On the relation between thermodynamic work extraction and distinguishability

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Assuming general principles of information theory, I show that the possibility of extracting work deterministically from a set of attributes implies that they must all be distinguishable from one another. This theorem provides an additional connection between thermodynamics and information theory, which is scale- and dynamics-independent, and goes via the law of conservation of energy. I also comment on its implications for the theory of von Neumann's universal constructor.

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There is a well known asymmetry in thermodynamics: while the law of conservation of energy can be formulated in a dynamics- and scale-independent way, the second law does not appear to have such a formulation, [1]. In currently known formulations, the second law is deemed only to apply at a certain macroscopic scale, which is never defined exactly. This is because the dynamical laws are time-reversal symmetric, hence laws prescribing the irreversibility of given transformations (like the second law does) are *prima facie* ruled out at the microscopic scale. Schemes such as Boltzmann's and Gibbs' to derive the second law from classical or quantum dynamics (supplemented with additional assumptions) provide a bridge with reversible dynamics, but they rely on approximation schemes such as ensembles and coarse-graining, which also make them scale-dependent.

Recently, quantum thermodynamics has provided a dramatic improvement, recasting thermodynamic laws within the quantum domain, relaxing various assumptions about thermodynamic equilibrium and asymptotic regimes, to cover single quantum systems [2–4]. Yet quantum thermodynamics (as the name suggests) relies on assuming quantum theory's formalism and laws – hence its 'second laws' are not dynamics-independent (unlike the conservation of energy).

It is still an open problem whether there exist scale-independent and dynamics-independent formulations of the second law of thermodynamics, compatible with dynamical laws we currently know, but also still meaningful under different dynamical laws (e.g. quantum theory's successor).

To address this problem, I shall examine the implications of a scale-independent, dynamics-independent definition of thermodynamic *work*. It includes as a special case the classical and quantum-thermodynamics definitions, but it is more general than either of those. In passing, I shall establish a further unexpected connection between information theory and thermodynamics, by explicitly linking the possibility of extracting work *deterministically* from a set of states, the law of *conservation of energy*, and the *distinguishability* of those states. This provides a further link between thermodynamics and information theory, via the first law in addition to the second.

Also, my definition of work allows one to distinguish work from heat independently of the dynamics and scale. Hence, it allows one to define heat in cases beyond the classical thermodynamic setting (where a specific scale is assumed) and beyond the quantum thermodynamics setting (where quantum dynamics is assumed).

Outline. Informally, the key result presented in this paper is that under a set of conjectured general principles satisfied by all dynamical theories that are at present reasonably conceivable, including quantum theory:

If it is possible to extract work deterministically from each of a set of attributes of a physical system, then the attributes in that set are all distinguishable from one another,

where 'attribute' here indicates a generalised state, as I shall define in the next section. Crucially, I shall define the concepts mentioned above (such as 'extracting work' and 'distinguishable') in a *scale-independent* and *dynamics-independent* way.

A proposition in a given physical theory is *scale-independent* if its applicability does not depend on the scale. For example, current formulations of the law of conservation of energy are scale-independent, because they apply both to individual microscopic systems and to macroscopic aggregates; while existing formulations of the second law are not, because they only apply at a certain macroscopic scale.

A proposition is *dynamics-independent* if it does not assume a specific dynamical law. For instance, consider the proposition that two states are *distinguishable* if and only if they are orthogonal: this proposition is dynamics-dependent, because it relies on the notion of orthogonality, which is defined in the formalism of quantum theory.

Likewise, consider the proposition that the work deterministically extractable, asymptotically, in a process taking ρ_1 to ρ_2 is given by: $F(\rho_1) - F(\rho_2)$, where

$F(\rho) = U(\rho) - \kappa_B TS(\rho)$, and $S(\rho) = -\mathrm{Tr}\{\rho \ln \rho\}$ while $U(\rho) = \mathrm{Tr}\{\rho H\}$, H being the Hamiltonian of the isolated system. This proposition is also dynamics-dependent (it depends on features of quantum theory's dynamics).

