

Dissipation, interaction, and relative entropy

B. Gaveau

Laboratoire analyse et physique mathématique, 14 avenue Félix Faure, F-75015 Paris, France

L. Granger

Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, D-01187 Dresden, Germany

M. Moreau

Université Pierre et Marie Curie, LPTMC, case 121, 4 place Jussieu, F-75252 Paris cedex 05, France

L. S. Schulman*

Physics Department, Clarkson University, Potsdam, New York 13699-5820, USA

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Many thermodynamic relations involve inequalities, with equality if a process does not involve dissipation. In this article we provide equalities in which the dissipative contribution is shown to involve the relative entropy (also called the Kullback-Leibler divergence). The processes considered are general time evolutions in both classical and quantum mechanics, and the initial state is sometimes thermal, sometimes partially so. As an application, the relative entropy is related to transport coefficients.

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I. INTRODUCTION

Dissipation reflects the profound distinction between work and heat in finite-time dynamical processes. In this article we relate dissipation to *relative entropy*, a quantity that we use to distinguish between actual and idealized time evolution as we explain below. This relation was introduced as a technical tool for calculations in our [1] and [2], in the context of stochastic dynamics, in order to extend the fluctuation-dissipation theorem as well as Onsager relations for the reduced dynamics of slow variables, even in the non-detailed-balance situation. In this article, we use exact unitary or symplectic dynamics; it follows immediately that the entropy of the true state remains constant during the exact evolution.

On the other hand, in thermodynamics, in kinetic theories, or in stochastic dynamics, by definition the true state of a system is replaced by an idealized coarse graining and as a consequence, the true evolution is replaced by an idealized evolution of the corresponding coarse-grained state (or by a quasistatic evolution in thermodynamics). There are two good reasons for using this idealization:

(1) It is impossible—even in principle—to specify the exact state of a large system. An attempt at extremely high precision would modify the system, even in a classical context (related to Maxwell’s demon). And it is even worse for quantum systems.

(2) Only slow variables can be measured with confidence and stability. As a result, an observer can describe the system only as a state of minimal information (or maximal entropy) compatible with the observed slow variables [3–6]. During the idealized evolution, information is lost by the observer and the increasing entropy of the idealized state measures this loss; however, under exact symplectic or unitary evolution the entropy of the true state remains constant. Thus, entropy flow

or production and dissipation measure the human observer’s partial inability to relate the exact microscopic theory of the evolution of a system to the macroscopic description of the same evolution.

Standard thermodynamics uses the maximal coarse graining of equilibrium, and the idealized evolution is not modeled explicitly, so the dissipation can be taken into account only by inequalities. For more detailed coarse graining (as in hydrodynamics, Boltzmann’s equation, kinetic theories, or stochastic thermodynamics) one can obtain an estimate for the dissipative effects, for example, by the calculation of transport coefficients.

In this article, our main purpose is to prove that the relative entropy terms between initial and final states measure the dissipation in the case of the exact dynamics, quantum or classical (as was noted already in [1,2] for stochastic dynamics), and to show that they are zero if and only if the interaction energy is zero. Generally, dissipative effects are measured by transport coefficients. Thus, we need prove that the relative entropy allows the calculation of transport coefficients. Indeed, we show below that the relative entropy terms provide the calculation of the thermal conductivity between two general quantum systems, initially at thermal equilibrium at different temperatures. This is a kind of Fourier law, except that we do not assume a linear regime, so that the dependence upon temperatures is more complicated than just their difference. Moreover, our exact calculation of the transport coefficient shows that it is indeed proportional to the square of the interaction energy, which confirms that for vanishingly small interaction energy, no transfer occurs in finite time. In other words, no power or finite rate of information flow can be extracted from a system if one does not have at the same time dissipative effects.

What emerges from our work is a general view in which dissipation comes from the loss of average microscopic information between the exact state and the information carried

*schulman@clarkson.edu

by the initial state, but averaged over the actual state: this quantity is exactly the relative entropy [1,7] (also known as the Kullback-Leibler divergence) between the actual true state and the coarse-grained initial state. As this quantity is always positive, it provides a lower bound for the interaction energy or an upper bound for the work that one can extract from the system.

