possible path $\eta$ yields the transformation law for $A$ in the internal vector spaces $\Psi_i$; it coincides with a spanning tree, $E = T$, has no cycles, hence it can only accomodate equilibrium systems. Then there exists a site function $\varphi_i = \beta u_i$ such that

$$w_{ij}/w_{ji} = e^{\beta(u_i-u_j)}, \hspace{1cm} ij \in T, \hspace{1cm}$$  \hspace{1cm} (32)

where we introduced an inverse temperature $\beta$, in units of Boltzmann’s constant. The inverse temperature and the energy $u_i$ are determined up to an energy shift and a rescaling of units, $u_i \rightarrow k(u_i + v)$, $\beta \rightarrow k^{-1}\beta$. In general, adding further edges $i_a, j_a$ to the graph will not result in a detailed balanced system, unless we fine-tune their rates. We then define a new set of temperatures $\beta_a$, such that

$$w_{i_a j_a}/w_{j_a i_a} = e^{\beta_a(u_{i_a}-u_{j_a})}, \hspace{1cm} i_a, j_a \in E \setminus T. \hspace{1cm}$$  \hspace{1cm} (33)

By definition, adding $i_a, j_a$ to the spanning tree generates a cycle $\gamma_a$, which can be oriented according to the orientation of $i_a, j_a$. By Euler’s formula, there are $|E| - |V| + 1$ such cycles. It is a basic graph-theoretical result that any loop can be decomposed in terms of the $\gamma_a$’s [31, Part I, Ch.4]. Let $c_{ij}^a = +1$ if $ij = i_a, j_a$, $-1$ if $ji = i_a, j_a$, otherwise it is zero. It can be shown that

$$\log \prod_a W(\gamma_a)^{c_{ij}^a} \sim A_{ij}. \hspace{1cm}$$  \hspace{1cm} (31)

Hence Wilson loops allow to reconstruct the gauge potential, up to gauge transformations [30]. By eq.(31), the choice of a spanning tree fixes the gauge by selecting one particular representative in the equivalence class of $A_{ij}$.

Spanning trees also allow to give a physical interpretation of the connection, as follows. Any graph which coincides with a spanning tree, $E = T$, has no cycles, hence it can only accomodate equilibrium systems. Then there exists a site function $\varphi_i = \beta u_i$ such that

$$w_{ij}/w_{ji} = e^{\beta(u_i-u_j)}, \hspace{1cm} ij \in T, \hspace{1cm}$$  \hspace{1cm} (32)

where we introduced an inverse temperature $\beta$, in units of Boltzmann’s constant. The inverse temperature and the energy $u_i$ are determined up to an energy shift and a rescaling of units, $u_i \rightarrow k(u_i + v)$, $\beta \rightarrow k^{-1}\beta$. In general, adding further edges $i_a, j_a$ to the graph will not result in a detailed balanced system, unless we fine-tune their rates. We then define a new set of temperatures $\beta_a$, such that

$$w_{i_a j_a}/w_{j_a i_a} = e^{\beta_a(u_{i_a}-u_{j_a})}, \hspace{1cm} i_a, j_a \in E \setminus T. \hspace{1cm}$$  \hspace{1cm} (33)

We just proved that the thermodynamics of any collection of transition rates can be described in terms of at most $|E| - |V|$ reservoirs, each at its own temperature, satisfying the condition of local detailed balance [32]. In this “minimal” case each transition is due to the interaction with exactly one reservoir. This ansatz allows to recast the basis Wilson loops in this form

$$W(\gamma_a) = \exp \left[ (\beta - \beta_a)(u_{i_a} - u_{j_a}) \right]. \hspace{1cm}$$  \hspace{1cm} (34)

Therefore, temperature differences are the fundamental thermodynamic forces of nonequilibrium systems, as one could expect. Since there is no external time-dependent driving, which would result in time-dependent transition rates, no work is performed by an external agent along one single realization of the process, and by the first law of stochastic thermodynamics [24], along a transition the energy gap $\delta u$ coincides with the heat exchanged $\delta q$. It is then illuminating to rewrite the geometric phase as

$$\log W(\gamma) = \int_\gamma \frac{\delta q}{T}, \hspace{1cm}$$  \hspace{1cm} (35)

yielding Clausius’s measure of irreversibility along one realization of a cyclic irreversible process. The length $\Sigma(\eta)$ is the entropy exchanged with the environment along any trajectory which performs a sequence of jumps, whichever the jumping times might be. This notion is completely independent of the time parametrization of the trajectory: it is purely geometrical.
REFERENCES


Final remarks. — The above construction can be easily generalized to Markov processes with time-dependent transition rates and to time-dependent gauge transformations. In this respect, our formalism has evident points of contact with stochastic pumping along cyclic protocols, whose geometrical nature has been recently studied [33]. It would be a conceptual advance to give a unified description of both aspects of NESM. We notice in passing that a Schnakenberg-type analysis is still lacking. The identification of ours as a gauge transformations is justified by the usage of the gauge machinery, which is analogous to well-established practice for the formalization of geometric phases in QM and of electromagnetism as a U(1) gauge theory. Employing analogies with the latter, C. Timm [37] discussed a slightly different gauge-theoretic structure for master equations.

To conclude, while we are conscious that the very simple gauge group makes the geometrization of irreversible thermodynamics unnecessary for all practical purposes, it allows to better appreciate the importance of macroscopic affinities as fundamental observables, and it might serve as a good starting ground for later generalizations. We point out that a Schnakenberg-type analysis is still lacking for quantum nonequilibrium systems, either described by a Lindblad-type equation or by a more general interaction of a system with reservoirs of quantum degrees of freedom. It is tenable that excursions to the quantum world might require more interesting gauge groups and a more pertinent application of gauge theory.

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REFERENCES


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