In this paper, I shall aim to be consistent with the existing dynamics-dependent notions of distinguishability and work extraction, while formulating them in a scale- and dynamics-independent way. To this end I shall use the recently proposed *constructor theory of information* [5, 6], which is an extremely useful tool for this purpose.

Constructor Theory. I shall now introduce the basics of constructor theory (the full definitions can be found in [6–8]). An *attribute* $\mathbf{x}$ of a physical system is a set of states all having a property x. For instance, in quantum theory, the set of all quantum states of a qubit where a given projector is sharp with value 1 is an attribute. I shall require attributes to be endowed with a topology. In the case of quantum theory it is the topology induced by the natural inner-product metric of Hilbert spaces. I shall also require that if $\mathbf{a}$ and $\mathbf{b}$ are attributes, the attribute $(\mathbf{a}, \mathbf{b})$ of the composite system $S_1 \oplus S_2$ is defined as the set of all states of the composite system where S_1 has attribute $\mathbf{a}$ and S_2 has attribute $\mathbf{b}$. This is required in order to conform to the *principle of locality*.

A *task* is the abstract specification of a physical transformation, represented as a finite set of ordered pairs of input/output attributes: $T = \{\mathbf{a_1} \to \mathbf{b_1}, \mathbf{a_2} \to \mathbf{b_2}, \cdots, \mathbf{a_n} \to \mathbf{b_n}\}$. Physical systems on which tasks can be performed are called *substrates*.

A *constructor* for a task T is a system which whenever presented with the substrate of the task T in one of the input attributes, it delivers it in one of the states of the allowed output attributes, and *retains the ability to do that again*. [17]

A task is *impossible* if the laws of physics impose a limit on how accurately it can be performed by a constructor. Otherwise, the task is *possible* - it can be performed by a *constructor* to arbitrarily high accuracy. In quantum information, gates for computational tasks are example of constructors [5]; and logically reversible computational tasks are possible tasks under unitary quantum theory.

Further examples of possible and impossible tasks under unitary quantum theory fall under the heading of cloning. Define the task of *cloning* a set of attributes X:

$$C(X) \doteq \bigcup_{x \in X} \{(\mathbf{x}, \mathbf{x_0}) \to (\mathbf{x}, \mathbf{x})\} \ . \tag{1}$$

When X is a boolean variable, $X = \{\mathbf{0}, \mathbf{1}\}$, $C(X)$ is the controlled-NOT task. This task is possible in quantum theory whenever all elements in X are orthogonal to one another; otherwise, if X consists of non-orthogonal states, it is impossible.

Constructor-theoretic statements never refer to specific constructors, only to the fact that tasks are possible or impossible. This is what allows one to achieve a scale-independent, dynamics-independent formulation of physical principles.

Tasks T_1 and T_2 can be composed in series (whenever the output set of attributes includes the input set of attributes of T_2), or in parallel, with the usual informal meaning of parallel and serial composition,[6]. I shall denote the serial composition of two tasks as $T_1 T_2$; the parallel composition as $T_1 \otimes T_2$.

Distinguishability. I shall now recall the definition of distinguishable variable, [6]. This allows one to express the concept of distinguishability via an operational criterion, without resorting to specific formal, dynamics-dependent properties such as orthogonality. First, one defines a class of substrates, *information media*.

An *information medium* is a substrate with a set of disjoint attributes X, called *information variable*, with the property that the task $C(X)$ and the permutation task:

$$\Pi(X) \doteq \bigcup_{x \in X} \{\mathbf{x} \to \Pi(\mathbf{x})\} \ , \tag{2}$$

are possible, for all permutation Π on the set of labels of the attributes in X and some attribute $\mathbf{x_0} \in X$.

As I said, the task $C(X)$ corresponds to *copying*, or cloning, the attributes of the first substrate onto the second, target, substrate; $\Pi(X)$, for a particular Π, corresponds to a logically reversible computation. For example, a qubit is an information medium with any set of two orthogonal quantum states, $X = \{\mathbf{0}, \mathbf{1}\}$, as defined above.

