Overview of Information Theory, Computer Science Theory, and Stochastic Thermodynamics for Thermodynamics of Computation

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Abstract: I give a quick overview of some of the theoretical background necessary for using modern nonequilibrium statistical physics to investigate the thermodynamics of computation. I first present some of the necessary concepts from information theory, and then introduce some of the most important types of computational machine considered in computer science theory.

After this I present a central result from modern nonequilibrium statistical physics: an exact expression for the entropy flow out of a system undergoing a given dynamics with a given initial distribution over states. This central expression is crucial for analyzing how the total entropy flow out of a computer depends on its global structure, since that global structure determines the initial distributions into all of the computer's subsystems, and therefore (via the central expression) the entropy flows generated by all of those subsystems. I illustrate these results by analyzing some of the subtleties concerning the benefits that are sometimes claimed for implementing an irreversible computation with a reversible circuit constructed out of Fredkin gates.

I. INTRODUCTION

In this chapter I give a quick overview of some of the theoretical background necessary for using modern nonequilibrium statistical physics to investigate the thermodynamics of computation.

I begin by presenting some general terminology, and then review some of the most directly relevant concepts from information theory. Next I introduce several of the most important kinds of computational machine studied in computer science theory. After this I summarize the parts of nonequilibrium statistical physics (more precisely, stochastic thermodynamics [1–3]) that are necessary for analyzing the thermodynamics of such computational machines. The interested reader is directed to [54] for a more detailed overview.

The key tool provided by stochastic thermodynamics is a decomposition of the entropy flow out of any open physical system that implements some desired map π on some initial distribution p_0 , into the sum of three terms [4]:

- 1. The "Landauer cost" of π . This is an information-theoretic quantity: the drop in Shannon entropy of the actual distribution over the states of the system as the system evolves. The Landauer cost depends only on π and p_0 , being independent of the precise details of the physical system implementing π .
- 2. The "mismatch cost" of implementing π with a particular physical system. This is also an information-theoretic quantity: a drop in Kullback-Leibler distance, between p_0 and a counterfactual "prior" distribution, q_0 , as those distributions both get transformed by π . The mismatch cost depends only on π , p_0 , and q_0 , being independent of any details of the physical system implementing π that are not captured in q_0 .
- 3. The "residual entropy production" due to using a particular physical system. This is a *linear* term, that depends on the graph-theoretic nature of π , on p_0 , and on the precise details of the physical system implementing π .

(See [5, 6] for earlier work that considered just the first two terms.)

This decomposition allows us to analyze how the thermodynamic costs of a fixed computational device vary if we change the physical environment of that device, i.e., change the distribution of inputs to the device. This decomposition also plays a key role in analyzing the thermodynamics of systems with multiple components that are interconnected, since the physical environment of each of those components is determined by the logical maps performed by the "upstream" components. (See [4, 7].)

To illustrate this decomposition of entropy flow, I end by using it to analyze the relative thermodynamic advantages and disadvantages of performing a computation with a logically reversible circuit (e.g. constructed out of Fredkin gates) rather than with a conventional circuit that uses logically irreversible gates.

II. TERMINOLOGY AND GENERAL NOTATION

As usual, for any set A, A^* is the set of all finite strings of elements from A. I write the Kronecker delta function as

$$\delta(a,b) = \begin{cases} 1 \text{ if } a = b \\ 0 \text{ otherwise} \end{cases}$$
 (1)

I write the indicator function for any Boolean function f(z) as

$$\mathbf{I}(f) = \begin{cases} 1 & \text{if } f(z) = 1\\ 0 & \text{otherwise} \end{cases}$$
 (2)

In general, random variables are written with upper case letters, and instances of those random variables are written with the corresponding lower case letters. When the context makes the meaning clear, I will often also use the upper case letter indicating a random variable, e.g., X, to indicate the set of possible outcomes of that random variable. For any distribution p(x) defined over the set X, and any $X' \subseteq X$, I write $p(X') = \sum_{x \in X'} p(x)$. Finally, given any conditional distribution $\pi(y|x)$ and a distribution p over X, I write πp for the distribution over Y induced by π and p,

$$(\pi p)(y) := \sum_{x \in X} \pi(y|x)p(x) \tag{3}$$

Computational machines are most often defined in terms of conditional distributions π that are (very good approximations of) single-valued state-update functions. That means that there are transitions in the state of the system that cannot occur in a single step, i.e. there are restrictions on which entries of the transition matrix can be nonzero. In order to analyze the entropy production in a physical system with this character, it helps to "decompose" the dynamics of the system, into the entropy production associated with a set of "sub-maps" defined by zero entries in the transition matrix.

Let f be a single-valued function from a set X into itself. An **island** of f is a pre-image $f^{-1}(x)$ for some $x \in f(X)$ [4]. I will write the set of all islands of a function f as L(f).

As an example, the logical AND operation,

$$\pi(c|a,b) = \delta(c,a \wedge b)$$

has two islands, corresponding to $(a,b) \in \{\{0,0\},\{0,1\},\{1,0\}\}\}$ and $(a,b) \in \{\{1,1\}\}$, respectively. I write the set of all distributions over an island $c \in L(f)$ as Δ_c . I make the obvious definitions that for any distribution p(x) and any $c \in L(f)$, the associated distribution over islands is $p(c) = \sum_{x \in c} p(x)$. As shorthand, I also write $p^c(x) = p(x|X \in c) = p(x)\mathbf{I}(x \in c)/p(c)$.

Intuitively, the islands of a function are different systems, isolated from one another for the duration of any process that implements that function. As this suggests, the islands of a dynamic process depends on how long it runs. For example, suppose $X = \{a, b, c\}$, and f(a) = a, f(b) = a, while f(c) = b. Then f has two islands, $\{a, b\}$ and $\{c\}$. However if we iterate f we have just a single island, since all three states get mapped under f^2 to the state a.

In the more general case where the physical process implements an arbitrary stochastic matrix π , the islands of π are the transitive closure of the equivalence relation,

$$x \sim x' \Leftrightarrow \exists x'' : \pi(x''|x) > 0, \pi(x''|x') > 0 \tag{4}$$

(Note that x and x' may be in the same island even if there is no x'' such that both P(x''|x) > 0 and P(x'|x) > 0, due to the transitive closure requirement.) Equivalently, the islands of π are a partition $\{X^i\}$ of X such that for all X^i , $x \notin X^i$,

$$\operatorname{supp} \pi(x'|x) \cap \bigcup_{x'' \in X^i} \operatorname{supp} \pi(x'|x'') = \varnothing$$
 (5)

Although the focus of this chapter is computers, which are typically viewed as implementing single-valued functions, all of the results below also hold for physical processes that implement general stochastic matrices as well, if one uses this more general definition of islands. Note that for either single-valued or non-single-valued stochastic matrices π , the islands of π will in general be a refinement of the islands of π^2 , since π may map two of its islands to (separate) regions that mapped on top of one another by π^2 . This will not be the case though if π permutes its islands.

III. INFORMATION THEORY

The Shannon entropy of a distribution over a set X, the Kullback-Leibler (KL) divergence between two distributions both defined over X (sometimes called the "relative entropy" of those two distributions), and the cross-entropy between two such distributions, respectively, are defined as

$$S(p(X)) = -\sum_{x \in X} p(x) \ln p(x)$$
(6)

$$D(p(X)||r(X)) = \sum_{x \in X} p(x) \ln \frac{p(x)}{r(x)}$$
 (7)

$$S(p(X)||r(X)) = S(p(X)) + D(p(X)||r(X))$$
(8)

$$= -\sum_{x \in X} p(x) \ln r(x) \tag{9}$$

(I adopt the convention of using natural logarithms rather than logarithms base 2 for most of this chapter.) I sometimes refer to the second arguments of KL divergence and of cross-entropy as a **reference distribution**. Note that the entropy of a distribution p is just the negative of the KL divergence from p to the uniform reference distribution, up to an overall (negative) constant.

The conditional entropy of a random variable X conditioned on a variable Y under joint distribution p is defined as

$$S(p(X|Y)) = \sum_{y \in Y} p(y)S(p(X|y))$$

$$= -\sum_{x \in X, y \in Y} p(y)p(x|y)\ln p(x|y)$$
(10)

and similarly for conditional KL divergence and conditional cross-entropy. The *chain rule* for entropy [8] says that

$$S(p(X|Y)) + S(p(Y)) = S(p(X,Y)) \tag{11}$$

Similarly, given any two distributions p and r, both defined over $X \times Y$, the conditional cross entropy between them equals the associated conditional entropy plus the associated conditional KL divergence:

$$S(p(X|Y)||r(X|Y)) = S(p(X|Y)) + D(p(X|Y)||r(X|Y))$$
(12)

$$= -\sum_{x \in X, y \in Y} p(x, y) \ln r(x|y) \tag{13}$$

The mutual information between two random variables X and Y jointly distributed according to p is defined as

$$I_p(X;Y) \equiv \mathcal{S}(p(X)) + \mathcal{S}(p(Y)) - \mathcal{S}(p(X,Y)) \tag{14}$$

$$= \mathcal{S}(p(X)) - \mathcal{S}(p(X|Y)) \tag{15}$$

(I drop the subscript p where the distribution is clear from context.) The data processing inequality for mutual information [8] states that if we have random variables X, Y, and Z, and Z is a stochastic function of Y, then $I(X;Z) \leq I(X;Y)$.

Where the random variable is clear from context, I sometimes simply write S(p), D(p||r), and S(p||r). I also sometimes abuse notation, and (for example) if a and b are specified, write S(A = a|B = b) to mean the conditional entropy of the random variable $\delta(A, a)$ conditioned on the event that the random variable B has the value b. When considering a set of random variables, I usually index them and their outcomes with subscripts, as in X_1, X_2, \ldots and x_1, x_2, \ldots I also use notation like $X_{1,2}$ to indicate the joint random variable (X_1, X_2) .

