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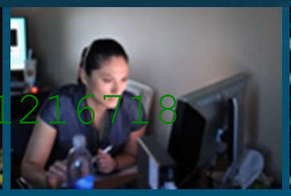
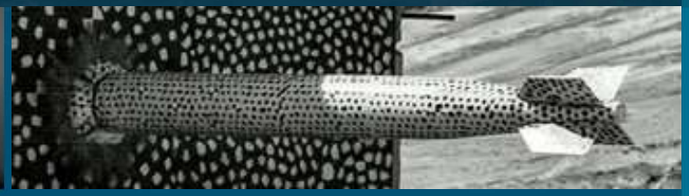
Quantum Foundations of Classical Reversible Computing





Thursday, May 27th, 2021

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Abstract of Article

The reversible computation paradigm aims to provide a new foundation for general classical digital computing that is capable of circumventing the thermodynamic limits to the energy efficiency of the conventional, non-reversible digital paradigm. However, to date, the essential rationale for and analysis of classical reversible computing (RC) has not yet been expressed in terms that leverage the modern formal methods of non-equilibrium quantum thermodynamics (NEQT). In this paper, we begin developing an NEQT-based foundation for the physics of reversible computing. We use the framework of Gorini-Kossakowski-Sudarshan-Lindblad dynamics (a.k.a. *Lindbladians*) with multiple asymptotic states, incorporating recent results from resource theory, full counting statistics, and stochastic thermodynamics. Important conclusions include that, as expected: (1) Landauer's Principle indeed sets a strict lower bound on entropy generation in traditional non-reversible architectures for deterministic computing machines when we account for the loss of correlations; and (2) implementations of the alternative *reversible* computation paradigm can potentially avoid such losses, and thereby circumvent the Landauer limit, potentially allowing the efficiency of future digital computing technologies to continue improving indefinitely. We also outline a research plan for identifying the fundamental minimum energy dissipation of reversible computing machines as a function of speed.

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Section I: Broad Theoretical Foundations

Quantum Foundations of Classical Reversible Computing

Big Picture (Non-Equilibrium Open Quantum System Framework)

Divide the model universe $\mathfrak{U}$ into the "system" (computing system) $\mathfrak{S}$ and its external environment $\mathfrak{E}$.

- System $\mathfrak{S}$ can contain its own free energy supply.
  - *E.g.*, a battery
- System $\mathfrak{S}$ can expel waste heat to the environment $\mathfrak{E}$.
  - To some extent, this is all just a formal convenience…
    - Since, a *large enough* closed system can approximate an open one.