Any two different information media (e.g. a neutron and a photon) must satisfy an *interoperability principle*, [6], which expresses elegantly the intuitive property that classical information must be copiable from one information medium to any other, irrespective of their physical details. Specifically, if S_1 and S_2 are information media, respectively with information variable X_1 and X_2, their composite system $S_1 \oplus S_2$ is an information medium with information variable $X_1 \times X_2$, where $\times$ denotes the Cartesian product of sets. This requires the task of copying information variables (as in eq. (1)) from one to the other to be possible.

A variable Y is *distinguishable* if the task

$$\bigcup_{y \in Y} \{\mathbf{y} \to \mathbf{q_y}\} \tag{3}$$

is possible, where the variable $\{\mathbf{q_y}\}$, of the same cardinality as Y, is an information variable.

Another principle of constructor theory relevant for my proof is the principle of *asymptotic distinguishability*. Let me define $S(n) \doteq \underbrace{S \oplus S \oplus ...S}_{n}$, a substrate consisting of n instances of the substrate S, and $x(n) \doteq \underbrace{(x, x, ..., x)}_{n}$, attribute of $S(n)$. Denote by $x(\infty)$ the attribute of $S(\infty)$, an unlimited supply of instances of S. This is of course a theoretical construct, which does not occur in reality. Consider any two disjoint, intrinsic attributes x and $x^{'}$.

Asymptotic distinguishability requires the attributes $x(\infty)$ and $x^{'}(\infty)$ of $S(\infty)$, whenever they are defined, to be distinguishable (as defined above). In quantum theory, this requirement corresponds to the fact that any two different quantum states are asymptotically distinguishable – which ensures the possibility of so-called quantum tomography.

In this paper I will be concerned with *pairwise* tasks, i.e. with tasks that only involve the transformation of one attribute into another, as in $\{\mathbf{a} \to \mathbf{b}\}$. I shall also use the notion of the transpose of a task T, denoted by $T^{\sim}$, which is defined as the task with the input/output pairs of T inverted: $T^{\sim} \doteq \{\mathbf{b} \to \mathbf{a}\}$. One requires that $(T^{\sim})^{\sim} = T$; and that $(T_1 \otimes T_2)^{\sim} = T_1^{\sim} \otimes T_2^{\sim}$.

The law of conservation of energy. I shall now express the law of conservation of energy in an explicitly dynamics-independent way [5]. Consider the set Σ of all pairwise tasks that one can define on a substrate S. A conservation law for an additive quantity of S (energy for instance) can be expressed by requiring that Σ can be partitioned into equivalence classes, defined as follows.

Each equivalence class X_E has the property that for any two tasks T_1 and T_2 belonging to X_E:

- Either the tasks $\{T_1, T_2\}$ and their trasposes $\{T_1^{\sim}, T_2^{\sim}\}$ are all *impossible*; or they are all possible.
- The task $T_1 \otimes T_2^{\sim}$ and its transpose are both possible tasks.

By using the properties of serial and parallel composition and the definition of transpose, [8], one can show that the two above conditions define an equivalence relation between tasks.

Using the properties of equivalence classes, I can now introduce a real-valued function F, with the property that for any two pairwise tasks T_1, T_2, $F(T_1) = F(T_2)$ if and only if they belong to the same equivalence class.

A little thought reveals that the label $F(T)$ represents the amount by which the task T violates the conservation law. Indeed, by the properties of parallel and serial composition, one can see that there is only one class where both T_1 and T_2 and their transposes are all possible: it is the class labelled by a zero change of the conserved quantity, so that $F(T) = 0$ for all tasks T in that class. In all the other classes, any task T and its transpose are both impossible and they violate the conservation law by opposite amounts, so that the task $T \otimes T^{\sim}$ is possible. Given that in this paper we are interested in the energy conservation, I shall call each equivalence class an *energy-equivalence class*; if two tasks T_1 and T_2 belong to the same energy-equivalence class, I will write: $T_1 \sim T_2$; which means that if T_1 and T_2 violate the conservation law, they do so by the same amount.