I write $S(\pi p)$ to refer to the entropy of distributions over Y induced by p(x) and the conditional distribution π , as defined in Eq. (3). I use similar shorthand for the other information-theoretic quantities, $D(\cdot||\cdot)$, $S(\cdot||\cdot)$ and $\mathcal{I}(\cdot)$. In particular, the *chain rule* for KL divergence and the *data-processing inequality* for KL divergence, respectively, are [8]:

1. For all distributions p, r over the space $X^a \times X^b$,

$$D(p(X^{a}, X^{b})||r(X^{a}, X^{b}))$$

$$= D(p(X^{b})||r(X^{b})) + D(p(X^{a}|X^{b})||r(X^{a}|X^{b}))$$
(16)

2. For all distributions p, r over the space X and conditional distributions $\pi(y|x)$,

$$D(p||r) \ge D(\pi p||\pi r) \tag{17}$$

(Note that by combining the chain rule for KL divergence with the chain rule for entropy, we get a chain rule for cross entropy.)

IV. COMPUTATIONAL MACHINES

A. Straight-line circuits

A (straight-line) circuit C is a tuple (V, E, F, X) that can be viewed as a special type of Bayes net [9–11]. The pair (V, E) specifies the vertices and edges of a directed acyclic graph (DAG). Intuitively, this DAG is the wiring diagram of the circuit. (In the circuit engineering industry, this is sometimes called the "netlist" of the circuit.) X is a Cartesian product $\prod_v X_v$, where each X_v

is the space of the variable associated with node v.¹ F is a set of conditional distributions, one for each non-root node v of the DAG, mapping the joint value of the (variables at the) parents of v, $x_{pa(v)}$, to the value of (the variable at) v, x_v . In conventional circuit theory, F is a set of single-valued functions.

Note that following the convention in the Bayes nets literature, with this definition of a circuit we orient edges in the direction of logical implication, i.e., in the direction of information flow. So the inputs to the circuit are the roots of the associated DAG, and the outputs are the leaves. The reader should be warned that this is the *opposite* of the convention in computer science theory. When there is no risk of confusion, I simply refer to a circuit C, with all references to V, E, F or X implicitly assumed as the associated elements defining C.

Straight line circuits are an example of **non-uniform** computers. These are computers that can only work with inputs of some fixed length. (In the case of a circuit, that length is specified by the number of root nodes in the circuit's DAG.) One can use a single circuit to compute the output for any input in a set of inputs, so long as all those inputs have the same length. If on the other hand one wishes to consider using circuits to compute the output for any input in a set that contains inputs of all possible lengths, then one must use a **circuit family**, i.e., an infinite set of circuits $\{C_i : i \in \mathbb{Z}^+\}$, where each circuit C_i has i root nodes.

In contrast to non-uniform computers, **uniform** computers are machines that can work with arbitrary length inputs.³ In general, the number of iterations a particular uniform computational machine requires to produce an output is not pre-fixed, in contrast to the case with any particular nonuniform computational machine. Indeed, for some inputs, a uniform computational machine may never finish computing. The rest of this section introduces some of the more prominent uniform computational machines.

B. Finite Automata

One important class of (uniform) computational machines are the finite automata. There are several different, very similar definitions of finite automata, some of which overlap with common definitions of "finite state machines". To fix the discussion, here I adopt the following definition:

¹In real electronic circuits, x_v will typically specify an element in a coarse-graining of the microstate space of the system, but as mentioned above, that is not relevant here.

²More general types of circuit than the one considered here allow branching conditions at the nodes and / or loops among the nodes. Such circuits cannot be represented as a Bayes net. To make clear what kind of circuit is being considered, sometimes the branch-free, loop-free type of circuit is called a "straight-line" circuit [12].

³The reader should be warned that computer scientists also consider "uniform circuit families", which is something that is related but different.

Definition 1. A finite automaton (FA) is a 5-tuple $(R, \Lambda, r^{\varnothing}, r^{A}, \rho)$ where:

- 1. R is a finite set of computational states;
- 2. Λ is a finite (input) **alphabet**;
- 3. $r^{\varnothing} \in R$ is the **start state**;
- 4. $r^A \in R$ is the accept state; and
- 5. $\rho: R \times \Lambda \to R$ is the **update function**, mapping a current input symbol and the current computational state to a next computational state.

A finite string of successive input symbols, i.e., an element of Λ^* , is sometimes called an **(input)** word, written as $\vec{\lambda}$. To operate a finite automaton on a particular input word, one begins with the automaton in its start state, and feeds that state together with the first symbol in the input word into the update function, to produce a new computational state. Then one feeds in the next symbol in the input word (if any), to produce a next computational state, and so on. I will sometimes say that the **head** is in some state $r \in R$, rather than say that the computational state of the automaton is r.

Often one is interested in whether the head is in state r^A after the last symbol from the input word is processed. If that is the case, one says that the automaton **accepts** that input word. In this way any given automaton uniquely specifies a **language** of all input words that that automaton accepts, which is called a **regular** language. As an example, any finite language (consisting of a finite set of words) is a regular language. On the other hand, the set of all palindromes over Λ , to give a simple example, is *not* a regular language.

Importantly, any particular FA can process input words of arbitrary length. This means that one cannot model a given FA as some specific (and therefore fixed width) circuit, in general. The FA will have properties that are not captured by that circuit. In this sense, individual FAs are computationally more powerful than individual circuits. (This does not mean that individual FAs are more powerful than entire circuit families however; see the discussion in Section IV D of how circuit families can be even more powerful than Turing machines.)

Finite automata play an important role in many different fields, including electrical engineering, linguistics, computer science, philosophy, biology, mathematics, and logic. In computer science specifically, they are widely used in the design of hardware digital systems, of compilers, of network protocols, and in the study of computation and languages more broadly.

To allow us to analyze a physical system that implements the running of an FA on many successive input words, we need a way to signal to the system when one input word ends and then another one begins. Accordingly, without loss of generality we assume that Λ contains a special blank state, written b, that delimits the end of a word. I write Λ_- for $\Lambda \setminus \{b\}$, so that words are elements of Λ_-^* .

In a **stochastic** finite automaton (sometimes called a "probabilistic automaton"), the singlevalued function ρ is replaced by a conditional distribution. In order to use notation that covers all iterations i of a stochastic finite automaton, I write this **update distribution** as $\pi(r_{i+1}|r_i,\lambda_i)$. The analogous extension of the word-based definition of finite automata into a word-based definition of a stochastic finite automata is immediate. For simplicity, from now on I will simply refer to "finite automaton", using the acronym "FA", to refer to a finite automaton that is either stochastic or deterministic.

Typically in the literature there is a set of multiple accept states — called "terminal states", or "accepting states" — not just one. Sometimes there are also multiple start states.

C. Transducers - Moore machines and Mealy machines

In the literature the definition of FA is sometimes extended so that in each transition from one computational state to the next an output symbol is generated. Such systems are also called "transducers" in the computer science community.

Definition 2. A transducer is a 6-tuple $(R, \Lambda, \Gamma, r^{\varnothing}, x^{A}, \rho)$ such that:

- 1. R is a finite set, the set of computational states;
- 2. Λ is a finite set, called the **input alphabet**;
- 3. Γ is a finite set, called the **output alphabet**;
- 4. $r^{\varnothing} \in R$ is the **start** state;
- 5. $r^A \in R$ is the accept state:
- 6. $\rho: R \times \Lambda \to R \times \Gamma$ is the **update rule**.

Sometimes the computational states of a transducer are referred to as the states of its **head**. I refer to the (semifinite) string of symbols that have yet to be processed by a transducer at some moment

as the **input** (data) stream at that moment. I refer to the string of symbols that have already been produced by the information ratchet at some moment as the **output** (data) stream at that moment.

To operate a transducer on a particular input data stream, one begins with the machine in its start state, and feeds that state together with the first symbol in the input stream into the update function, to produce a new computational state, and a new output symbol. Then one feeds in the next symbol in the input stream (if any), to produce a next computational state and associated output symbol, and so on.

In a **stochastic** transducer, the single-valued function ρ is replaced by a conditional distribution. In order to use notation that covers all iterations i of the transducer, I write this **update distribution** as $\pi(\gamma_{i+1}, r_{i+1}|r_i, \lambda_i)$. Stochastic transducers are used in fields ranging from linguistics to natural language processing (in particular machine translation) to machine learning more broadly. From now on I implicitly mean "stochastic transducer" when I use the term "transducer".

As with FAs, typically in the literature transducers are defined to have a set of multiple accept states, not just one. Sometimes there are also multiple start states. Similarly, in some of the literature the transition function allows the transducer to receive the empty string as an input and/or produce the empty string as an output.

A Moore machine is a transducer where the output γ is determined purely by the current state of the transducer, r. In contrast, a transducer in which the output depends on both the current state x and the current input λ is called a Mealy machine.

As a final comment, an interesting variant of the transducers defined in Def. 2 arises if we remove the requirement that there be accept states (and maybe even remove the requirement of start states). In this variant, rather than feeding an infinite sequence of input words into the system, each of which results in its own output word, one feeds in a single input word, which is infinitely long, producing a single (infinitely long) output word. This variant is used to define so-called "automata groups" or "self-similar groups" [13].

Somewhat confusingly, although the computational properties of this variant of transducers differs in crucial ways from those defined in Def. 2, this variant is also called "transducers" in the literature on "computational mechanics", a branch of hidden Markov model theory [14]. Fortunately, this same variant have also been given a different name, **information ratchets**, in work analyzing

⁴The reader should be warned that some of the literature refers to both FAs and transducers as "finite state machines", using the term "acceptor" or "recognizer" to refer to the system defined in Def. 1. Similarly, the word "transducer" is sometimes used loosely in the physics community, to apply to a specific system that transforms one variable — typically energy — into another variable, or even just into another form.

their statistical physics properties [15]. Accordingly, here I adopt that term for this variant of (computer science) transducers.

D. Turing machines

Perhaps the most famous class of computational machines are Turing machines [12, 16, 17]. One reason for their fame is that it seems that one can model any computational machine that is constructable by humans as a Turing machine. A bit more formally, the *Church-Turing thesis* states that, "A function on the natural numbers is computable by a human being following an algorithm, ignoring resource limitations, if and only if it is computable by a Turing machine." The "physical Church-Turing thesis" modifies that to say that the set of Turing machines includes all mechanical algorithmic procedures admissible by the laws of physics.