In the following material, we first consider a two-component system A and B . There is no hypothesis on the size of the systems, and we do not introduce thermal reservoirs. Thus, the identities we derive are exact. In Secs. III–V, we recall various identities, including a derivation of the Brillouin-Landauer estimate, an estimate of the work that can be extracted from a two-part system in interaction with an external source of work in terms of nonequilibrium free energies and the relative entropy of the state before and after the evolution. Similar identities were also obtained recently in [8,9] and [10]. Continuing, we study the effect of an external agent on an (otherwise) isolated system; again we obtain an identity relating the work to the difference of internal (not free) energies and the usual dissipative terms. In this we go beyond Refs. [8–10]. Finally, we derive the relation between the relative entropy and the heat conductivity in a quantum system. In some of our examples one or both systems are initially at thermal equilibrium, but only the initial temperatures appear explicitly in the definition of the nonequilibrium free energies. These free energies are no longer state functions because they depend explicitly on the initial temperature and not on the actual effective temperature. No coarse graining by an effective final or intermediate thermal state is used, and neither system is a reservoir.

II. DEFINITIONS AND NOTATION

Denote the state of a classical or quantum system by ρ . “Tr A ” indicates either an integral in phase space (classical observable) or the trace in Hilbert space (quantum observable). For both, $\rho \geq 0$ and $\text{Tr} \rho = 1$. The entropy of ρ is defined as $S(\rho) \equiv -\text{Tr} \rho \log \rho$ (the logarithm is to base e throughout). For states ρ and ρ' , the relative entropy is $S(\rho|\rho') \equiv \text{Tr}[\rho(\log \rho - \log \rho')]$. It is known [7] that $S(\rho|\rho') \geq 0$, with equality iff $\rho = \rho'$. It is identically true that

$$S(\rho|\rho') = S(\rho') - S(\rho) - \text{Tr}[(\rho - \rho') \log \rho'], \quad (1)$$

and this identity lies behind all results in the present article. If U is an evolution operator for some time interval, either symplectic or unitary, and A an observable, let $A^{(U)}$ denote the evolute of A ; e.g., in the quantum case, $\rho^{(U)} = U\rho U^\dagger$. For Φ a function of ρ , we also define $\delta^{(U)}\Phi(\rho) \equiv \Phi(\rho^{(U)}) - \Phi(\rho)$.

In particular, if $\Phi(\rho) = \text{Tr}_B \rho = \rho_A$, then

$$\delta^{(U)}\rho_A = \rho_A^{(U)} - \rho_A, \quad (2)$$

where

$$\rho_A^{(U)} = \text{Tr}_B \rho^{(U)}. \quad (3)$$

Notice that $\rho_A^{(U)}$ is the partial trace over B of the evolved state $\rho^{(U)}$, not the evolution of ρ_A by an internal dynamics of A (this would be nonphysical in the case where A is coupled to other systems).

III. INFORMATION AND ENERGY TRANSFERS IN INTERACTING SYSTEMS

Let A and B denote interacting systems, with respective Hamiltonians H_A and H_B , and interaction energy V . The energy expectations are $E_A(\rho) = \text{Tr}(H_A\rho)$, $E_V(\rho) = \text{Tr}(V\rho)$, etc. Energy conservation under evolution by U requires

$$\delta^{(U)}[E_A(\rho) + E_B(\rho) + E_V(\rho)] = 0. \quad (4)$$

For ρ a state of $A + B$, let $\rho_A \equiv \text{Tr}_B \rho$ and $\rho_B \equiv \text{Tr}_A \rho$. We take the initial (time-0) state of $A + B$ to be

$$\rho_0 = \rho_A(\beta_A) \otimes \rho_{B0}, \quad (5)$$

where $\rho_A(\beta_A) = \exp(-\beta_A H_A)/Z_A(\beta_A)$ is the thermal state at temperature $T_A \equiv \beta_A^{-1}$ and ρ_{B0} is any state of B . We immediately deduce from Eq. (1)

$$\begin{aligned} \beta_A \delta^{(U)} E_A(\rho) &= -\delta^{(U)} S(\rho_B) + [S(\rho^{(U)}|\rho_A^{(U)} \otimes \rho_B^{(U)}) \\ &\quad + S(\rho_A^{(U)}|\rho_A(\beta_A))]. \end{aligned} \quad (6)$$

