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Thermodynamics of Weakly Coherent Collisional Models

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We introduce the idea of weakly coherent collisional models, where the elements of an environment interacting with a system of interest are prepared in states that are approximately thermal but have an amount of coherence proportional to a short system-environment interaction time in a scenario akin to well-known collisional models. We show that, in the continuous-time limit, the model allows for a clear formulation of the first and second laws of thermodynamics, which are modified to include a nontrivial contribution related to quantum coherence. Remarkably, we derive a bound showing that the degree of such coherence in the state of the elements of the environment represents a resource, which can be consumed to convert heat into an ordered (unitarylike) energy term in the system, even though no work is performed in the global dynamics. Our results therefore represent an instance where thermodynamics can be extended beyond thermal systems, opening the way for combining classical and quantum resources.

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Introduction.—The laws of thermodynamics provide operationally meaningful prescriptions on the tasks one may perform, given a set of available resources. The second law, in particular, sets strict bounds on the amount of work that can be extracted in a certain protocol. Most processes in nature, however, are not thermodynamic and therefore do not enjoy such a simple and far-reaching set of rules. One is then led to ask whether there exists scenarios “beyond thermal” for which a clear set of thermodynamic rules can nonetheless be constructed. This issue has recently been addressed, e.g., in the context of nonthermal heat engines [1–3], squeezed thermal baths [4–6], coherence amplification [7], information flows [8], and quantum resource theories [9–11]. The question also acquires additional meaning in light of recent experimental demonstrations that quantum effects can indeed be used as thermodynamic resources [12,13].

A framework that is particularly suited for addressing the thermodynamics of engineered reservoirs is that of collisional models (also called repeated interactions) [14–27]. They draw inspiration from Boltzmann’s original *Stosszahlansatz*: At any given interval of time, the system S will only interact with a tiny fraction of the environment. For instance, in Brownian motion, a particle interacts with only a few water molecules at a time. Moreover, this interaction lasts for an extremely short time, after which the molecule moves on, never to return [28]. Since the environment is large, the next molecule to arrive will be completely uncorrelated from the previous one, so the process repeats anew.

In the context of quantum systems, this process is depicted in Fig. 1, where the system S interacts sequentially

with a multiparty environment whose elements, henceforth dubbed ancillae A_n , are assumed to be mutually independent and prepared, in general, in arbitrary states. This process generates a stroboscopic evolution for the reduced density matrix of the system, akin to a discrete-time Markov chain. A continuous-time description in terms of a Lindblad master equation can be derived in the short-time limit, provided some assumptions are made about the system-ancilla interaction [16,18,27].

When the ancillae are prepared in thermal states, it is possible to quantitatively address quantities of key thermodynamic relevance, from work to heat currents and entropy [22–26]. This process includes both the stroboscopic case, where formal relations can be drawn with the resource theory of athermality [29,30], and the continuous-time limit [19,31]. The framework is also readily extended to systems coupled to multiple baths in an entirely consistent way [20,21,32]. Conversely, when the state of the ancillae is not

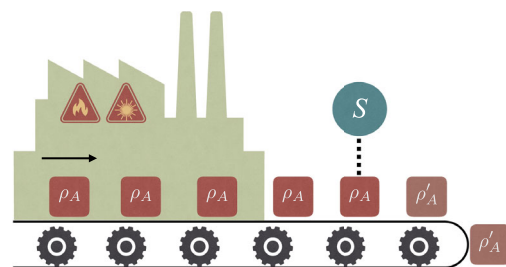


FIG. 1. Basic setup of weakly coherent collisional models. The system is allowed to interact sequentially with a series of independent ancillae prepared in states ρ_A , which are close to being thermal but have a small amount of coherence [cf. Eq. (5)].

thermal, much less can be said about its thermodynamic properties.

An important contribution in this direction was given in Refs. [19,33], which put forth a general framework for describing the thermodynamics of collisional models. However, for general ancillary states, the second law of thermodynamics is expressed in terms of system-ancilla correlations and the changes in the state of the ancillae [cf. Eq. (3) below]. These quantities are rarely accessible in practice, which greatly limits the operational use of such formulations.