In part due to this thesis, Turing machines form one of the keystones of the entire field of computer science theory, and in particular of computational complexity [18]. For example, the famous Clay prize question of whether P = NP — widely considered one of the deepest and most profound open questions in mathematics — concerns the properties of Turing machines. As another example, the theory of Turing machines is intimately related to deep results on the limitations of mathematics, like Gödel's incompleteness theorems, and has broader, philosophical implications [19]. As a result, it seems that the foundations of physics may be restricted by some of the properties of Turing machines [20, 21].

Along these lines, some authors have suggested that the foundations of statistical physics should be modified to account for the properties of Turing machines, e.g., by adding terms to the definition of entropy. After all, given the Church-Turing hypothesis, one might argue that the probability distributions at the heart of statistical physics are distributions "stored in the mind" of the human being analyzing a given statistical physical system (i.e., of a human being running a particular algorithm to compute a property of a given system). See [22–24].

There are many different definitions of Turing machines that are "computationally equivalent" to one another. This means that any computation that can be done with one type of Turing machine can be done with the other. It also means that the "scaling function" of one type of Turing machine, mapping the size of a computation to the minimal amount of resources needed to perform that computation by that type of Turing machine, is at most a polynomial function of the scaling function of any other type of Turing machine. (See for example the relation between the scaling functions of single-tape and multi-tape Turing machines [17].) The following definition will

be useful for our purposes, even though it is more complicated than strictly needed:

Definition 3. A Turing machine (TM) is a 7-tuple $(R, \Lambda, b, v, r^{\varnothing}, r^{A}, \rho)$ where:

- 1. R is a finite set of computational states;
- 2. Λ is a finite **alphabet**;
- 3. $b \in \Lambda$ is a special **blank** symbol;
- 4. $v \in \mathbb{Z}$ is a **pointer**;
- 5. $r^{\varnothing} \in R$ is the **start** state;
- 6. $r^A \in R$ is the accept state; and
- 7. $\rho: R \times \mathbb{Z} \times \Lambda^{\infty} \to R \times \mathbb{Z} \times \Lambda^{\infty}$ is the **update function**. It is required that for all triples (r, v, T), that if we write $(r', v', T') = \rho(r, v, T)$, then v' does not differ by more than 1 from v, and the vector T' is identical to the vectors T for all components with the possible exception of the component with index v;⁵

 r^A is often called the "halt state" of the TM rather than the accept state. In addition, in some alternative (computationally equivalent) definitions, there is a set of multiple accept states rather than a single accept state. ρ is sometimes called the "transition function" of the TM. We sometimes refer to R as the states of the "head" of the TM, and refer to the third argument of ρ as a **tape**, writing a value of the tape (i.e., semi-infinite string of elements of the alphabet) as T. The set of triples that are possible arguments to the update function of a given TM are sometimes called the set of **instantaneous descriptions** (IDs) of the TM. (These are sometimes instead referred to as "configurations".) Note that as an alternative to Def. 3, we could define any TM as a map over an associated space of IDs.

Any TM $(R, \Sigma, b, v, \rho, r^{\varnothing}, \rho)$ starts with $r = r^{\varnothing}$, the counter set to a specific initial value (e.g, 0), and with T consisting of a finite contiguous set of non-blank symbols, with all other symbols equal to b. The TM operates by iteratively applying ρ , until the computational state falls in r^A , at which time it stops. (Note that the definition of ρ for $r = r^A$ is arbitrary and irrelevant.)

⁵Technically the update function only needs to be defined on the "finitary" subset of $\mathbb{R} \times \mathbb{Z} \times \Lambda^{\infty}$, namely, those elements of $\mathbb{R} \times \mathbb{Z} \times \Lambda^{\infty}$ for which the tape contents has a non-blank value in only finitely many positions.

If running a TM on a given initial state of the tape results in the TM eventually halting, the state of T when it halts is called the TM's **output**. The initial state of T (excluding the blanks) is sometimes called the associated **input**, or **program**. (However, the reader should be warned that the term "program" has been used by some physicists to mean specifically the shortest input to a TM that results in it computing a given output.) We also say that the TM **computes** an output from an input. In general, there will be inputs for which the TM never halts. The set of all those inputs to a TM that cause it to eventually halt is called its **halting set**.

As mentioned, there are many variants of the definition of TMs provided above. In one particularly popular variant the single tape in Definition 3 is replaced by multiple tapes. Typically one of those tapes contains the input, one contains the TM's output (if and) when the TM halts, and there are one or more intermediate "work tapes" that are in essence used as scratch pads. The advantage of using this more complicated variant of TMs is that it is often easier to prove theorems for such machines than for single-tape TMs. However, there is no difference in their computational power.

Returning to the TM variant defined in Definition 3, a **universal Turing machine** (UTM), M, is one that can be used to emulate any other TM. More precisely, a UTM M has the property that for any other TM M', there is an invertible map f from the set of possible states of the tape of M' into the set of possible states of the tape of M, such that if we:

- 1. apply f to an input string σ' of M' to fix an input string σ of M;
- 2. run M on σ until it halts;
- 3. apply f^{-1} to the resultant output of M;

then we get exactly the output computed by M' if it is run directly on σ' .

An important theorem of computer science is that there exists universal TMs. Intuitively, this just means that there exists programming languages which are "universal", in that we can use them to implement any desired program in any other language, after appropriate translation of that program from that other language. This universality leads to a very important concept:

Definition 4. The Kolmogorov complexity of a UTM M computing a string $\sigma \in \Lambda^*$ is the length of the shortest input string s such that M computes σ from s.

Intuitively, (output) strings that have low Kolmogorov complexity for some specific UTM M are those with short, simple programs in the language of M. For example, in all common (universal)

programming languages (e.g., C, Python, Java, etc.), the first m digits of π have low Kolmogorov complexity, since those digits can be generated using a relatively short program. Strings that have high (Kolmogorov) complexity are sometimes referred to as "incompressible". These strings have no patterns in them that can be generated by a simple program. As a result, it is often argued that the expression "random string" should only be used for strings that are incompressible.

A **prefix** (free) TM is one such that no one input in its halting set is a proper prefix of another string in its halting set (when both are viewed as symbol strings). The **coin-flipping prior** of a prefix TM M is the probability distribution over the strings in M's halting set generated by IID "tossing a coin" to generate those strings, in a Bernoulli process, and then normalizing.⁶ So any string σ in the halting set has probability $2^{-|\sigma|}/\Omega$ under the coin-flipping prior, where Ω is the normalization constant for the TM in question.

The coin-flipping prior provides a simple Bayesian interpretation of Kolmogorov complexity: Under that prior, the Kolmogorov complexity of any string σ for any prefix TM M is just (the log of) the maximum a posterior (MAP) probability that any string σ' in the halting set of M was the input to M, conditioned on σ being the output of that TM. (Strictly speaking, this result is only true up to an additive constant, given by the log of the normalization constant of the coin-flipping prior for M.)

The normalization constant Ω for any fixed prefix UTM, sometimes called "Chaitin's Omega", has some extraordinary properties. For example, the successive digits of Ω provide the answers to all well-posed mathematical problems. So if we knew Chaitin's Omega for some particular prefix UTM, we could answer every problem in mathematics. Alas, the value of Ω for any prefix UTM M cannot be computed by any TM (either M or some other one). So under the Church-Turing hypothesis, we cannot calculate Ω . (See also [26] for a discussion of a "statistical physics" interpretation of Ω that results if we view the coin-flipping prior as a Boltzmann distribution for an appropriate Hamiltonian, so that Ω plays the role of a partition function.)

It is now conventional to analyze Kolmogorov complexity using prefix UTMs, with the coinflipping prior, since this removes some undesirable technical properties that Kolmogorov complexity has for more general TMs and priors. Reflecting this, all analyses in the physics community that concern TMs assume prefix UTMs. (See [25] for a discussion of related concepts like conditional Kolmogorov complexity.)

Interestingly, for all their computational power, there are some surprising ways in which TMs

⁶Kraft's inequality guarantees that since the set of strings in the halting set is a prefix-free set, the sum over all its elements of their probabilities cannot exceed 1, and so can be normalized. See [25].

are weaker than the other computational machines introduced above. For example, there are an infinite number of TMs that are more powerful than any given circuit, i.e., given any circuit C, there are an infinite number of TMs that compute the same function as C. Indeed, any single UTM is more powerful than every circuit in this sense. On the other hand, it turns out that there are circuit families that are more powerful than any single TM. In particular, there are circuit families that can solve the halting problem [17].

V. ENTROPY DYNAMICS

This section reviews those aspects of stochastic thermodynamics that are necessary to analyze the dynamics of various types of entropy during the evolution of computational machines. As illustrated with examples, the familiar quantities at the heart of thermodynamics (e.g., heat, dissipation, thermodynamic entropy, work) arise in special cases of this analysis.

In the first subsection, I review the conventional decomposition of the entropy flow (EF) out of a physical system into the change in entropy of that system plus the (irreversible) entropy creation (EP) produced as that system evolves [1, 2]. To fix details, I will concentrate on the total amount of EF, EP and entropy change that arise over a time-interval [0, 1].

In the second subsection, I review recent results [4] that specify how the EP generated by the evolution of some system depends on the initial distribution of states of the system. These recent results allow us to evaluate how the EF of an arbitrary system, whose dynamics implements some conditional distribution π of final states given initial states, depends on the initial distribution of states of the system that evolves according to π . (As elaborated in subsequent sections, this dependence is one of the central features determining the entropic costs of running any computational machine.)

I end this section with some general cautions about translating a computer science definition of a computational machine into a physics definition of a system that implements that machine.

⁷In this paper I will not specify units of time, and often implicitly change them. For example, when analyzing the entropy dynamics of a given circuit, sometimes the time interval [0, 1] will refer to the time to run the entire circuit, and the attendant entropic costs. However at other times [0, 1] will refer to the time to run a single gate within that circuit, and the entropic costs of running just that gate. In addition, for computational machines that take more than one iteration to run, I will usually just refer to a "time interval [0, 1]" without specifying which iteration of the machine that interval corresponds to. Always the context will make the meaning clear.