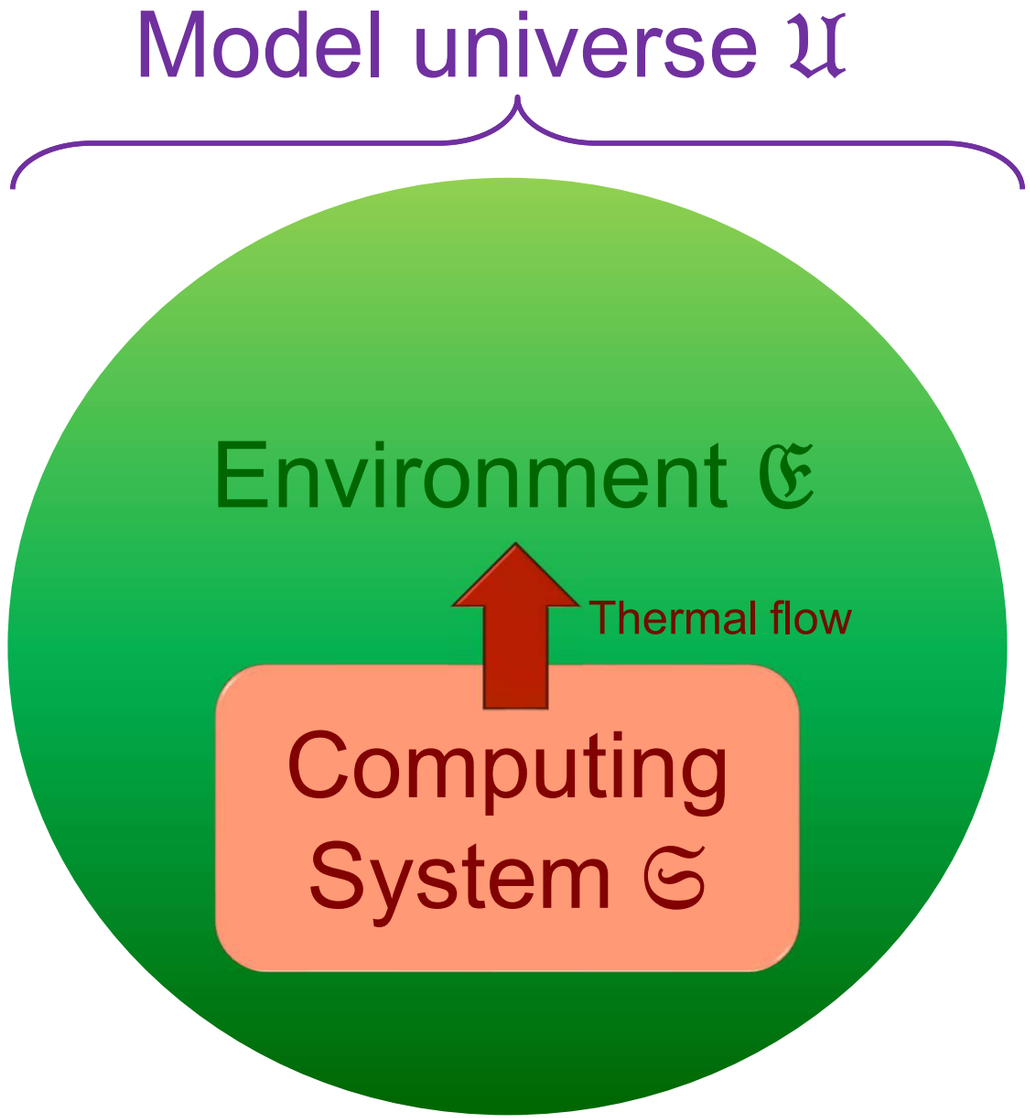
Assume the universe's Hilbert space factorizes:

- $\mathcal{H}_{\mathfrak{U}} = \mathcal{H}_{\mathfrak{E}} \otimes \mathcal{H}_{\mathfrak{S}}$ ← We mostly focus on $\mathcal{H}_{\mathfrak{S}}$.

Also important assumption: Correlations between $\mathfrak{S}$ and $\mathfrak{E}$ aren't effectively tracked or modeled…

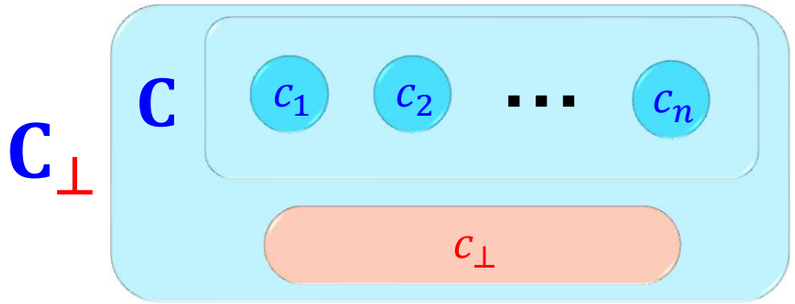
- $\therefore \rho_{\mathfrak{U}} = \rho_{\mathfrak{E}} \otimes \rho_{\mathfrak{S}}$
  - Effectively, after a short thermalization timescale after emitting energy ΔQ. → Markovian approximation.

Generally model environment $\mathfrak{E}$ as being in a uniform thermal state at some constant temperature T.