By noting that each task is an ordered pair of attributes, the partition into equivalence classes of the set of pairwise tasks also induces a partition into classes of the set of attributes Σ of the substrate S. One can choose a function E that labels each class by a real number, with the property that $E(\mathbf{a}) = E(\mathbf{b})$ if and only if the two attributes belong to the same class, and if $T = \{\mathbf{a} \to \mathbf{b}\}$, then the function labelling the equivalence class of tasks is related to the function E by the following relation: $F(T) = E(\mathbf{b}) - E(\mathbf{a})$. The labelling of attributes defined by E can be thought of as an energy function (defined up to a constant). Thus I shall say that an attribute has a particular value of energy if it belongs to one of these classes labelled by that particular value of energy, under a fixed labelling E compatible with the partition into equivalence classes of the set of all pairwise tasks.

Hence as promised the law conservation of energy is expressible as the scale-independent, dynamics-independent requirement that the possible and impossible tasks on substrates S obey the two conditions listed above.

Work media. The concept of a *work repository* in classical thermodynamics is never exactly defined; but there is a general consensus, following Planck, on identifying a work repository with a system that behaves 'in the same way' as a weight in a uniform gravitational field, which can be raised or lowered to different heights, [1]. In quantum thermodynamics, it is common practice to define a work repository as a system in any eigenstates of its Hamiltonian, such as a set of bound states in an atom; there are also other proposed notions of work repositories (see [3] for a review). Here my intention is to be more general than those notions, but compatible with all of them. I shall do so by generalising the class of work repositories to that of *work media*, [8].

In constructor theory I shall define work media as a particular class of substrates satisfying an operational criterion (just like information media): certain tasks must be possible on a substrate for it to qualify as a work medium. This will provide a conjectured scale-independent, dynamics-independent generalisation of the notion of work repository, building on the classical definition of Planck's and Clausius'.

A work medium is a substrate $\mathbf{Q}$ with a set W of three attributes $\mathbf{w}+, \mathbf{w_0}, \mathbf{w}_-$ with the property that:

- The task

$$\{(\mathbf{w}_+, \mathbf{w_0}) \to (\mathbf{w_0}, \mathbf{w}_+), (\mathbf{w_0}, \mathbf{w_0}) \to (\mathbf{w}_+, \mathbf{w}_-)\} \tag{4}$$

  is possible;

- The task $T_{m,n} = \{\mathbf{w_m} \to \mathbf{w_n}\}$ is not possible, for all $\mathbf{m} \neq \mathbf{n}$ belonging to W; and all the tasks $T_{m,n}$ belong to the same energy-equivalence class.

A set of attributes $W = \{\mathbf{w_0}, \mathbf{w}_+, \mathbf{w}_-\}$ having these properties is a *work variable*.

Let me explain the physical meaning of the above definition. A quantum system with at least 3 equally spaced energy levels satisfies the definition of work media. As an example, consider an atom Q with three different energy levels, in decreasing order of energy as follows: $\mathbf{w}_+, \mathbf{w}_-, \mathbf{w_0}$. The key fact about the first requirement is that it is *not* satisfied by purely thermal degrees of freedom, as defined in traditional thermodynamics. For example, it is not satisfied by assuming $\mathbf{w}_\alpha = \mathbf{T}_\alpha$, where the attributes $\mathbf{T}_+, \mathbf{T}_-, \mathbf{T_0}$ of, say, a volume of water each correspond to a thermal state with given temperature T_α. Because of the second law of thermodynamics, the first condition above is not satisfied, because it requires an equilibrium state $(\mathbf{T_0}, \mathbf{T_0})$ to give rise to two different temperature attributes $(\mathbf{T}_+, \mathbf{T}_-)$, with no other side effects. Thus, systems endowed with thermal degrees of freedom within the standard definitions of thermodynamics do not qualify as work media.