A. Entropy flow, entropy production, and Landauer cost

To make explicit connection with thermodynamics, consider a physical system with countable state space X that evolves over time interval $t \in [0,1]$ while in contact with one or more thermal reservoirs, while possibly also undergoing driving by one or more work reservoirs.⁸ In this chapter I focus on the scenario where the system dynamics over the time interval is governed by a continuous-time Markov chain (CTMC). However many of the results presented below are more general.

Let $W_{x;x'}(t)$ be the rate matrix of the CTMC. So the probability that the system is in state x at time t evolves according to the linear, time-dependent equation

$$\frac{d}{dt}p_x(t) = \sum_{x'} W_{x;x'}(t)p_{x'}(t)$$
(18)

which I can write in vector form as $\dot{p}(t) = W(t)p(t)$. I just write "W" to refer to the entire timehistory of the rate matrix. W and p(0) jointly fix the conditional distribution of the system's state at t = 1 given its state at t = 0, which I write as π . As shorthand, I sometimes abbreviate x(0) as x, and sometimes abbreviate the initial distribution p(0) as p. (So for example, πp is the ending distribution over states.) I will also sometimes abbreviate p(1) as p', and x(1) as x'; the context should always make the meaning clear.

Next, define the entropy flow (rate) at time t as

$$\sum_{x',x''} W_{x';x''}(t) p_{x''}(t) \ln \left[\frac{W_{x';x''}}{W_{x'';x'}} \right]$$
 (19)

Physically, this corresponds to an entropy flow rate out of the system, into reservoirs it is coupled to.

In order to define an associated total amount of entropy flow during a non-infinitesimal time interval (EF), define $\mathbf{x} = (N, \vec{x}, \vec{\tau})$ as a trajectory of N+1 successive states $\vec{x} = (x(0), x(1), \dots, x(N))$, along with times $\vec{\tau} = (\tau_0 = 0, \tau_1, \tau_2, \dots, \tau_{N-1})$ of the associated state transitions, where $\tau_{N-1} \leq 1$, the time of the end of the process, x(0) is the beginning, t = 0 state of the system, and x(N) is the ending, t = 1 state of the system. Then under the dynamics of Eq. (18), the probability of that \mathbf{x} given the initial state x_0 is [1, 3, 27]

$$p(\boldsymbol{x}|x(0)) = \left(\prod_{i=1}^{N-1} S_{\tau_{i-1}}^{\tau_i}(x(i-1))W_{x(i);x(i-1)}(\tau_i)\right) S_{\tau_{N-1}}^1(x_N)$$
(20)

 $^{^{8}}$ In statistical physics, a "reservoir" R in contact with a system S is loosely taken to mean an infinitely large system that interacts with S on time scales infinitely faster than the explicitly modeled dynamical evolution of the state of S. For example, a "particle reservoir" exchanges particles with the system, a "thermal reservoir" exchanges heat, and a "work reservoir" is an external system that changes the energy spectrum of the system S.

where $S_{\tau}^{\tau'}(x) = e^{\int_{\tau}^{\tau'} W_{x;x}(t)dt}$ is the "survival probability" of remaining in state x throughout the interval $t \in [\tau, \tau']$. The total EF out of the system during the interval can be written as an integral weighted by these probabilities:

$$Q(p_0) = \int p_0(x_0) p(\boldsymbol{x}|x(0)) \sum_{i=1}^{N-1} W_{x(i);x(i-1)}(\tau_i) \ln \frac{W_{x(i);x(i-1)}(\tau_i)}{W_{x(i-1);x(i)}(\tau_i)} D\boldsymbol{x}$$
(21)

(Note that I use the convention that EF reflects total entropy flow *out* of the system, whereas much of the literature defines EF as the entropy flow *into* the system.)

EF will be the central concern in the analysis below. By plugging in the evolution equation for a CTMC, we can decompose EF as the sum of two terms. The first is just the change in entropy of the system during the time interval. The second, is the **(total) entropy production** (EP) in the system during the process [1, 28, 29]. I write EP as $\sigma(p)$. It is the integral over the interval of the instantaneous EP rate,

$$\sum_{x',x''} W_{x';x''}(t) p_{x''}(t) \ln \left[\frac{W_{x';x''} p_{x''}(t)}{W_{x'';x''} p_{x'}'(t)} \right]$$
(22)

I will use the expressions "EF incurred by running a process", "EF to run a process", or "EF generated by a process" interchangeably, and similarly for EP.⁹ EF can be positive or negative. However, for any CTMC, the EP rate given in Eq. (22) is non-negative [1, 28], and therefore so is the EP generated by the process. So

$$Q(p_0) = \sigma(p_0) + S(p_0) - S(\pi p_0)$$
(23)

$$\geq S(p_0) - S(\pi p_0) \tag{24}$$

where throughout this section, π refers to the conditional distribution of the state of the system at t = 1 given its state at t = 0, which is implicitly fixed by W(t).

Total entropy flow across a time interval can be written as a linear function of the initial distribution:

$$Q(p_0) = \sum_{x_0} \mathcal{F}(x_0) p_0(x_0)$$
 (25)

for a function $\mathcal{F}(x)$ that depends on the entire function $W_{x;x'}(t)$ for all $t \in [0,1)$, and so is related to the discrete time dynamics of the entire process, $\pi(x_1|x_0)$. (See Eq. (21).) However, the minimal entropy flow for a fixed transition matrix π is the drop in entropy from $S(p_0)$ to $S(\pi P_0)$. This

⁹Confusingly, sometimes in the literature the term "dissipation" is used to refer to EP, and sometimes it is used to refer to EF. Similarly, sometimes EP is instead referred to as "irreversible EP", to contrast it with any change in the entropy of the system that arises due to entropy flow.

is not a linear function of the initial distribution p_0 . In addition, the entropy production – the difference between actual entropy flow and minimal entropy flow – is not a linear function of p_0 . These nonlinearities are the basis of much of the richness of statistical physics, and in particular of its relation with information theory.

There are no temperatures in any of this analysis. Indeed, in this very general setting, temperatures need not even be defined. However, often the system is coupled to a heat bath, with a well-defined temperature T.¹⁰ If in addition the Hamiltonian of the system obeys "detailed balance" (DB) with that heat bath, EF can be written as [3]

$$Q = k_B T^{-1} Q \tag{26}$$

where k_B is Boltzmann constant, and Q is the expected amount of heat transferred from the system into bath ν during the course of the process.

Example 1. Consider the special case of an isothermal process, meaning there is a single heat bath at temperature T (although possibly one or more work reservoirs and particle reservoirs). Suppose that the process transforms an initial distribution p and Hamiltonian p into a final distribution p' and Hamiltonian p'. There are no a priori requirements that either p or p' is at equilibrium for the associated Hamiltonian,

As mentioned, in this scenario EF equals $(k_BT)^{-1}$ times the total heat flow into the bath. EP, on the other hand, equals $(k_BT)^{-1}$ times the dissipated work of the process, which is the work done on the system over and above the minimal work required by any isothermal process that performs the transformation $(p, H) \mapsto (p', H')$ [30]. So by Eq. (24) and energy conservation, the minimal work is the change in the expected energy of the system plus $(k_BT \text{ times})$ the drop in Shannon entropy of the system. This is just the change in the nonequilibrium free energy of the system from the beginning to the end of the process [30–32].

There are many different physical phenomena that can result in nonzero EP. One broad class of such phenomena arises if we take an "inclusive" approach, modeling the dynamics of the system and bath together:

Example 2. Continuing with the special case of an isothermal process, suppose that the heat bath never produces any entropy by itself, i.e., that the change in the entropy of the bath equals the EF

¹⁰Sometimes in the literature a "heat bath" is defined to be a thermal reservoir at (canonical ensemble) equilibrium, which is sometimes also presumed to be infinite. The context will make it clear whenever the discussion requires this presumption.

from the system into the bath. Then the change in the sum, {marginal entropy of the system} + {marginal entropy of the heat bath} must equal the EF from the system to the bath plus the change in the marginal entropy of the system by itself. By Eq. (23) though, this is just the EP of the system

On the other hand, Liouville's theorem tells us that the joint entropy of the system and the bath is constant. Combining establishes that EP of the system equals the change in the difference between the joint entropy and the sum of the marginal entropies, i.e., EP equals the change in the mutual information between the system and the bath.

To illustrate this, suppose we start with system and bath statistically independent. So the mutual information between them originally equals zero. Since mutual information cannot be negative, the change of that mutual information during the process is non-negative. This confirms that EP is non-negative, for this particular case where we start with no statistical dependence between the system and the bath. See [33].

Variants of Eq. (24) are sometimes referred to in the literature as the **generalized Landauer's bound**. To motivate this name, suppose that there is a single heat bath, at temperature T, and that the system has two possible states $X = \{0, 1\}$. Suppose further that the initial distribution p(x) is uniform over these two states, and that the conditional distribution π implements the function $\{0, 1\} \mapsto 0$, i.e., a 2-to-1 'bit-erasure' map. So by Eq. (26) and the non-negativity of EP, the minimal heat flow out of the system accompanying any process that performs that bit erasure is $k_B T(\ln 2 - \ln 1) = k_B T \ln 2$, in accord with the bound proposed by Landauer [34].

Note though that in contrast to the bound proposed by Landauer, the generalized Landauer's bound holds for systems with an arbitrary number of states, an arbitrary initial distribution over their states, and an arbitrary conditional distribution π . Most strikingly, the generalized Landauer bound holds even if the system is coupled to multiple thermal reservoirs, all at different temperatures, e.g., in a steady state heat engine [35, 36] (see Ex. 4 below). In such a case $k_BT \ln 2$ is not defined. Indeed, the generalized Landauer bound holds even if the system does not obey detailed balance with any of the one or more reservoirs it's coupled to.