Computational State Abstraction

There is no need to worry, at the start, about exactly *how* the digital computing machine will be organized (*e.g.*, into bits)…



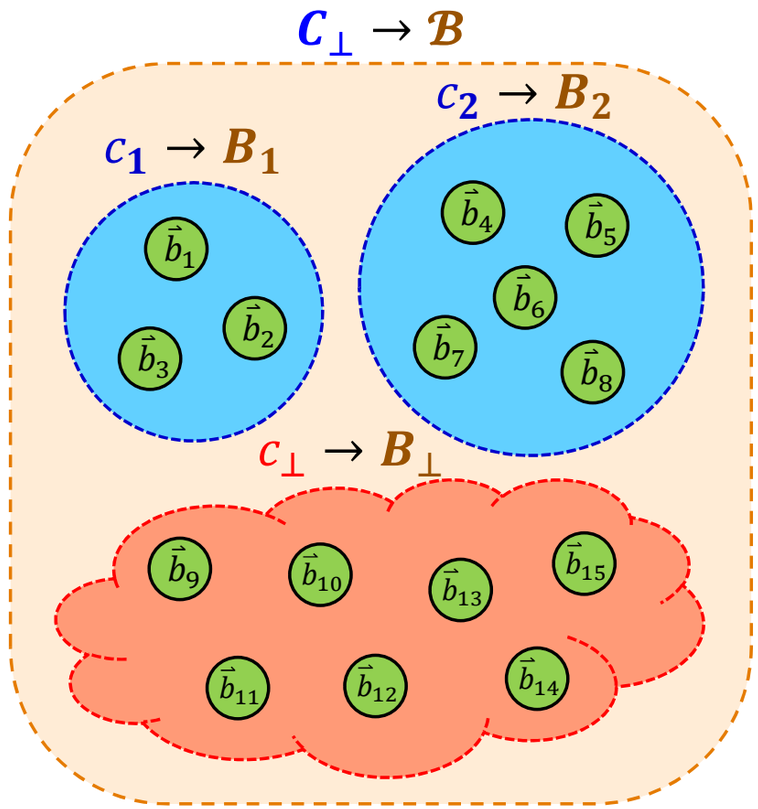
- Instead, just say that, at any given time, we can define some number n of valid discrete *computational states* $c_1, c_2, \ldots, c_n$ that the machine could theoretically be in
  - The set of *all* of these defined computational states is called $\mathbf{C}$.
- We can add a single extra "dummy computational state" $c_\perp$ to represent the generic circumstance that the system is not currently strictly occupying *any* of these defined computational states.
  - The computer might be powered down, broken, vaporized, or, just one of its state bits might just be a *little* bit outside of its defined error margins.
  - The set of *all* "computational states" *including* $c_\perp$ is called $\mathbf{C}_\perp$.
    - Call this "the augmented computational state set."

Note we can always break down the computational model in more detail later as needed.

Proto-Computational Basis

A *proto-computational basis* for the computing system $\mathfrak{S}$ just means *any* appropriate orthonormal basis $\mathcal{B}$ for the system's Hilbert space $\mathcal{H}_{\mathfrak{S}}$ such that the exact computational state $c \in \boldsymbol{C}_{\perp}$ would be consistently and unambiguously determined by a (hypothetical) complete projective measurement of the *quantum* state of the machine onto the basis $\mathcal{B}$.

- Given such a $\mathcal{B}$, it follows that $\boldsymbol{C}_{\perp}$ can then be identified (i.e. put into correspondence) with a set-theoretic *partition* of the set $\mathcal{B}$.



Example of a computational state space $\boldsymbol{C}$ consisting of 3 distinct computational states $c_1, c_2, c_\perp$, each identified with an equivalence class of basis states in $\mathcal{B}$. The catch-all state $c_\perp = \mathcal{B} - \bigcup_{i=1}^{n} c_i$ is considered computationally invalid.