Motivated by this search for “thermodynamics beyond thermal states,” in this Letter we draw a theoretical formulation of the laws of thermodynamics for the class of weakly coherent collisional models (Fig. 1), i.e., situations where the ancillae are prepared in states that, albeit close to thermal ones, retain a small amount of coherence. This case is realistic, as perfect thermal equilibrium is unlikely to be achieved in practice.

We show that, despite their weakness, the implications of such residual coherence for both the first and second laws of thermodynamics are striking, in that nontrivial contributions to the continuous-time open dynamics arise to affect the phenomenology of energy exchanges between system and environment [22]. In order to illustrate these features in a clear manner, we choose a scenario where no work is externally performed on the global system-ancilla compound [20,21,32], so all changes in the energy of the system can be faithfully attributed to heat flowing from or into the environment. Despite this choice, we derive a bound showing how coherence in the ancillae (quantified by the relative entropy of coherence) is consumed to convert part of the heat into a coherent (worklike) term in the system.

Our analysis thus entails that quantum coherence can embody a faithful resource in the energetics of open quantum systems [31]. Such a resource can be consumed to transform disordered energy (heat) into an ordered one (work), thus catalyzing the interconversion of thermodynamic energy exchanges of profoundly different nature and paving the way to the control and steering of the thermodynamics of quantum processes.

Collisional models.—We begin by describing the general structure of collisional models. A system S interacts with an arbitrary number of environmental ancillae A_1, A_2, \dots , all identically prepared in a certain state ρ_A . Each system-ancilla interaction lasts for a time τ and is governed by a unitary U_{SA_n} . The state of S after its interaction with A_n is embodied by the stroboscopic map

$$\rho_S((n+1)\tau) = \text{tr}_{A_n}(\rho'_{SA_n}) \equiv \text{tr}_{A_n}[U_{SA_n}(\rho_S(n\tau) \otimes \rho_A)U_{SA_n}^\dagger], \quad (1)$$

where $\rho_S(n\tau)$ is the state of S before the n th system-ancilla interaction.

Next, let H_S and H_{A_n} denote the free Hamiltonians of the system and ancillae. We define the heat exchanged in each interaction as the change in energy in the state of the ancilla [34–36] $Q_{A_n} = \text{tr}\{H_{A_n}(\rho'_{A_n} - \rho_{A_n})\}$, where $\rho'_{A_n} = \text{tr}_S \rho'_{SA_n}$. Work is then defined as the mismatch between Q_{A_n} and the change in energy of the system, $\Delta E_n = \text{tr}\{H_S[\rho_S((n+1)\tau) - \rho_S(n\tau)]\}$, leading to the usual first law of thermodynamics

$$\Delta E_n = W_n - Q_{A_n}. \quad (2)$$

As the global dynamics is unitary, the definition of work in this case is unambiguous, being associated with the cost of switching the S - A_n interaction on and off [20,21,32]. This work cost will be strictly zero whenever the system satisfies the condition [29,30] $[U_{SA_n}, H_S + H_{A_n}] = 0$, which states strict energy conservation. In this case, Eq. (2) reduces to $\Delta E_n = -Q_{A_n}$, which implies that all energy changes in the system can be unambiguously attributed to energy flowing to or from the ancillae. In order to highlight the role of quantum coherence, we assume this is the case throughout the Letter. The extension to the case where work is also present is straightforward.

The second law of thermodynamics for the map in Eq. (1) can be expressed as the positivity of the entropy production in each stroke, defined as [19,33]

$$\Sigma_n = \mathcal{I}(\rho'_{SA_n}) + S(\rho'_{A_n} \parallel \rho_{A_n}), \quad (3)$$

where $\mathcal{I}(\rho'_{SA_n}) = S(\rho'_S) + S(\rho'_{A_n}) - S(\rho'_{SA_n})$ is the mutual information between S and A_n after their joint evolution, $S(\rho'_{A_n} \parallel \rho_{A_n}) = \text{tr}(\rho'_{A_n} \ln \rho'_{A_n} - \rho'_{A_n} \ln \rho_{A_n})$ is the relative entropy between the initial and final states of A_n , and $S(\rho) = -\text{tr}(\rho \ln \rho)$ is the von Neumann entropy. Equation (3) quantifies the degree of irreversibility associated with tracing out the ancillae. It accounts not only for the system-ancilla correlations that are irretrievably lost in this process but also for the change in state of the ancilla, represented by the last term in Eq. (3). The two terms were recently compared in Refs. [24,37] and in the context of Landauer’s principle [34].