Motivated by the generalized Landauer's bound, we define the (unconstrained) Landauer cost as the minimal EF required to compute π on initial distribution p using any process, with no constraints:

$$\mathcal{L}(p,\pi) := \mathcal{S}(p) - \mathcal{S}(\pi p). \tag{27}$$

With this definition we can write

$$Q(p) = \mathcal{L}(p, \pi) + \sigma(p) \tag{28}$$

Example 3. Landauer's bound is often stated in terms of the minimal amount of work that must be done in order to perform a given computation, rather than the heat that must be generated. This is appropriate for physical processes that both begin and end with a constant, state-independent energy function. For such processes, there cannot be any change in expected energy between the beginning and end of the process. Moreover, by the first Law of thermodynamics,

$$\Delta E = W - \mathcal{Q}(p)$$

where ΔE is the change in expected energy from the beginning and end of the process, W is work incurred by the process, and as before, $\mathcal{Q}(p)$ is the expected amount of heat that leaves the system and enters the bath. Since $\Delta E = 0$, W = Q. So the bounds in Example 1 on the minimal heat that must flow out of the system also give the minimal work that must be done on the system.

Any process which achieves $\sigma = 0$ (i.e., the generalized Landauer's bound) for some particular initial distribution p is said to be **thermodynamically reversible**, when run on that distribution. A necessary condition for a process to be thermodynamically reversible is that if we run it forward on an initial distribution p to produce p', and then "run the process backward", by changing the signs of all momenta and reversing the time-sequence of any driving, we return to p. (See [2, 37–39].)

A process being "logically reversible" means it implements an invertible map over its state space. However, a process being "thermodynamically reversible" does *not* mean it implements an invertible map over the space of all distributions. Indeed, unless a process implements a logically reversible map over the state space, in general it will map multiple initial distributions to the same final distribution, up to any desired accuracy [40].

As an example, bit erasure is a non-invertible map over the associated unit simplex. However, for any initial distribution q_0 , there is a process that implements bit erasure on q_0 thermodynamically reversibly [41]. Note though that if we run the bit erasure process backwards from the ending (delta function) distribution, we have to arrive back at the initial distribution q_0 , to satisfy the necessary condition for thermodynamic reversibility when run on q_0 . So if we run that bit-erasure process on any initial distribution $p_0 \neq q_0$ and then run it backwards, we would not arrive back at p_0 (we arrive at q_0 instead). This proves that the bit-erasure process cannot be thermodynamically reversible when run on any such $p_0 \neq q_0$.

This bit-erasure example underscores that thermodynamic reversibility is a joint property of a process W and the initial distribution p_0 ; if we run the same process on a different initial distribution, in general the amount of EP it generates will change. This dependence of EP on the initial

distribution is a central issue in analyzing the entropic costs of computation, and is addressed in the next subsection.

B. Mismatch cost and residual EP

Computational machines are built of multiple interconnected computational devices. A crucial concern in calculating the entropic costs of running such a computational machine is how the costs incurred by running any of its component devices, implementing some distribution π , depends on the distribution over the inputs to that device, p_0 . It is crucial how the entropic cost of running an AND gate depends on its inputs, how the cost of running an OR gate depends on its inputs, etc.

For a fixed π , we can write Landauer cost of any process that implements π as a single-valued function of the initial distribution p_0 ; no properties of the rate matrix W matter for calculating Landauer cost, beyond the fact that that matrix implements π . However, even if we fix π , we cannot write EP as a single-valued function of p_0 , because EP does depend on the details of how W implements π . (Intuitively, it is the EP, not the Landauer cost, that reflects the "nitty gritty details" of the dynamics of the rate matrix implementing the computation.) In this subsection I review recent results establishing precisely how W determines the dependence of EP on p_0 .

It has long been known how the entropy production rate, at a single moment t, jointly depends on the rate matrix W(t) and on the distribution over states p_t . (In fact, those dependencies are given by the expression in Eq. (22).) On the other hand, until recently nothing was known about how the EP of a discrete time process, evolving over an extended time interval, depends on the initial distribution over states. Initial progress was made in [5], in which the dependence of EP on the initial distribution was derived for the special case where $\pi(x_1|x_0)$ is nonzero for all x_0, x_1 . However, this restriction on the form of π is violated in deterministic computations.

Motivated by this difficulty, [4] extended the earlier work in [5], to give the full dependence of EP on the initial distribution for arbitrary π . That extended analysis shows that EP can always be written as a sum of two terms. Each of those terms depends on p_0 , as well as on the "nitty gritty details" of the process, embodied in W(t).

The first of those EP terms depends on p_0 linearly. By appropriately constructing the nitty gritty details of the system (e.g., by having the system implementing π run a quasi-static process), it is possible to have this first term equal zero identically, for all p_0 . The second of the EP terms instead is given by a drop in the KL divergence between p and a distribution q that is specified by the nitty gritty details, during the time interval $t \in [0, 1]$. For nontrivial distributions π , this term

can not be made to equal zero for any distribution p_0 that differs from q_0 . This is unavoidable EP incurred in running the system, which arises whenever one changes the a.

To review these recent results, recall the definition of islands c and associated distributions Δ_c from Section II. Nest make the following definition:

Definition 5. For any conditional distribution π implemented by a CTMC, and any island $c \in L(\pi)$, the associated **prior** is

$$q^c \in \underset{r: \text{supp}(r) \in \Delta_c}{\arg \min} \sigma(r)$$

We write the associated lower bound on EP as

$$\sigma^{min}(c) := \min_{r: \operatorname{supp}(r) \in \Delta_c} \sigma(r)$$

It will simplify the exposition to introduce an arbitrary distribution over islands, q(c), and define

$$q(x) := \sum_{c \in L(\pi)} q(c)q^{c}(x)$$

In [4] it is shown that

$$\sigma(p) = D(p||q) - D(\pi p||\pi q) + \sum_{c \in L(\pi)} p(c)\sigma^{min}(c)$$
(29)

(Due to the definition of islands, while the choice of distribution q(c) affects the precise distribution q inside the two KL divergences, it has no effect on their difference, and so has no effect on EP; see [4].)

The drop of KL divergences on the RHS of Eq. (29) is called the the **mismatch cost** of running the CTMC on the initial distribution p, and is written as $\mathcal{E}(p)$.¹¹ Given the priors q^c , both of these KL divergences in the mismatch cost depend only on p and on π . By the data-processing inequality for KL divergence, mismatch cost is non-negative. It equals zero if $p^c = q^c$ for all c, or if π is a measure-preserving map, i.e., a permutation of the elements of X.

The remaining sum on the RHS of Eq. (29) is called the **residual EP** of the CTMC. It is a linear function of p(c), without any information theoretic character. In addition, it has no explicit dependence on π . It is (the p(c)-weighted average of) the minimal EP within each island. $\sigma^{min}(c) \geq 0$ for all c, and residual EP equals zero if and only if the process is thermodynamically reversible. I will refer to $\sigma^{min}(c)$ as the **residual EP** (**parameter**) vector of the process. The

¹¹In [5], due to a Bayesian interpretation of q, the mismatch cost is instead called the "dissipation due to incorrect priors".

"nitty-gritty" physics details of how the process operates is captured by the residual EP vector together with the priors.

Combining Eq. (29) with the definitions of EF and of cross entropy establishes the following set of equivalent ways of expressing the EF:

Proposition 1. The total EF incurred in running a process that applies map π to an initial distribution p is

$$Q(p) = \mathcal{L}(p, \pi) + \mathcal{E}(p) + \sum_{c \in L(\pi)} p(c)\sigma^{min}(c)$$
$$= [S(p||q) - S(\pi p||\pi q)] + \sum_{c} p(c)\sigma^{min}(c)$$

Unlike the generalized Landauer's bound, which is an inequality, Prop. 1 is exact. It holds for both macroscopic and microscopic systems, whether they are computational devices or not.

I will use the term **entropic cost** to broadly refer to entropy flow, entropy production, mismatch cost, residual entropy, or Landauer cost. Note that the entropic cost of any computational device is only properly defined if we have fixed the distribution over possible inputs of the device.

It is important to realize that we cannot ignore the residual EP when calculating EF of real-world computational devices. In particular, in real-world computers — even real-world quantum computers, presuming they are coupled to input/output devices — a sizable portion of the heat generation occurs in the wires connecting the devices inside the computer (often a majority of the heat generation, in fact). However, wires are designed to simply copy their inputs to their outputs, which is a logically invertible map. As a result, the Landauer cost of running a wire is zero (to within the accuracy of the wire's implementing the copy operation with zero error), no matter what the initial distribution over states of the wire p_0 is. For the same reason, the mismatch cost of any wire is zero. This means that the entire EF incurred by running any wire is just the residual EP incurred by running that wire. So in real-world wires, in which $\sigma^{min}(c)$ invariably varies with c (i.e., in which the heat generated by using the wire depends on whether it transmits a 0 or a 1), the dependence of EF on the initial distribution p_0 must be linear. In contrast, for the other devices in a computer (e.g., the digital gates in the computer), both Landauer cost and mismatch cost can be quite large, resulting in nonlinear dependencies on the initial distribution.

Example 4. It is common in the literature to decompose the rate matrix into a sum of rate matrices

of one or more mechanisms v:

$$W_{x;x'}(t) = \sum_{\nu} W_{x,x'}^{\nu}(t) \tag{30}$$

In such cases one replaces the definitions of the EF rate and EP rate in Eq. (19), (22), with the similar definitions,

$$\sum_{x',x'',\nu} W^{\nu}_{x',x''}(t) p_{x''}(t) \ln \left[\frac{W^{\nu}_{x',x''}}{W^{\nu}_{x'',x'}} \right]$$
(31)

and

$$\sum_{x',x'',\nu} W^{\nu}_{x',x''}(t) p_{x''}(t) \ln \left[\frac{W^{\nu}_{x',x''} p_{x''}(t)}{W^{\nu}_{x'',x'} p'_{x}(t)} \right]$$
(32)

respectively.

When there is more than one mechanism, since the log of a sum is not the same as the sum of a log, these redefined EF and EP rates differ from the analogous quantities given by plugging $\sum_{\nu} W_{x,x'}^{\nu}(t)$ into Eq. (19),(22). For example, if we were to evaluate Eq. (19) for this multiple-mechanism W(t), we would get

$$\sum_{x',x'',\nu} W_{x',x''}^{\nu}(t) p_{x''}(t) \ln \left[\frac{\sum_{\nu'} W_{x',x''}^{\nu'}}{\sum_{\nu''} W_{x'',x'}^{\nu''}} \right]$$
(33)

which differs from the expression in Eq. (31).