The above definition therefore singles out the attributes that can be used to provide and absorb energy from another system, reversibly, with no other side-effects. It is therefore consistent with the traditional notion of 'work repository', but it is applicable to general systems that need not be mechanical, e.g. an atom in an excited state. In addition, it advances existing definitions, such as those declaring eigenstates of energy to be work repositories by fiat. One can also express elegantly that all work media are interoperable, just like for information media, implying that the composite system of two work media is still a work medium, [8]. This interoperability defines a class of physical systems – whether classical, quantum or obeying as yet unknown laws of physics – provided that they conform to the above conditions.

A deterministic work extractor. Consider now a substrate $\mathbf{S}$ with a set of attributes X each belonging to an energy-equivalence class. I define the task of deterministically extracting work for the variable X as the following task on the composite system of $\mathbf{S}$ and of a work medium $\mathbf{M}$:

$$\bigcup_{x\in X} \{(\mathbf{x}, \mathbf{w_0}) \to (\mathbf{f_x}, \mathbf{w_x})\} \tag{5}$$

where $\{\mathbf{f_x}\}$ are some attributes of $\mathbf{S}$ and $\mathbf{w_x} \in W$ for some work variable W of $\mathbf{M}$. For example, $\mathbf{M}$ here could be an atom that gets excited or de-excited by interaction with another system $\mathbf{S}$.

The operation of a constructor for the above task, if possible, is deterministic because it delivers one and only one output for any particular input, retaining the ability to cause it again; and without there being any other side-effects.

The relation between cloning and deterministic work extraction. Now we can state more precisely the theorem informally expressed at the outset:

Theorem 1. *A work variable is a distinguishable variable.*

In quantum theory, this means that deterministic work extractors must operate on sets of orthogonal subspaces. The proof goes as follows. First, we prove that any work variable W is a distinguishable variable, as defined above. Consider the following task, as the generalisation of (5) to having n substrates as the target:

$$\begin{aligned}&\{(\mathbf{w}_+, (\mathbf{w_0})^{(2n)}) \to (\mathbf{w}_+, (\mathbf{w}_+, \mathbf{w}_-)^{(n)});\\ &(\mathbf{w_0}, (\mathbf{w_0})^{(2n)}) \to (\mathbf{w_0}, (\mathbf{w}_-, \mathbf{w}_+)^{(n)})\}.\end{aligned} \tag{6}$$

When n tends to infinity, $(\mathbf{w}_+, \mathbf{w}_-)^{(n)})$ is asymptotically distinguishable from $(\mathbf{w}_-, \mathbf{w}_+)^{(n)}$, by the asymptotic-distinguishability principle. Thus, the attributes $\mathbf{w}_+$ and $\mathbf{w_0}$ of a work medium are distinguishable from one another, by definition of distinguishability.

Hence, by the definition of deterministic work extraction and by the above proof, any variable X from which one can extract work deterministically, must also be distinguishable. This concludes the proof that a deterministic work extractor is also a perfect distinguisher of states.

Implications for the second law. This theorem (being scale- and dynamics-independent) tackles the issue of distinguishing work from heat, and of formulating the second law of thermodynamics in a scale-independent way, [8]. I can illustrate how by recalling the concept of adiabatic accessibility, which is the basis of the axiomatic approach to thermodynamics, [11, 12].

I will propose a variant of the definition of adiabatic accessibility, appealing to the notion of *adiabatic possibility*. A task $\{\mathbf{x} \to \mathbf{y}\}$ is adiabatically possible if the task:

$$\{(\mathbf{x}, \mathbf{w_0}) \to (\mathbf{y}, \mathbf{w_1})\}$$

is possible for some two work attributes $\mathbf{w_1}, \mathbf{w_2}$ belonging to a work variable.

Unlike previous definitions of adiabatic possibility (see [12]), this definition does not rely on ensembles or similar approximations. Therefore it allows one to formulate the second law, as expressed in the axiomatic approach, as a scale-independent, and dynamics-independent law. It can be stated as follows:

There are tasks that are adiabatically possible, whose transpose is not adiabatically possible.

Based on this idea, one can introduce an exact, scale-independent distinction between work and heat - as intended in classical thermodynamics – see [8] for a discussion of these aspects.