This equation can be checked directly, as follows. One has

$$S(\rho^{(U)}|\rho_A^{(U)} \otimes \rho_B^{(U)}) = -S(\rho^{(U)}) + S(\rho_A^{(U)}) + S(\rho_B^{(U)}). \quad (7)$$

But $S(\rho^{(U)}) = S(\rho_0) = S(\rho_A(\beta_A)) + S(\rho_{B0})$. This is because for the exact evolution the entropy remains constant. Therefore

$$S(\rho^{(U)}|\rho_A^{(U)} \otimes \rho_B^{(U)}) = \delta^{(U)} S(\rho_B) + S(\rho_A^{(U)}) - S(\rho_A(\beta_A)). \quad (8)$$

Then

$$\begin{aligned} S(\rho_A^{(U)}|\rho_A(\beta_A)) &= -S(\rho_A^{(U)}) + \beta_A [E_A(\rho_A^{(U)}) - F_A(\beta_A)] \\ &= -S(\rho_A^{(U)}) + \beta_A \delta^{(U)} E_A(\rho_A) + S(\rho_A(\beta_A)). \end{aligned} \quad (9)$$

Adding Eqs. (8) and (9), we obtain the identity (6).

For similar results, see [9] and [8]. In particular, if the evolution U is such that $\delta^{(U)} S(\rho_B) \leq 0$ (so that the information content of B has increased), then

$$\beta_A \delta^{(U)} E_A(\rho) \geq |\delta^{(U)} S(\rho_B)|. \quad (10)$$

This implies that the energy of A has *increased* [or that the energy $E_B(\rho) + E_V(\rho)$ has decreased]. Thus a transfer of information to B implies a transfer of energy from B to A [11,12,14–16]. Moreover, the equality (10) is attained only when $\rho_A^{(U)} = \rho_A(\beta_A)$ and $\rho^{(U)} = \rho_A^{(U)} \otimes \rho_B^{(U)}$, in which case $\delta^{(U)} E_A(\rho) = 0$, $\delta^{(U)} S(\rho_B) = 0$, and no transfer has occurred. Finally, if $\rho_A^{(U)} = \rho_A(\beta_A)$, then $\delta^{(U)} E_A(\rho) = 0$ and from Eq. (10), $\delta^{(U)} S(\rho_B) = 0$. In particular, if A is a true thermal bath (unchanged by the evolution) it cannot be used to lower the entropy of another system, B .

Remark. In Eq. (6) the expression in square brackets is positive. Note too that $S(\rho^{(U)}|\rho_A^{(U)} \otimes \rho_B^{(U)})$ is the mutual information between A and B in the state $\rho_A^{(U)}$. We further remark that Eq. (6) is true even if U does not conserve energy and if H_B is time dependent (but H_A must be time independent). However, Eq. (6) does demand of U that entropy be constant under its action.

IV. WHEN THE SYSTEMS ARE INITIALLY IN EQUILIBRIUM

Assume now that A and B are in thermal equilibrium states (with $T_B \equiv \beta_B^{-1}$) at $t = 0$ so that

$$\rho_0 = \rho_A(\beta_A) \otimes \rho_B(\beta_B). \quad (11)$$

Then the following identities can be deduced:

$$-\delta^{(U)} E_V(\rho) = (1 - \beta_A/\beta_B)\delta^{(U)} E_A(\rho) + T_B S(\rho^{(U)}|\rho_0), \quad (12)$$

$$\beta_A \delta^{(U)} E_A(\rho) + \beta_B \delta^{(U)} E_B(\rho) = S(\rho^{(U)}|\rho_0), \quad (13)$$

$$\begin{aligned} \delta^{(U)} E_A(\rho) + \delta^{(U)} E_B(\rho) &= T_A \delta^{(U)} S(\rho_A) + T_B \delta^{(U)} S(\rho_B) \\ &+ [T_A \delta^{(U)} S(\rho_A^{(U)}|\rho_A(\beta_A)) \\ &+ T_B \delta^{(U)} S(\rho_B^{(U)}|\rho_B(\beta_B))]. \end{aligned} \quad (14)$$