Computational and Non-Computational Subspaces

In some cases, we may be able to factor the Hilbert space $\mathcal{H}_{\mathfrak{S}}$ of the computing system into separate Hilbert spaces for "computational" and "non-computational" degrees of freedom:

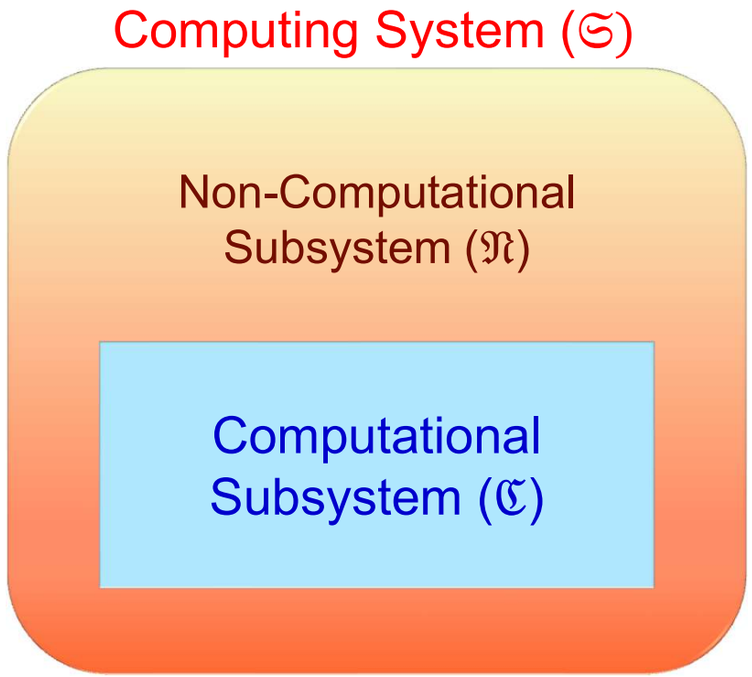
- $\mathcal{H}_{\mathfrak{S}} = \mathcal{H}_{\mathfrak{C}} \otimes \mathcal{H}_{\mathfrak{N}}$

But, this may not always be possible!

- *E.g.* different states of the computational subsystem $\mathfrak{C}$ may put differing constraints on the $\mathfrak{N}$ system, such that we can't properly describe the $\mathfrak{N}$ system by itself using the very *same* Hilbert space for all cases.

However, in such cases, we can still represent $\mathcal{H}_{\mathfrak{S}}$ via a direct sum of subspaces for different comp. states:

- $\mathcal{H}_{\mathfrak{S}} = \oplus_{i=0}^{n} \mathcal{H}_{\mathfrak{N}}^{(i)}$, where $\mathcal{H}_{\mathfrak{N}}^{(i)}$ is a Hilbert space for the $\mathfrak{N}$ subsystem that is applicable when the $\mathfrak{C}$ state happens to be c_i. (Let $c_0 = c_\perp$.)
  - This is the same as treating the various $\mathfrak{N}$ subspaces $\mathcal{H}_{\mathfrak{N}}^{(i)}$ as orthogonal; which is true since they are just the subspaces spanned by the basis vectors in $\boldsymbol{B}_i$.



$\mathbf{C}_\perp = \{c_0, \ldots, c_n\}$; $\boldsymbol{B}_i = \{\vec{b}_{i,1}, \ldots, \vec{b}_{i,n_i}\}$

General state of $\mathfrak{N}$ system for computational state c_i:

$$\vec{v}_i^{\,\mathfrak{N}} = \sum_{j=0}^{n_i} a_{i,j}\vec{b}_{i,j}$$

General state of complete computing system $\mathfrak{S}$:

$$\vec{v}^{\,\mathfrak{S}} = \sum_{i=0}^{n}\sum_{j=1}^{n_i} a_{i,j}\vec{b}_{i,j}$$

(Before normalization)

Time-Dependent Description

In general, the definition of the accessible computational states could be *time-dependent*.