Continuous-time limit.—In the limit of small τ , Eq. (1) can be approximated by a Lindblad master equation. Such a limit requires a value of τ sufficiently small to allow us to approximate $\rho_S((n+1)\tau) - \rho_S(n\tau)$ as a sufficiently smooth derivative. Mathematically, in order to implement this, it is convenient to rescale the interaction potential V_{SA_n} between S and A_n by a factor $1/\sqrt{\tau}$ [16,18,27]. In other words, one assumes that the total S - A_n Hamiltonian is of the form

$$H_{SA_n} = H_S + H_{A_n} + V_{SA_n}/\sqrt{\tau} \quad (4)$$

with the unitary evolution $U_{SA_n} = \exp[-i\tau H_{SA_n}]$. This kind of rescaling, which enables the performance of the

continuous-time limit, is frequent in stochastic processes, e.g., in classical Brownian motion [38] or in the interaction with the radiation field [40].

Weakly coherent ancillae.—Finally, we specify the state of the ancillae, which is the main feature of our construction. We assume that the ancillae are prepared in a state of the form

$$\rho_A = \rho_A^{\text{th}} + \sqrt{\tau}\lambda\chi_A, \quad (5)$$

where $\rho_A^{\text{th}} = e^{-\beta H_A}/Z_A$ is a thermal state at the inverse temperature β (Z_A is the corresponding partition function). Here, χ_A is a Hermitian operator having no diagonal elements in the energy basis of H_A . Moreover, λ is a control parameter that measures the magnitude of the coherences. Notice that the term “weak coherences” is used here in the sense that we are interested specifically in the case where $\tau \rightarrow 0$, in which case the second term in Eq. (5) is much smaller in magnitude than the first. For finite τ , not all choices of χ_A lead to a positive semidefinite ρ_A . However, in the limit $\tau \rightarrow 0$, these constraints are relaxed, and any form of χ_A having no diagonal entries becomes allowed.

The scaling in Eq. (5) highlights an interesting feature of coherent collisional models, namely, that for a short τ and strong V_{SA_n} , even weak coherences already produce non-negligible contributions.

We use the unitary U_{SA_n} generated by Eq. (4) and the state in Eq. (5) in the map stated in Eq. (1). We then expand the latter in a power series of τ and take the limit $\tau \rightarrow 0$. This process then leads to the quantum master equation (cf. Ref. [41] for details)

$$\dot{\rho}_S = -i[H_S + \lambda G, \rho_S] + D(\rho_S), \quad (6)$$

where $\dot{\rho}_S = \lim_{\tau \rightarrow 0} [\rho_S((n+1)\tau) - \rho_S(n\tau)]/\tau$. We also define

$$D(\rho_S) = -\text{tr}_A[V_{SA}, [V_{SA}, \rho_S \otimes \rho_A^{\text{th}}]]/2, \quad (7)$$

representing the usual Lindblad dissipator associated with the thermal part ρ_A^{th} , and

$$G = \text{tr}_A(V_{SA}\chi_A), \quad (8)$$

representing a new unitary contribution stemming from the coherent part of ρ_A . In deriving Eq. (6), we have assumed that $\text{tr}_A(V_{SA}\rho_A^{\text{th}}) = 0$, as customary [42]. Equations (6)–(8) provide a general recipe for deriving quantum master equations in the presence of weak coherences. All one requires is the form of the system-ancilla interaction potential and the state of the ancillae. In the limit $\lambda \rightarrow 0$, one recovers the standard thermal master equation [16,18,27,32].