From this one can derive corresponding inequalities, for example,

$$-\delta^{(U)} E_V(\rho) \geq (1 - \beta_A/\beta_B)\delta^{(U)} E_A(\rho), \quad (15)$$

$$\beta_A \delta^{(U)} E_A(\rho) + \beta_B \delta^{(U)} E_B(\rho) \geq 0, \quad (16)$$

$$\delta^{(U)} E_A(\rho) + \delta^{(U)} E_B(\rho) \geq T_A \delta^{(U)} S(\rho_A) + T_B \delta^{(U)} S(\rho_B). \quad (17)$$

These relations imply important theoretical and practical conclusions. If, for instance, $T_A > T_B$ and $\delta^{(U)} E_A(\rho) < 0$, it follows from (15) that $\delta^{(U)} E_V(\rho) < 0$ and that the interaction energy cannot be neglected, contrary to current approximations. On the other hand, one sees that (16) is the Clausius inequality. It should be pointed out that the equalities (12)–(14) are much stronger than the corresponding inequalities (15)–(17). In particular, (12)–(14) show that these inequalities are changed into equalities iff there are no changes under the evolution operator U . On the other hand, the last term in the right-hand side of (14) can be interpreted as the energy dissipation, which is thus expressed in terms of relative entropies.

Remark. Some of the above relations have greater validity than so far stated. For example, Eqs. (14) and (17) are valid even if U is a general evolution, not even conserving energy. On the other hand, Eqs. (12), (13) and (15), (16) require conservation of energy as well as of entropy, which is satisfied for unitary or symplectic evolution. Finally, since all these equations refer to the temperature of B , it is clear that ρ_B must be thermal.

V. INTERACTING SYSTEMS COUPLED TO A WORK SOURCE

As before, A and B interact, but now A is coupled to an external source of work and its Hamiltonian becomes $H_A(\lambda)$, with the parameter λ taking the value λ_0 at time 0. The initial state is now written $\rho_0 = \rho_{A,0} \otimes \rho(\beta_B)$ (so B is in a thermal state, but A may not be). The external observer can modify λ , and at the end of the evolution U , λ has some value $\lambda^{(U)}$. Then

the work $\delta^{(U)} W$ received by the external observer is

$$\begin{aligned} \delta^{(U)} W &= -\delta^{(U)} E_V(\rho) - \delta^{(U)} F_A(\rho_A, \beta_B) \\ &- T_B [S(\rho^{(U)}|\rho_A^{(U)} \otimes \rho_B^{(U)}) + S(\rho_B^{(U)}|\rho_B(\beta_B))], \end{aligned} \quad (18)$$

where

$$\begin{aligned} \delta^{(U)} F_A(\rho_A, \beta_B) &= [E_A(\rho_A^{(U)}) - T_B S(\rho_A^{(U)})] \\ &- [E_A(\rho_{A,0}) - T_B S(\rho_{A,0})] \end{aligned} \quad (19)$$

is the variation of the (nonequilibrium) free energy of A , calculated at temperature T_B , and

$$\begin{aligned} E_A(\rho_A^{(U)}) &= \text{Tr}[\rho_A^{(U)} H_A(\lambda^{(U)})], \\ E_A(\rho_{A,0}) &= \text{Tr}[\rho_{A,0} H_A(\lambda_0)]. \end{aligned} \quad (20)$$

In particular we deduce

$$\delta^{(U)} W \leq -\delta^{(U)} E_V(\rho) - \delta^{(U)} F_A(\rho_A, \beta_B). \quad (21)$$