Discussion. Under my operational definition of work and the general information-theoretic principles expressed earlier, if work can be extracted from a set of attributes of a physical substrate, these states must be distinguishable - therefore this theorem establishes a novel connection between thermodynamics and information theory, which is scale- and dynamics-independent.

The principles I assumed are robust and general, and they are satisfied by quantum theory and classical mechanics. In quantum theory, the theorem I proved implies that if one can extract work deterministically from any of a set of states, these states must be orthogonal to each other. In this regard, one might be puzzled by the following fact. A classical heat engine is capable of extracting work deterministically from the composite system of two heat reservoirs, each set initially at two different temperatures. The maximum extractable work is a function of the two temperatures and of the heat capacity of the two reservoirs, (see e.g. [13]). Consider now two different attributes of the two reservoirs, ($\mathbf{T}_+$, $\mathbf{T}_-$) and ($\tilde{\mathbf{T}}_+$, $\tilde{\mathbf{T}}_-$). By Carnot's theorem, there is a classical heat engine that acts deterministically as an optimal work extractor from a system prepared in either $(\mathbf{T}_+, \mathbf{T}_-)$ or $(\tilde{\mathbf{T}}_+, \tilde{\mathbf{T}}_-)$. Are these two attributes distinguishable? The theorem I proved implies that they are.

Yet, if each is represented by a quantum thermal state, they should not be distinguishable! This seems to contradict my result. But it does not. The heat engine works as a deterministic work extractor on those states only *asymptotically*, when the number of constituents of the reservoirs tends to infinity. In this case, the states of the reservoir corresponding to two different temperature differences are asymptotically distinguishable, because they correspond each to having infinitely-many copies of a thermal state. My result is therefore consistent with the fact that different thermal states of a single quantum system are not distinguishable. In other words, deterministic work extractors cannot extract work perfectly from each of a set of different thermal states, away from the asymptotic regime, [14].

Another notable fact is that this theorem outlines an interesting parallel between a programmable quantum computer (which behaves as such only with a set of programs from the computational basis [15, 16]) and a deterministic work extractor. The variables that can serve as input to a deterministic work extractor must be a set of distinguishable attributes (orthogonal subspaces in quantum theory). This constitutes the only possible 'work basis', which, in complete analogy with the computational basis, has to be made of orthogonal subspaces. This could be either a set of sharp energy states; or a set of states that are not diagonal in the energy basis, each provided with orthogonal labels. In other words, it is impossible to extract work deterministically in a single-shot fashion from a set of unknown quantum states with a given average work content, for instance produced by a naturally occurring phenomenon. This fact has important implications for quantum thermodynamics, specifically for the work that can be extracted deterministically from states that have coherence in the energy basis, [14]. In these studies one considers a process that extracts work optimally and deterministically from a particular quantum state with some non-zero coherence in the energy basis, as compared to the corresponding thermal state with the same mean energy. However, the process in question is a special-purpose machine, which requires to know a priori which state has been prepared. Therefore, it is not a universal work-extractor for a set of input states, in the sense I defined, not more than a Szilard engine without its memory is. Therefore the result of this paper is compatible with those other results.

Because the theorem assumes only those general principles, it applies to quantum theory and classical mechanics as a special cases, but it does not rely on their specific formal structure. For instance, the theorem could apply to what I call hybrid systems, consisting of a quantum system interacting with a physical system whose dynamics is not fully specified or intractable. It could also apply to the potential successors of quantum theories - e.g. theories of coupled gravity and quantum matter.

I have thus established the promised connection between the work extraction, the conservation of energy, and information theory. This result provides the foundation for formulating thermodynamics in an information-theoretic, dynamics-independent and scale-independent way; it is also a first step towards a theory of programmable constructors in quantum theory, which will generalise the theory of quantum computation to general tasks, in a way already envisaged by von Neumann and his theory of the universal constructor. In order to devise this theory, one will have to merge quantum thermodynamics with general principles of constructor theory. I leave the exploration of this possibility to further research.

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