- *E.g.*, if the computing system is clocked in phases, and different numbers of bits are active in different phases. Or, if the system is being built up over time.
- We will typically assume there exists some discrete set of times $t = \tau_\ell \in \mathbb{R}$ at which the computational states are well-defined.

Abstract computational concepts:

- $\boldsymbol{C}(t)$ – The discrete set of computational states defined for the computing system at time t.
- $n(t) = |\boldsymbol{C}(t)|$ – The number of computational states defined for the computing system at time t.
- $c_i(t)$ – The i^{th} computational state in $\boldsymbol{C}(t)$, in some arbitrary enumeration of computational states.
- $\boldsymbol{C}_\perp(t) = \boldsymbol{C}(t) \cup \{\boldsymbol{c}_\perp(t)\}$ – The augmented computational state space at time t.
- $c(t)$ – The actual computational state at time t (if fully decohered, & deterministic).

Physical concepts:

- $\boldsymbol{\mathcal{B}}(t)$ – A protocomputational basis for $\mathcal{H}_{\Subset}$ that can be used to define the computational states at time t.
- $\vec{b}_j(t)$ – The j^{th} particular protocomputational basis state in $\boldsymbol{\mathcal{B}}(t)$.
- $\boldsymbol{B}_i(t) \subseteq \boldsymbol{\mathcal{B}}(t)$ – The subset of protocomputational basis states that corresponds to $c_i(t)$.
  - As before, this is a partition of $\boldsymbol{\mathcal{B}}(t)$.
- $\boldsymbol{B}_\perp(t) = \boldsymbol{\mathcal{B}}(t) - \bigcup_{i=1}^{n} \boldsymbol{B}_i$ – The subset of protocomputational basis states for which the computational state is *undefined* ($\perp$) at time t.

Fundamental Theorem of the Thermodynamics of Computation

NOTE: We distinguish this from Landauer's Principle proper.

Let $\phi \in \mathcal{H}_{\mathfrak{S}}$ represent a microstate (pure quantum state) of the computing system $\mathfrak{S}$.

- Let ϕ be hypothetically sampled by applying a complete projective measurement of $\mathfrak{S}$ onto some protocomputational basis $\boldsymbol{\mathcal{B}}$.
  - Thus ϕ can be identified as ϕ_i, corresponding to some $\vec{b}_i \in \boldsymbol{\mathcal{B}}$.
- The probability distribution $p(\phi_i)$ is given as usual by the Born rule, or equivalently by the diagonal elements of the $\rho_{\mathfrak{S}}$ density matrix in the $\boldsymbol{\mathcal{B}}$ basis.

Note that the distribution $p(\phi_i)$ implies a *derived* distribution over the *computational* states:

$$P(c_j) = \sum_{\phi_i \in c_j} p(\phi_i) \,.$$

And, the total entropy of the physical system (random variable Φ for the state ϕ) can always be written as $S(\Phi) = H(C) + S(\Phi|C)$,