This inequality is analogous to, but more general than, the standard thermodynamic inequality concerning the work that can be extracted isothermally. Here the process need not be isothermal, B is not a heat bath, and A 's final state need not be equilibrium at temperature T_B . Moreover, we have equality in Eq. (21) iff $\rho_B^{(U)} = \rho_B(\beta_B)$ and $\rho^{(U)} = \rho_A^{(U)} \otimes \rho_B(\beta_B)$. Assume now that A and B are initially in thermal states at T_A and T_B , so that $\rho_0 = \rho_A(\beta_A, \lambda_0) \otimes \rho_B(\beta_B)$. The work received by the external observer is then

$$\begin{aligned} \delta^{(U)} W &= -\delta^{(U)} E_V(\rho) - (1 - \beta_B/\beta_A)\delta^{(U)} E_B(\rho) \\ &+ [F_A(\beta_A, \lambda_0) - F_A^{(U)}] \\ &- T_A [S(\rho^{(U)}|\rho_A^{(U)} \otimes \rho_B^{(U)}) + S(\rho_B^{(U)}|\rho_B(\beta_B))], \end{aligned} \quad (22)$$

where $F_A(\beta_A, \lambda_0)$ is the equilibrium free energy of A and $F_A^{(U)}$ is the final (nonequilibrium) free energy at temperature T_A ,

$$F_A^{(U)} = \text{Tr}[H_A(\lambda^{(U)})\rho_A^{(U)}] - T_A S(\rho_A^{(U)}). \quad (23)$$

If $\beta_A = \beta_B$ one obtains the inequality

$$\delta^{(U)} W \leq -\delta^{(U)} E_V(\rho) + F_A(\beta_A, \lambda_0) - F_A^{(U)}, \quad (24)$$

with equality iff $\rho_B^{(U)} = \rho_B(\beta_B)$ and $\rho^{(U)} = \rho_A^{(U)} \otimes \rho_B(\beta_A)$. Equation (24) is more general than the usual thermodynamic relation [5] in two ways: it includes the interaction energy $\delta^{(U)} E_V(\rho)$ and it involves a nonequilibrium free energy $F_A^{(U)}$ [defined by Eq. (23)] which, being equal to or greater than the equilibrium value, strengthens the inequality.

VI. SINGLE SYSTEM COUPLED TO A WORK SOURCE

A single system has Hamiltonian $H(\lambda)$, with changes in the external parameter λ corresponding to work. At $t = 0$, $\lambda = \lambda_0$, and we assume the state to be thermal: $\rho_0 = \exp[-\beta_0 H(\lambda_0)]/Z(\beta_0, \lambda_0)$. The external observer changes λ to $\lambda^{(U)}$, inducing an evolution U of the system which ultimately reaches the state $\rho^{(U)}$. Define the *adiabatic* temperature $\beta_a^{(U)}$ by

$$S(\rho^{(U)}) = S(\beta_a^{(U)}, \lambda^{(U)}), \quad (25)$$

with $S(\beta, \lambda)$ the entropy of the thermal state [17]. Then one has

$$\delta^{(U)}W = E(\beta_0, \lambda_0) - E(\beta_a^{(U)}, \lambda^{(U)}) - \frac{1}{\beta_a^{(U)}} S(\rho^{(U)} | \rho(\beta_a^{(U)}, \lambda^{(U)})), \quad (26)$$

with $E(\beta, \lambda)$ the energy of the thermal state. From this one deduces the standard [5] thermodynamic inequality for adiabatic processes,

$$\delta^{(U)}W \leq E(\beta_0, \lambda_0) - E(\beta_a^{(U)}, \lambda^{(U)}), \quad (27)$$

with equality iff $\rho^{(U)} = \rho(\beta_a^{(U)}, \lambda^{(U)})$. In particular, if the external observer imposes a cycle, namely, $\lambda^{(U)} = \lambda_0$, then $\beta_a^{(U)} = \beta_0$ and

$$\delta^{(U)}W = -\frac{1}{\beta_0} S(\rho^{(U)} | \rho(\beta_0, \lambda_0)) \leq 0. \quad (28)$$

Remark. The inequality Eq. (27) is different from those in the works of Jarzynski [18] and Kawai *et al.* [19]. One difference is that we use the *adiabatic* temperature [in Eq. (27)], while they use the initial temperature β_A . Although we have not proved it, it is possible that our Eq. (27) is the best possible. In addition, we use *internal* energy rather than free energy, which is more appropriate for an adiabatic process.