Nonetheless, all the results presented above apply just as well with these redefinitions of EF and EP. In particular, under these redefinitions the time-derivative of the entropy still equals the difference between the EP rate and the EF rate, total EP is still non-negative, and total EF is still a linear function of the initial distribution. Moreover, that linearity of EF means that with this redefinition we can still write (total) EP as a sum of the mismatch cost, defined in terms of a prior, and a residual EP that is a linear function of the initial distribution.

By themselves, neither the pair of definitions in Eq. (19),(22) nor the pair in Eq. (31),(32) is "right" or "wrong". Rather, the primary basis for choosing between them arises when we try to apply the resulting mathematics to analyze specific thermodynamic scenarios. The development starting from Eq. (19),(22), for a single mechanism, can be interpreted as giving heat flow rates and work rates for the thermodynamic scenario of a single heat bath coupled to the system. (See Ex. 2 and 3 above.) However, in many thermodynamic scenarios there are multiple heat baths coupled to the system. The standard approach for analyzing these scenarios is to identify each heat bath with a separate mechanism, so that there is a separate temperature for each mechanism, T^{ν} . Typically

one then assumes local detailed balance (LDB), meaning that separately for each mechanism ν , the associated matrix $W^{\nu}(t)$ obeys detailed balance for the (shared) Hamiltonian H(t) and resultant (ν -specific) Boltzmann distribution defined in terms of the temperature T^{ν} , i.e., for all ν, x, x', t ,

$$\frac{W_{x,x'}^{\nu}(t)}{W_{x',x}^{\nu}(t)} = e^{[H_{x'}(t) - H_x(t)]/T^{\nu}}$$
(34)

This allows us to identify the EF rate in Eq. (31) as the rate of heat flow to all of the baths. So the EP rate in Eq. (32) is the rate of irreversible gain in entropy that remains after accounting for that EF rate and for the change in entropy of the system. See [1?, 2].

As a final comment, it is important to emphasize that all of the analysis above assumes that there are no constraints on how the physical system can implement π . For example, the Landauer cost given in Eq. (27) and Proposition 1 is the unconstrained minimal amount of EF necessary to implement the conditional distribution π on any physical system, when there are no restrictions on the rate matrix underlying the dynamics of that system. However, in practice there will always be some constraints on what rate matrices the engineer of a system can use to implement a desired logical state dynamics. In particular, the architectures of the computational machines defined in Section IV constrain which variables in a system implementing those machines are allowed to be directly coupled with one another by the rate matrix.

The minimal amount of EF needed to implement a desired distribution π if one is constrained to use a particular computational machine to implement that dynamics is called the **machine** Landauer cost. Trivially, since it is the solution to the same optimization problem that defines Landauer cost, only with extra constraints imposed, the machine Landauer cost is never less than the (unconstrained) Landauer cost, i.e. the machine Landauer cost of some particular computational machine is never less than the value given in Eq. (27). In fact, the machine Landauer cost can be substantially greater than the unconstrained Landauer cost, as illustrated by the following simple example.

Example 5. Suppose our computational machine's state space is two bits, x^1 and x^2 , and that the function f(x) erases both of those bits. Let $p_0(x)$ be the initial distribution over joint states of the two bits. (As a practical matter, p_0 would be determined by the preferences of the users of the system, e.g., as given by the frequency counts over a long time interval in which they repeatedly use the system.) In this scenario, the unconstrained Landauer cost is

$$S(p_0(X)) - S(p_1(X)) = S(p_0(X))$$

$$= S(p_0(X^1)) + S(p_0(X^2|X^1))$$
(35)

Now modify this scenario by supposing that we are constrained to implement the parallel bit erasure with two subsystems acting independently of one another, one subsystem acting on the first bit and one subsystem acting on the second bit. This changes the Landauer cost to

$$S(p_0(X^1)) - S(p_1(X^1)) + S(p_0(X^2)) - S(p_1(X^2)) = S(p_0(X^1)) + S(p_0(X^2))$$
(36)

The gain in Landauer cost due to the constraint — the machine Landauer cost — is $S(p_0(X^2))$ — $S(p_0(X^2|X^1))$. This is just the mutual information between the two bits under the initial distribution p_0 , which in general is nonzero.

To understand the implications of this phenomenon, suppose that the parallel bit erasing subsystems are thermodynamically reversible when considered by themselves. It is still the case that if they are run in parallel as two subsystems of an overall system, and if their initial states are statistically correlated, then that overall system is not thermodynamically reversible. Indeed, if we start with p_0 , implement the parallel bit erasure using two thermodynamically reversible bit-erasers, and then run that process in reverse, we end up with the distribution $p_0(x^1)p_0(x^1)$ rather than $p_0(x^1, x^2)$.

A general analysis of how the architecture of a computational machine affects the associated machine Landauer cost can be found in [4]. The special case when the open system in question is an information ratchet, there is only a single heat bath, and local detailed balance holds, is considered in [42]. See also [7, 43].

It is important to emphasize that all of the results in this section for mismatch costs and residual EP hold for processes that implement general stochastic matrices as well as those that implement single-valued functions, if one uses the appropriate generalization of islands. Finally, despite the importance of EP to the entropic costs of real world systems, from now on I will assume that the residual EP of any island of any device I consider equals zero. The resultant analysis gives the least possible EF, which would arise if (as is almost always the case in the real world) we don't design the prior of a device to match the actual distribution of its input states, and so must account for its possible mismatch cost. In addition, this assumption simplifies the calculations, since we no longer have to consider the islands of the processes.

VI. ENTROPY DYNAMICS OF LOGICALLY REVERSIBLE CIRCUITS

Our modern understanding of nonequilibrium statistical physics makes clear that there is no a priori relation between the logical reversibility of a function taking inputs to outputs, $f: X^{IN} \to \mathbb{R}$

 X^{OUT} , and the thermodynamic reversibility of a system that implements f [38, 41, 44–47]. This should not be surprising; logical reversibility is all about maps from the *state* of a system at one time to its state at another, whereas thermodynamic reversibility is all about trajectories of *marginal probability distributions* over the states of the system as the system evolves from one time to another (together with properties of any external reservoirs the system is coupled to, etc.). These are completely different kinds of mathematical structures, with the result that thermodynamic reversibility need not imply anything about logical reversibility, or vice versa.

However, the pioneering work of Landauer and Bennett [34, 48, 49] on the thermodynamics of computation led to a common misperception that logical and thermodynamic reversibility are in fact identical. This has in turn motivated research on "reversible circuits". In this research one is presented with a conventional circuit C made of logically <u>ir</u>reversible gates which implements some logically irreversible function f, and tries to construct a logically <u>reversible</u> circuit, C', that emulates C. The underlying insight is that we can always do this, by appropriately wiring together a set of logically reversible gates (e.g., Fredkin gates) to create a circuit C' that maps any input bits $x^{IN} \in X^{IN}$ to a set of output bits that contain both $f(x^{IN})$ and a copy of x^{IN} [50–53]. Tautologically, the entropy of the distribution over the states of this circuit after the map has completed is identical to the entropy of the initial distribution over states. So the Landauer cost is zero, it would appear. This has led to claims in the literature suggesting that by replacing a conventional logically irreversible circuit with an equivalent logically reversible circuit, we can reduce the "thermodynamic cost" of computing $f(x^{IN})$ to zero. More precisely, it would appear that we can reduce the total EF expended to zero.

This general line of reasoning should be worrisome. As mentioned, we now know that we can directly implement any logically irreversible map $x^{IN} \to f(x^{IN})$ in a thermodynamically reversible manner. So by running such a direct implementation of a logically irreversible f in reverse (which can be done thermodynamically reversibly), we would extract heat from a heat bath. If we do that, and then implement f forward using a logically reversible circuit, we would return the system to its starting distribution, seemingly having extracting heat from the heat bath, thereby violating the second law.

As it turns out, there are some thermodynamic advantages to using a logically reversible circuit rather than an equivalent logically irreversible circuit. However, there are also some disadvantages to using logically reversible circuits. Moreover, the advantages of logically reversible circuits cannot be calculated simply by counting "the number of bit erasures" performed by the equivalent logically irreversible circuit. In the following two subsections I elaborate these relative advantages and

disadvantages of using reversible circuits, in order to illustrate the results presented in the sections above.

Before doing that though, in the remainder of this subsection I present some needed details concerning logically reversible circuits that are constructed out of logically reversible gates. One of the properties of logically reversible gates that initially caused problems in designing circuits out of them is that running those gates typically produces "garbage" bits, to go with the bits that provide the output of the conventional gate that they emulate. The problem is that these garbage bits need to be reinitialized after the gate is used, so that the gate can be used again. Recognizing this problem, [50] shows how to avoid the costs of reinitializing any garbage bits produced by using a reversible gate in a reversible circuit C', by extending C' with yet more reversible gates (e.g., Fredkin gates). The result is an **extended circuit** that takes as input a binary string of input data x, along with a binary string of "control signals" $m \in M$, whose role is to control the operation of the reversible gates in the circuit. The output of the extended circuit is a binary string of the desired output for input x^{IN} , $x^{OUT} = f(x^{IN})$, together with a copy of m, and a copy of x^{IN} , which I will write as x^{IN}_{copy} . So in particular, none of the output garbage bits produced by the individual gates in the original, unextended circuit of reversible gates still exists by the time we get to the output bits of the extended circuit.¹²

While it removes the problem of erasing the garbage bits, this extension of the original circuit with more gates does not come for free. In general it requires doubling the total number of gates (i.e., the circuit's size), doubling the running time of the circuit (i.e., the circuit's depth), and increasing the number of edges coming out of each gate, by up to a factor of 3. (In special cases though, these extra cost can be reduced, sometimes substantially.)