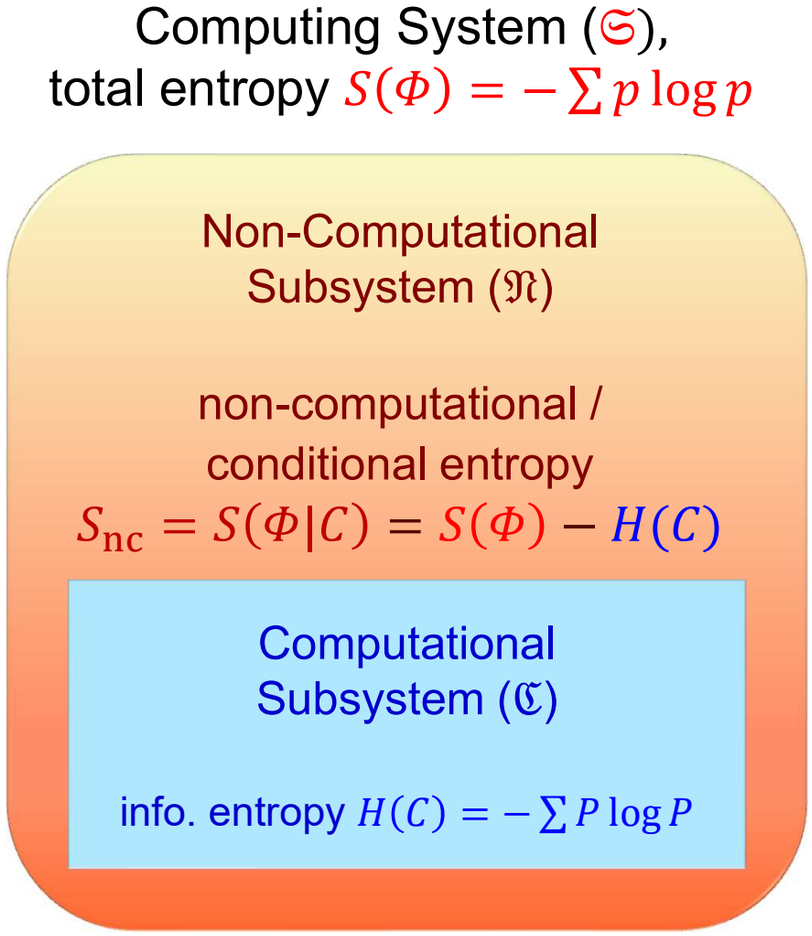
- where C is a random variable for the *computational* state, and S, H are the entropies based on the probability distributions p, P respectively.

Cite Physical Foundations of Landauer's Principle

Fundamental Theorem Illustrated

The total entropy of any given computing system $\mathfrak{S}$ can always be partitioned as a sum of the entropies associated to its computational vs. non-computational subsystems.

- In this picture, we are implicitly imagining hypothetically sampling $\mathfrak{S}$ by measuring it in an appropriate protocomputational basis $\boldsymbol{\mathcal{B}}$…
  - When this is not the case, or at times when the system becomes (perhaps briefly) entangled with its environment $\mathfrak{E}$, we need to be a little bit more careful.



Computational Operations

For our purposes, a (classical) *computational operation* O *on* a computational state set $\boldsymbol{C}$ is a (potentially stochastic) map:

$$O: \boldsymbol{C} \rightarrow \mathcal{P}(\boldsymbol{C})$$

- Maps each initial state $c_i \in \boldsymbol{C}$ to a corresponding probability distribution $P_i \in \mathcal{P}(\mathbf{C})$ over final states.

A computational operation O is called *deterministic* (for our purposes) when the final state entropy $H(P_i) = 0$ for all i.

- Also we can have that O is just *deterministic over a subset* $\boldsymbol{A} \subset \boldsymbol{C}$ of initial states, but not the whole set $\boldsymbol{C}$.
- If O is not deterministic, we call it *stochastic*.
  - So as not to be confused with the computer science meaning of *nondeterministic*.

Logically Reversible Operations

We say that an operation O is *(unconditionally, logically) reversible* if and only if there is no final state $c_k \in C$ that is reachable from two different c_i, c_j $(i \neq j)$, *i.e.*, where:

$$P_i(c_k) \neq 0 \text{ and } P_j(c_k) \neq 0.$$

- Otherwise, we say that O is *logically irreversible*.

We say that O is *conditionally (logically) reversible under the precondition that the initial state* $c \in A$, for some $A \subseteq C$, if and only if there is no final state $c_k \in C$ reachable from two $c_i, c_j \in A$ $(i \neq j)$.

- Although it's not very widely known, it's only this weaker, *conditional* form of reversibility (given a context where the precondition is guaranteed to be satisfied) that's required to avoid the information loss that causes necessary dissipation under Landauer's Principle!
  - Models of reversible (as well as quantum) computing can be generalized in ways that take advantage of this.