Eigenoperator interaction.—The physics of Eqs. (6)–(8) becomes clearer if one assumes a specific form for the interaction V_{SA} . A structure that is particularly illuminating, in light of the strict energy-conservation condition, is

$$V_{SA} = \sum_k g_k L_k^\dagger A_k + \text{H.c.}, \quad (9)$$

where g_k are complex coefficients and L_k and A_k are eigenoperators for the system and ancilla, respectively [43]. In other words, they satisfy the conditions $[H_S, L_k] = -\omega_k L_k$ and $[H_A, A_k] = -\omega_k A_k$, for the same set of Bohr frequencies $\{\omega_k\}$. This means that they function as lowering and raising operators for the energy basis of S and A . As both have the same ω_k , all of the energy leaving the system enters an ancilla and vice versa, so strict energy conservation is always satisfied.

The form taken by the dissipator in Eq. (7) when V_{SA} , as given above, is the standard thermal one,

$$D(\rho_S) = \sum_k \{\gamma_k^- \mathcal{D}[L_k] + \gamma_k^+ \mathcal{D}[L_k^\dagger]\}, \quad (10)$$

where $\mathcal{D}[L] = L\rho_S L^\dagger - \frac{1}{2}\{L^\dagger L, \rho\}$. We also define the jump coefficients $\gamma_k^- = |g_k|^2 \langle A_k A_k^\dagger \rangle_{\text{th}}$ and $\gamma_k^+ = |g_k|^2 \langle A_k^\dagger A_k \rangle_{\text{th}}$, with $\langle \dots \rangle_{\text{th}} = \text{tr}\{(\dots)\rho_A^{\text{th}}\}$. As shown, e.g., in Ref. [43], since the A_k are eigenoperators, these coefficients satisfy detailed balance $\gamma_k^+/\gamma_k^- = e^{-\beta\omega_k}$. As for the new coherent contribution in Eq. (8), we now find

$$G = \sum_k \{g_k \langle A_k \rangle_\chi L_k^\dagger + g_k^* \langle A_k^\dagger \rangle_\chi L_k\}, \quad (11)$$

where $\langle \dots \rangle_\chi = \text{tr}\{(\dots)\chi\}$ means an average over the coherent part χ of the ancillae.

Qubit example.—As an illustrative example, suppose both system and ancillae are resonant qubits with $H_{S(A)} = (\Omega/2)\sigma_z^{S(A)}$ and $V_{SA} = g(\sigma_+^S \sigma_-^A + \sigma_-^S \sigma_+^A)$. Moreover, we take $\chi_A = |0\rangle\langle 1| + |1\rangle\langle 0|$, so Eq. (10) reduces to the simple amplitude damping dissipator $D(\rho_S) = \sum_{j=\pm} \gamma^j \mathcal{D}[\sigma_j^S]$, whereas the coherent contribution in Eq. (11) goes to $G = g\sigma_x^S$. The dynamics of the system will then mimic that of a two-level atom driven by classical light, with $D(\rho_S)$ representing the incoherent emission or absorption of radiation and G a coherent driving term.

Modified first law.—Collisional models enable the unambiguous distinctions between heat and work, which is, in general, not the case [44], due to the full access to the global dynamics offered by such approaches [19,32]. In particular, Eq. (6) was derived under the assumption of strong energy conservation, so no work by an external agent is required to perform the unitary. Any energy changes in the system are thus solely due to energy leaving or entering the ancillae.

The evolution of $\langle H_S \rangle$ is easily evaluated as

$$d\langle H_S \rangle / dt = i\lambda \langle [G, H_S] \rangle + \text{tr}[H_S D(\rho_S)]. \quad (12)$$

The basic structure of these two terms is clearly different. The second term represents the typical *incoherent* energy usually associated with heat, whereas the first represents a coherent contribution more akin to quantum mechanical work. Indeed, we show below that the first term in Eq. (12) satisfies the properties expected from quantum mechanical work. We thus refer to it as the coherent work, $\dot{\mathcal{W}}_C = i\lambda \langle [G, H_S] \rangle$. We also refer to the last term in Eq. (12) as the incoherent heat, $\dot{\mathcal{Q}}_{\text{inc}} = \text{tr}\{H_S D(\rho_S)\}$. As the ancillae are not thermal, they will act as both thermal and work reservoirs (in the sense specified in Ref. [19]). As a consequence, classifying their change of energy as heat or work is prone to a certain level of ambiguity. For weakly coherent ancillae, however, this separation becomes unambiguous.