A. Reversible circuits compared to all-at-once devices

In practice, typically we will want to reuse any given circuit many times, with different inputs each time. Most simply, we can assume that those inputs are generated by IID sampling a fixed distribution (which is ultimately determined by the user of the circuit). To ensure that the (average) entropic costs are independent of how many times the circuit has been used, we need to reinitialize $\overline{}^{12}$ More precisely, in one popular form of reversible circuits, a map $f: X^{IN} \to X^{OUT}$ is implemented in several steps. First, in a "forward pass", the circuit made out of reversible gates sends $(x^{IN}, m, \vec{0}^{GARBAGE}, \vec{0}^{OUT}) \to$

steps. First, in a "forward pass", the circuit made out of reversible gates sends $(x^{IN}, m, \vec{0}^{GARBAGE}, \vec{0}^{OUT}) \rightarrow (x^{IN}, m, m', f(x^{IN}))$, where m' is the set of "garbage bits", $\vec{0}^{OUT}$ is defined as the initialized state of the output bits, and similarly for $\vec{0}^{GARBAGE}$. After completing this forward pass, an offboard copy is made of x^{OUT} , i.e., of $f(x^{IN})$. Then the original circuit is run "in reverse", sending $(x^{IN}, m, m', f(x^{IN})) \rightarrow (x^{IN}, m, \vec{0}^{GARBAGE}, \vec{0}^{OUT})$. The end result is a process that transforms the input bit string x^{IN} into the offboard copy of $f(x^{IN})$, together with a copy of x^{IN} (conventionally stored in the same physical variables that contained the original version of x^{IN}), all while leaving the control bit string m unchanged.

the output variables of the circuit after each use. I will refer to a process that does this as the answer-reinitialization of that circuit.

Now in general, there are many different "basis sets" of allowed gates we can use to construct a conventional (logically irreversible) circuit that computes any given logically irreversible function f. Indeed, even once we fix a set of allowed gates, in general there are an infinite number of logically irreversible circuits that implement f using that set of gates. Due to this, we need to clarify precisely what "logically irreversible circuit" we wish to compare to any given extended circuit that implements the same function f as that circuit.

One extreme possibility is to compare the extended circuit to a single, monolithic gate that computes the same function, i.e., to a physical system that directly maps $(x^{IN}, \vec{0}^{OUT}) \rightarrow (x^{IN}, f(x^{IN}))$. However, this map is logically reversible, just like the extended circuit, and so not of interest for the comparison.

A second possibility is to compare the extended circuit to a system with a state space X that directly maps $x \in X \to f(x) \in X$, without distinguishing input variables and output variables. Such a map is *not* logically reversible, but (as mentioned above) can be implemented with a thermodynamically reversible system, whatever the initial distribution over X. I will refer to such a physical system that maps $x \to f(x)$ in a manner that is thermodynamically reversible for some initial distribution q(x) as an **all at once** (AO) device, or AO circuit. (The reason for this terminology is that the underlying Hamiltonian may need to simultaneously couple all components of x in order to achieve thermodynamic reversibility). If we implement f with an AO device, then the minimal EF we must expend to calculate f is the drop in entropy of the distribution over X as that distribution evolves according to f. This drop is nonzero (assuming f is not logically invertible). This would seem to mean that there is an advantage to using the equivalent extended circuit rather than the AO device, since the minimal EF with the extended circuit is zero.

However, we must be careful to compare apples to apples. The number of information-carrying bits in the extended circuit after it completes computing f is $\log |X^{IN}| + \log |X^{OUT}| + \log |M|$. The number of information-carrying bits in the AO device when it completes is just $\log |X^{OUT}|$. Therefore the minimal number of bits there must be in the AO device is $\max(\log |X^{OUT}|, \log |X^{IN}|)$. So it may be that the extended circuit and the AO circuit implement functions over different spaces, of different sizes.

This means that the entropic costs of answer-reinitializing the two circuits (i.e., reinitializing their variables in preparation for the next inputs) will differ. In general, the Landauer cost and mismatch cost of answer-reinitialization of an extended circuit will be greater than the corresponding

answer-reinitialization costs of an equivalent AO device. This is for the simple reason that the answer-reinitialization of the extended circuit must reinitialize the bits containing copies of x and m, which do not even exist in the AO device.

To be more quantitative, first, for simplicity, assume that the initial distribution over the bits in the extended circuit that encode m is a delta function. (This would be the case if we do not want the physical circuit to implement a different computation from one run to the next, so only one vector of control signals m is allowed.) This means that the ending distribution over those bits is also a delta function. The Landauer cost of reinitializing those bits is zero, and assuming that we perform the reinitialization using a prior that equals the delta function over m, the mismatch cost is also zero. So assuming the residual EP of reinitialization those bits containing a copy of m is zero, we can we can ignore those bits from now on.

To proceed further in our comparison of the entropic costs of the answer reinitialization of an AO device with those of an equivalent extended circuit, we need to specify the detailed dynamics of the answer-reinitialization process that is applied to the two devices. Both the AO device and the equivalent extended circuit have a set of output bits that contain $f(x^{IN})$ that need to be reinitialized, with some associated entropic costs. In addition though, the extended circuit needs to reinitialize its ending copy of x^{IN} , whereas there is no such requirement of the equivalent AO device. To explore the consequences of this, I now consider several natural models of the answer-reinitialization:

1) In one model, we require that the answer-reinitialization of the circuit is performed within each output bit g itself, separately from all other variables. Define Fr(C) to mean an extended circuit that computes the same input-output function f^C as a conventional circuit C, and define AO(C) similarly. Assuming for simplicity that the residual entropy of reinitializing all output bits is zero, the EF for the answer-reinitialization of Fr(C) using such a bit-by-bit process is

$$Q_{C'}(p,q) = \sum_{g \in V^{\text{OUT}}} S(p_g || q_g)$$
(37)

where $V^{\rm OUT}$ indicates the set of all bits containing the final values of x^{OUT} and x^{IN}_{copy} .

Using gate-by-gate answer-reinitialization, the EF needed to erase the output bits containing $f^{C}(x^{IN})$ is the same for both AO(C) and Fr(C). Therefore the additional Landauer cost incurred in answer-reinitialization due to using Fr(C) rather than AO(C) is the Landauer cost of erasing

the output bits in Fr(C) that store x_{copy}^{IN}

$$\Delta \mathcal{S}_{Fr(C),C}(p) := \sum_{v \in V_{IN}} \mathcal{S}(p_v) \tag{38}$$

where I write " $v \in V_{IN}$ " to mean the output bits that contain x_{copy}^{IN} , and p_v to mean the ending marginal distributions over those bits. Similarly, the difference in mismatch cost is

$$\Delta D_{Fr(C),C}(p,q) := \sum_{v \in V_{IN}} D_v(p^v || q^v)$$
(39)

where q_v refers to a prior used to reinitialize the output bits in $v \in V_{IN}$.

However, independent of issues of answer-reinitialization, the Landauer cost of implementing a function using an AO device that is optimized for an initial distribution p_{IN} can be bounded as follows:

$$S(p_{\text{IN}}) - S(f^C p_{\text{IN}}) \le S(p_{\text{IN}})$$

$$\le \sum_{v \in V_{\text{IN}}} S_v(p_v)$$

$$= \Delta S_{Fr(C),C}(p)$$
(40)

Combining this with Eq. (38) shows that under gate-by-gate answer-reinitialization, the total Landauer cost of implementing a function using an AO device — including the costs of reinitializing the gates containing the value $f^C(x^{IN})$ — is upper-bounded by the extra Landauer cost of implementing that same function with an equivalent extended circuit, i.e., just that portion of the cost that occurs in answer-reinitializing the extra output bits of the extended circuit. This disadvantage of using the extended circuit holds even if the equivalent AO device is logically irreversible. So as far as Landauer cost is concerned there is no reason to consider using an extended circuit to implement a logically irreversible computation with this first type of answer-reinitialization.

On the other hand, in some situations, the mismatch cost of running the AO device will be greater than the mismatch cost of the answer-reinitialization of x_{copy}^{IN} in the equivalent extended circuit. This illustrated in the following example:

Example 6. Suppose that the input to the circuit consists of two bits, a and b, where the actual distribution over those bits, p, and prior distribution over those bits, q, are:

$$p(x_b) = \delta(x_b, 0)$$
$$p(x_a|x_b = 0) = 1/2 \quad \forall x_a$$

$$q(x_b) = \delta(x_b, 1)$$

$$q(x_a|x_b = 0) = 1/2 \quad \forall x_a$$

$$q(x_a|x_b = 1) = \delta(x_a, 0)$$

Suppose as well that f^C is a many-to-one map. Then plugging in gives

$$D(p_{\text{IN}} || q_{\text{IN}}) - D(f^C p_{\text{IN}} || f^C q_{\text{IN}}) = D(p_{\text{IN}} || q_{\text{IN}})$$

$$> \sum_{v \in V_{\text{IN}}} D(p_v || q_v)$$

This sum equals the mismatch cost of the answer-reinitialization of x_{copy}^{IN} , which establishes the claim.

However, care should be taken in interpreting this result, since there are subtleties in comparing mismatch costs between circuits and AO devices, due to the need to compare apples to apples (see discussion of this point in [4]).

2) A second way we could answer-reinitialize an extended circuit involves using a system that simultaneously accesses all of the output bits to reinitialize x_{copy}^{IN} , including the bits storing $f(x^{IN})$.

To analyze this approach, for simplicity assume there are no restrictions on how this reinitializing system operates, i.e., that it is an AO device. The Landauer cost of this type of answer-reinitialization of x_{copy}^{IN} is just $\mathcal{S}(p(X^{IN}|X^{OUT})) - \ln[1]$, since this answer-reinitialization process is a many-to-one map over the state of x_{copy}^{IN} . Assuming f^C is a deterministic map though, by Bayes' theorem

$$S(p(X^{IN}|X^{OUT})) = S(p(X^{IN})) - S(p(X^{OUT}))$$
(41)

So in this type of answer-reinitialization, the extra Landauer cost of the answer-reinitialization in the extended circuit that computes f^C is identical to the total Landauer cost of the AO device that computes the same function f^C . On the other hand, in this type of answer-reinitialization process the mismatch cost of the extended circuit may be either greater or smaller than that of the AO device, depending on the associated priors.