VII. RELATIVE ENTROPY AND TRANSPORT COEFFICIENTS

The previous identities can be transformed into inequalities similar to the standard inequalities of nonequilibrium thermodynamics using the positivity of the relative entropies appearing in these identities. Thus the relative entropy terms measure exactly the dissipative effects, coming from the fact that actual evolutions differ from idealized quasistatic processes. As an example, we deduce the transport coefficients, confirming the significance of the relative entropy.

Consider systems A and B , initially in equilibrium at temperatures β_A^{-1} and β_B^{-1} , respectively. The joint system $A + B$ evolves until a final time t . Let U or $U(t)$ denote the overall evolution operator from 0 to t . We wish to evaluate the flow of energy from A to B , and deduce an expression for the thermal conductivity.

Let $\rho(t)$ be the state at time t . Then, as shown above [Eq. (12)],

$$(\beta_A - \beta_B) \delta^{(U)} E_A(\rho_A) = \beta_B \delta^{(U)} E_V(\rho) + S(\rho(t) | \rho_A(\beta_A) \otimes \rho_B(\beta_B)). \quad (29)$$

We can estimate each term of the second member of Eq. (29) in the Born approximation, for systems A and B in the limits of continuous spectrum and t large. Then the interaction term $\delta^{(U)} E_V(\rho)$ becomes negligible, and in a calculation whose details we will present elsewhere [20], one obtains

$$\begin{aligned} \delta^{(U)} E_A(\rho_A) &\approx \frac{S(\rho(t) | \rho_A(\beta_A) \otimes \rho_B(\beta_B))}{\beta_A - \beta_B} \\ &\approx (\beta_A - \beta_B) K t. \end{aligned} \quad (30)$$

In this expression the term of principal interest is K , a thermal conductivity coefficient proportional to the square of the matrix element of the interaction energy V . In particular,

$$K = \frac{\pi}{\hbar Z_A(\beta_A) Z_B(\beta_B)} \int dE_A dE'_A dE_B dE'_B \times \phi(E_A, E'_A, E_B, E'_B), \quad (31)$$

where

$$\begin{aligned} \phi &= f_A(E_A) f_A(E'_A) f_B(E_B) f_B(E'_B) \\ &\times e^{-\beta_A E'_A - \beta_B E'_B} |V(E'_A, E'_B | E_A, E_B)|^2 \\ &\times \delta(E_A + E_B - E'_A - E'_B) \frac{E_A - E'_A}{\beta_A - \beta_B} \\ &\times (1 - e^{(\beta_A - \beta_B)(E_A - E'_A)}) > 0, \end{aligned} \quad (32)$$

and f_A and f_B are the densities of states of systems A and B . Equation (30) is a form of the Fourier heat law.

VIII. CONCLUSIONS

Equations (6) and (14) are identities for the energy exchange or information exchange between parts of a classical or quantum system evolving under the exact true dynamics, starting from a thermal state. The state of the system during its evolution is the true state and is a nonequilibrium state. In particular its entropy remains constant during the evolution. Thus there is no coarse graining of the evolution and these identities do not depend on a choice of a specific model (stochastic or kinetic). These identities contain relative entropy terms between the actual evolved state and the initial state, and because the relative entropy is positive, the consequences of these identities are inequalities which generalize the inequalities of nonequilibrium thermodynamics. See Eqs. (10) and (15)–(17). The relative entropy terms can be considered as general expressions measuring dissipation effects occurring internally between interacting parts of the system during its evolution. This is confirmed by the fact that one can deduce the thermal conductivity coefficient between two interacting parts of a system from an estimate of the relative entropy, as is seen in Eqs. (30) and (31). The same method also gives an identity, Eqs. (22) and (26), for the work exchanged between a system and an external agent and thus an inequality [Eqs. (24) and (27)] for the work that can be extracted from a system, together with an exact expression for the dissipation. We have also seen that the interaction energy, which is often neglected, can be used to give additional precision [cf. Eq. (22)] and is important in calculating transport coefficients [see Eqs. (31) and (32)].

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