Combining this with Eq. (2) gives the modified first law

$$d\langle H_S \rangle / dt \equiv -\dot{\mathcal{Q}}_A = \dot{\mathcal{W}}_C + \dot{\mathcal{Q}}_{\text{inc}}, \quad (13)$$

where $\dot{\mathcal{Q}}_A = \lim_{\tau \rightarrow 0} \mathcal{Q}_{A_n} / \tau$ is the change in energy of each ancilla. Such a modified first law is one of our key results. It reflects a transformation process, where part of the heat flowing in or out of the ancillae is converted into a coherent energy change \mathcal{W}_C , with the remainder being the incoherent heat $\dot{\mathcal{Q}}_{\text{inc}}$. Next, we show that this transformation process is made possible by consuming coherence in the ancillae.

Modified second law.—We now turn to the second law in Eq. (3). All entropic quantities can be computed using perturbation theory in τ , leading to results that become exact in the limit $\tau \rightarrow 0$. The details are given in Ref. [41]. We find

$$\mathcal{I}(\rho'_{SA_n}) = -\beta \Delta F - \Delta C_{A_n}, \quad (14)$$

$$S(\rho'_{A_n} \| \rho_A) = \beta \mathcal{W}_C + \Delta C_{A_n}, \quad (15)$$

where ΔF is the change in nonequilibrium free energy of the system, $F(\rho_S) = \langle H_S \rangle - TS(\rho_S)$ and $\mathcal{W}_C \simeq \dot{\mathcal{W}}_C \tau$. Moreover, $\Delta C_{A_n} = C(\rho'_{A_n}) - C(\rho_{A_n})$ is the change in the relative entropy of coherence [45,46] in the state of the ancillae with $\mathcal{C}(\rho_A) = S(\rho_A^d) - S(\rho_A)$, with ρ_A^d the diagonal part of ρ_A in the eigenbasis of H_A . If $\lambda = 0$ in Eq. (5), we get $\mathcal{W}_C = \Delta C_{A_n} = 0$ (so that $\Sigma = -\beta \Delta F$).

The positivity of the relative entropy in Eq. (15) implies that in each system-ancilla interaction, the coherent work is always bounded by

$$\beta \mathcal{W}_C \geq -\Delta C_{A_n}. \quad (16)$$

This is the core result of our investigation: It shows that the coherent work is bounded by the loss of coherence in the state of the ancillae, which needs to be consumed in order to enable the transformation process described in Eq. (13). Coherence can, in this case, therefore be interpreted as a thermodynamic resource, which must be used to convert disordered energy in the ancillae into an ordered type of energy usable for the system.

On a more general level, the resource in question here is the athermality of ρ_A [29,30,47] (i.e., its nonpassive character [48]). However, the specifics of how this resource can be extracted (which requires knowledge of the operator G) and, most importantly, into *what* it can be converted will depend on the form of ρ_A . This argument can be further strengthened by studying the ergotropy [49] in the state (5), which is defined as the maximum amount of work extractable from ρ_A . As we show in Ref. [41], for weakly coherent states, it follows that $\mathcal{W} = TC(\rho_A)$. This result provides additional physical grounds to the bound in Eq. (16): The optimal process for extracting coherent work is when the ancillae lose all their coherence so that $-\Delta C(\rho_A) = C(\rho_A)$.