3) A third way we could answer-reinitialize x_{copy}^{IN} in an extended circuit arises if, after running the circuit, we happened upon a set of initialized external bits, just lying around, as it were, ready to be exploited. In this case, after running the circuit, we could simply swap those external bits with x_{copy}^{IN} , thereby answer-reinitializing the output bits at zero cost.

Arguably, this is more sleight-of-hand than a real proposal for how to re-initialize the output bits. Even so, it's worth pointing out that rather than use those initialized external bits to contain a copy of x_{copy}^{IN} , we could have used them as an information battery, extracting up to a maximum of $k_BT \ln 2$ from each one by thermalizing it. So the opportunity cost in using those external bits to reinitialize the output bits of the extended circuit rather than use them as a conventional battery is $|V_{IN}|k_BT \ln 2$. This is an upper bound on the Landauer cost of implementing the desired computation using an AO device. So again, as far as Landauer cost is concerned, there is no advantage to using an extended circuit to implement a logically irreversible computation with this third type of answer-reinitialization.

Summarizing, it is not clear that there is a way to implement a logically irreversible function with an extended circuit built out of logically reversible gates that reduces the Landauer cost below the Landauer cost of an equivalent AO device. The effect on the mismatch cost of using such a circuit rather than an AO device is more nuanced, varying with the priors, the actual distribution, etc.

B. Reversible circuits versus irreversible circuits

I now extend the analysis from comparing the entropic costs of an extended circuit and those of a computationally equivalent AO device, to also consider the costs of a computationally equivalent conventional circuit, built with multiple logically irreversible gates. As illustrated below, the entropic costs of the answer-reinitialization of a conventional circuit (appropriately modeled) are the same as the entropic costs of the answer-reinitialization of a computationally equivalent AO device. So the analysis of the preceding subsection carries over, giving the relationship between the entropic costs of answer-reinitialization of conventional circuits and the entropic costs of answer-reinitialization of conventional circuits. In particular, the minimal EF required to answer-reinitialize a conventional circuit is in general lower than the minimal EF required to answer-reinitialize a computationally equivalent extended circuit.

Accordingly, in this subsection I focus instead on comparing the entropic costs of running conventional circuits, before they undergo any answer-reinitialization, with the entropic costs of running computationally equivalent extended circuits, before they undergo any answer-reinitialization. While the full analysis of the entropic costs of running conventional circuits is rather elaborate [4], some of the essential points can be illustrated with the following simple example.

Suppose we have a system that comprises two input bits and two output bits, with state space written as $X = X_1^{IN} \times X_2^{IN} \times X_1^{OUT} \times X_2^{OUT}$. Consider mapping the input bits to the output bits by running the "parallel bit erasure" function. Suppose that while doing that we simultaneously reinitialize the input bits x_1^{IN} and x_2^{IN} , in preparation for the next run of the system on a new set of inputs. So assuming both of the output bits are initialized before the process begins to the erased value 0, the state space evolves according to the function $f:(x_1^{IN},x_2^{IN},0,0)\to(0,0,0,0)$.

Consider the following three systems that implement this f:

- 1. An AO device operating over $X_1^{IN} \times X_2^{IN} \times X_1^{OUT} \times X_2^{OUT}$ that directly implements f;
- 2. A system that implements f using two bit-erasure gates that are physically isolated from one another, as briefly described in Example 5. Under this model the system first uses one bit-erasure gate to send $(X_1^{IN}, X_1^{OUT}) = (x_1^{IN}, 0) \to (0, 0)$, and then uses a second bit-erasure gate to apply the same map to the second pair of bits, (X_2^{IN}, X_2^{OUT}) .

The requirement that the gates be physically isolated means that the rate matrix of the first gate is only allowed to involve the pair of bits (X_1^{IN}, X_1^{OUT}) , i.e., it is of the form $W_{x_1^{IN}, x_1^{OUT}; (x_1^{IN})', (x_1^{OUT})'}(t)$. So the dynamics of (x_1^{IN}, x_1^{OUT}) is independent of the values of the other variables, (x_2^{IN}, x_2^{OUT}) . Similar restrictions apply to the rate matrix of the second gate. (So in the language of [4], the two gates each run a "solitary process".)

- 3. A system that uses two bit-erasure gates to implement f, just as in (2), but does not require that those gates run in sequence and that they be physically isolated. In other words, the rate matrix that drives the first bit-erasure gate as it updates the variables (x_1^{IN}, x_1^{OUT}) is allowed to do so based on the values (x_2^{IN}, x_2^{OUT}) , and vice-versa. Formally, this means that both of those rate matrices are of the form $W_{x_1^{IN}, x_1^{OUT}, x_2^{IN}, x_2^{OUT}; (x_1^{IN})', (x_2^{OUT})'; (x_2^{IN})', (x_2^{OUT})'}(t)$.
- (2) and (3) are both physical models of a conventional circuit made out of two gates that each implement logically-irreversible functions. However, they differ in whether they only allow physical coupling among the variables in the circuit that are logically needed for the circuit to compute the desired function (model (2)), or instead allow arbitrary coupling, e.g., to reduce entropic costs (model (3)).

The Landauer cost of the first model, (1), is the minimal EF needed to implement the parallel bit erasure with a single monolithic gate,

$$S(p_0(X_1^{IN}, X_2^{IN}, X_1^{OUT}, X_2^{OUT})) - S(\hat{f}_{1,2} \ p_0(X_1^{IN}, X_2^{IN}, X_1^{OUT}, X_2^{OUT}))$$

$$= S(p_0(X_1^{IN}, X_2^{IN}, X_1^{OUT}, X_2^{OUT}))$$

$$= S(p_0(X_1^{IN}, X_2^{IN}))$$
(42)

where $\hat{f}_{1,2}$ is the conditional distribution implementing the parallel bit erasure, so that $\hat{f}_{1,2} p_0(x)$ is the ending distribution, which is a delta function centered at (0,0,0,0).

Next, assume that both of the gates in (2) are thermodynamically reversible, if they are considered in isolation, separately from any other systems (and if they are run on the appropriate initial distributions). In other words, considered in isolation from any other systems, they are both AO devices. So the minimal EF needed to run the first of those gates is

$$S(p_0(X_1^{IN}) - S(\hat{f}_1 \ p_0(X_1^{IN}, X_1^{OUT})) = S(p_0(X_1^{IN})$$
(43)

Similarly, the minimal EF needed to run the second gate is $S(p_0(X_2^{IN}))$.

Combining, we see that the difference between {the minimal EF needed to run a conventional circuit constructed as in model (2)} and {the minimal EF needed to run a computationally equivalent AO device (model (1))} is

$$S(p_0(X_1^{IN}) + S(p_0(X_2^{IN}) - S(p_0(X_1^{IN}, X_2^{IN})))$$
(44)

This is just the initial mutual information between X_1^{IN} and X_2^{IN} . So the minimal EF needed to run model (2) will exceed the minimal EF needed to run model (1) whenever X_1^{IN} and X_2^{IN} are statistically coupled under the initial distribution, p_0 . (See Example 5.)

On the other hand, because of the increased flexibility in their rate matrices, we can assume that the bit-erasure gates in the circuit defined in (3) each achieve zero EP even when considered as systems operating over the full set of four bits. So each of those bit-erasure gates is thermodynamically reversible even when considered in the context of the full system. As a result, running the circuit defined in model (3) requires the same minimal EF as running an AO device. So in general, the minimal EF needed to run to the conventional circuit defined in model (3) is less than the minimal EF of running a circuit as modeled in (2) compared to a circuit as modeled in (3) is precisely the difference between machine Landauer cost and (unconstrained) Landauer cost, discussed at the end of Section V. (A detailed analysis of this difference in costs, involving explicit rate matrices, can be found in the appendices in [4].)

Next, note that we only need to reinitialize the two output bits after running any of the three models (1), (2) and (3). In contrast, the extended circuit that runs f needs to reinitialize its input

bits as well, in preparation for receiving a new set of inputs for a next run of the system. So models (1), (2) and (3) have lower minimal EF for answer-reinitialization than the computationally equivalent extended circuit, in general.

Summarizing, the minimal total EF (including both the EF needed to run the system and to answer-reinitialize it) that is needed by model (2) exceeds the minimal total EF needed by either the equivalent AO device (model (1)) or the equivalent conventional circuit as defined by model (3), with the difference equal to the mutual information of the inputs bits under p_0 . In turn, the minimal EFs to (only) run either model (1) or model (3) exceeds the minimal EF needed to run an equivalent extended circuit, by $S(p_0(X_1^{IN}, X_2^{IN}))$. However, the minimal total EF of the models (1) and (3) will in general be no greater than the minimal total EF of the extended circuit, and may be smaller (depending on the details of the answer-reinitialization process in the extended circuit).

On the other hand, as a purely practical matter, constructing a conventional circuit as in (3) for circuits substantially larger than parallel bit-erasures may be quite challenging; to do so requires that identify all sets of variables that are *statistically* coupled, at any stage of running the circuit, and make sure that our gates are designed to *physically* couple those variables. There are no such difficulties with constructed an extended circuit. Another advantage of an extended circuit is that no matter what the true distribution p_0 is, an extended circuit has zero mismatch cost, since there is no drop of KL divergence between p_0 and $any q_0$ under a logically reversible dynamics. In contrast, all three models (1) - (3) can have nonzero mismatch cost, in general.

As yet another point of comparison, an extended circuit will often have far more wires than an equivalent conventional circuit. And as mentioned above, the residual EP generated in wires is one of the major sources of EF in modern digital gates. So even in a situation where a conventional circuit has nonzero mismatch cost, when the EF generated in the wires is taken into account, there may be no disadvantage to using that conventional circuit rather a computationally equivalent extended circuit.

Clearly there is a rich relationship between the detailed wiring diagram of a conventional logically irreversible circuit, the procedure for answer-reinitializing the outputs of a computationally equivalent extended circuit, the distribution over the input bits of those circuits, and how the aggregate entropic costs of those two circuits compare. Precisely delineating this relationship is a topic for future research.

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