Time-Dependent Case

We can write O_s^t to denote a computational operation being applied over the time interval between starting time $s \in \mathbb{R}$ and terminating time $t \in \mathbb{R}$, with $t > s$:

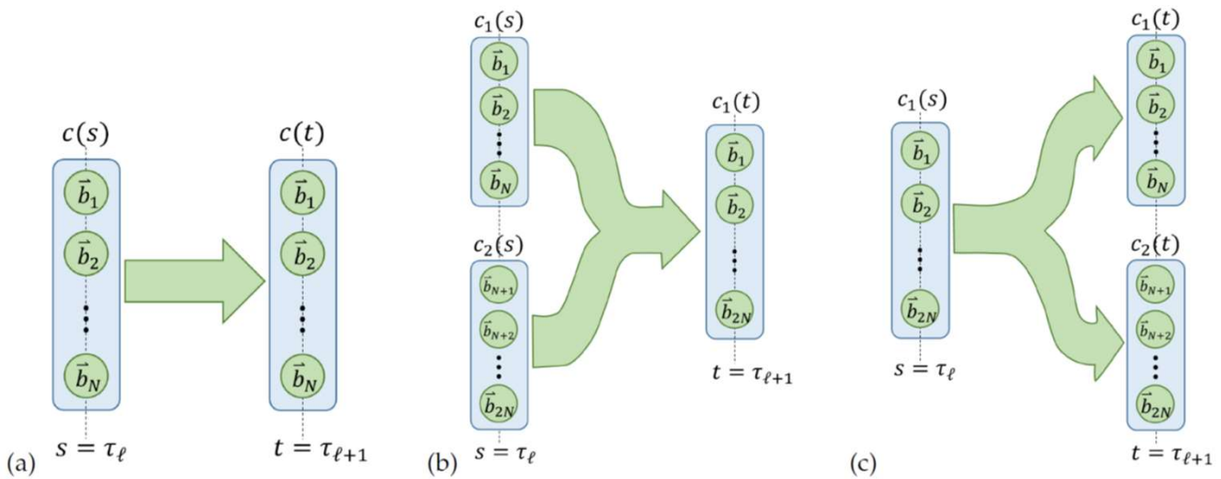
$$O_s^t : \boldsymbol{C}(s) \to \mathcal{P}\big(\boldsymbol{C}(t)\big)$$