Inserting Eqs. (14) and (15) in Eq. (3) and taking the limit $\tau \rightarrow 0$, one finds that the entropy production rate $\Pi = \lim_{\tau \rightarrow 0} \Sigma_n / \tau$ can be expressed as

$$\Pi = \beta(\dot{\mathcal{W}}_C - \dot{F}) = \dot{S}(\rho_S) - \beta \dot{\mathcal{Q}}_{\text{inc}}. \quad (17)$$

This equation embodies a modified second law of thermodynamics in the presence of weak coherences. It is structurally identical to the classical second law [50] but with the coherent work \mathcal{W}_C instead. The positivity of Π sets the bound $\dot{\mathcal{W}}_C \geq \dot{F}$ that, albeit looser than the one in Eq. (16), has the advantage of depending solely on system-related quantities.

Extension to multiple environments.—An extremely powerful feature of collisional models is the ability to describe systems coupled to multiple baths. The typical idea is represented in Fig. 2. The system is placed to interact with multiple species of ancillae, with each species being independent and identically prepared in states ρ_A, ρ_B, ρ_C , etc. This can be used to model nonequilibrium steady states, e.g., of systems coupled to multiple baths. In the stroboscopic scenario, the state of the system will be constantly bouncing back and forth with each interaction,

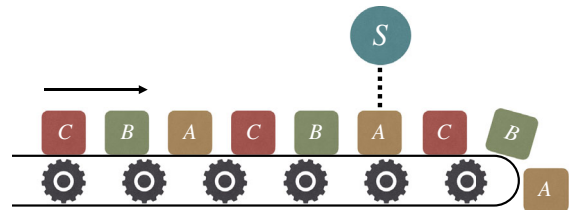


FIG. 2. Example of a collisional model where the system interacts with multiple species of ancillae.

even in the long-time limit. But the stroboscopic state after sequences of repeated interactions with the ancillae will, in general, converge to a steady state.

The remarkable feature of this construction is that the contributions from each species become *additive* in the continuous-time limit, in contrast to models where the bath is constantly coupled to the system [51]. We assume that each interaction lasts for a time τ/m , where m is the number of ancilla species (e.g., $m = 3$ in Fig. 2). Moreover, let $i = A, B, C, \dots, m$ label the different species. To obtain a well-behaved continuous-time limit, one must rescale the interaction potential V_{S_i} with each species [Eq. (4)] by $m/\sqrt{\tau}$ while keeping the coherent terms in Eq. (5) proportional to $\sqrt{\tau}$. Using this recipe, we find the master equation

$$\dot{\rho} = -i \left[H_S + \sum_j \lambda_j G_{S_j} \rho_S \right] + \sum_j D_j(\rho_S), \quad (18)$$

where the sums are over the various species involved, while G_{S_j} and D_j are exactly the same as those given in Eqs. (7) and (8). This is extremely useful, as it provides a recipe to construct complex master equations, with nontrivial steady states, from fundamental underlying building blocks.

This approach translates neatly into the first and second laws of thermodynamics, which now become

$$d\langle H_S \rangle / dt \equiv - \sum_j \dot{Q}_j = \sum_j (\dot{W}_C^j + \dot{Q}_{\text{inc}}^j) \quad (19)$$

and

$$\Pi = \dot{S}(\rho_S) - \sum_j \beta_j \dot{Q}_{\text{inc}}^j, \quad (20)$$

where β_j is the inverse temperature of species j . Both have the same structure as the usual first and second laws for systems coupled to multiple environments.

Conclusions.—We have introduced a scenario beyond the standard system plus thermal bath, for which operationally useful thermodynamic laws can be constructed. The key feature of our scenario is the use of weakly coherent states. For strong system-ancilla interactions, even weak coherences already lead to a nontrivial contribution. This leads to a modified continuous-time Lindblad master equation that encompasses a nontrivial coherent term giving rise to an effective work contribution to the energetics of the open system, although no external work is exerted at the global level. Incoherent (thermal) energy provided by the environment is catalyzed into worklike terms for the system to use by the (weak) coherence with which the former is endowed.

We believe that this analysis thus provides a striking example of the resourcelike role that coherence can play in nonequilibrium thermodynamic processes [31], with

applications, for instance, in the design of heat engines mixing classical and quantum resources.

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