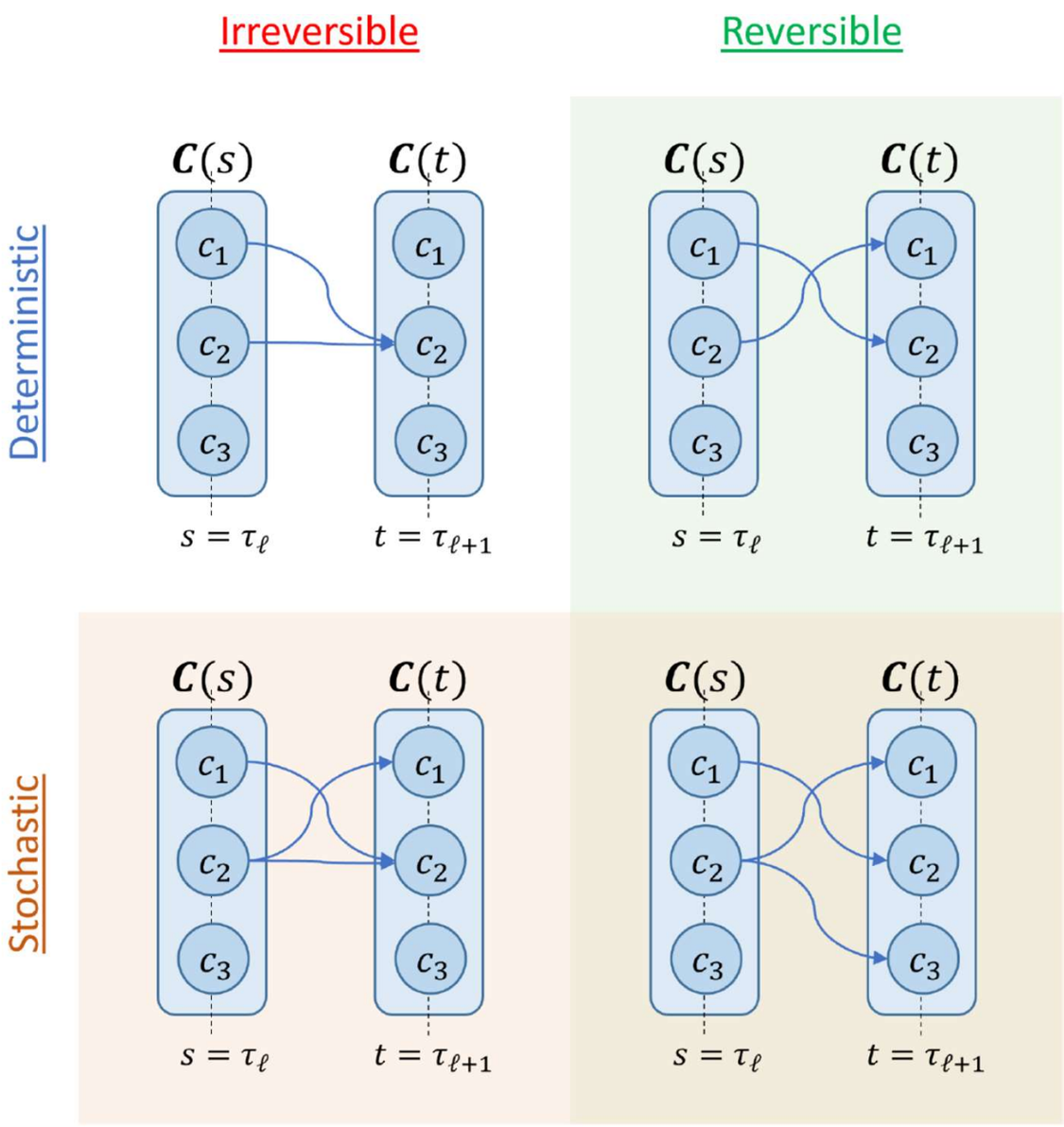
The remaining definitions (for determinism, reversibility, etc.) change correspondingly in the obvious ways.

Operations and Transitions

We can easily illustrate various categories of computational operations in terms of the state transitions making them up →

- We can think about the transitions in terms of what they do to the basis state sets (below).
  - Note that, in unitary evolution, the *aggregate* size of the basis state sets is conserved.
    - In open-system dynamics, this need not be the case, as entropy may transfer to/from the environment.





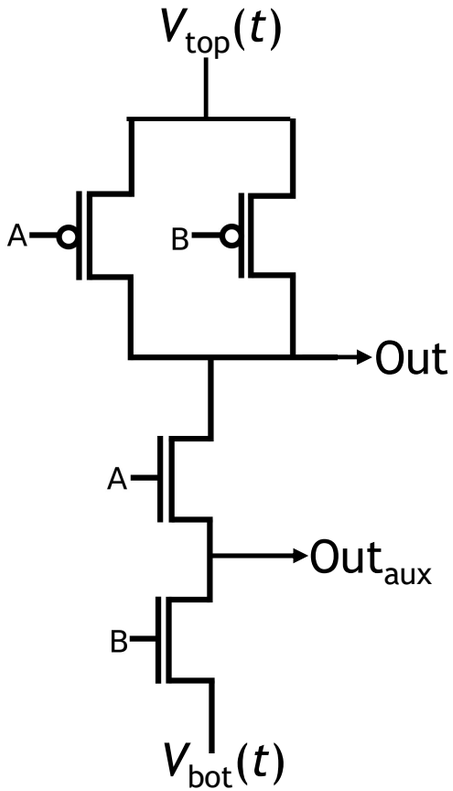
Gates vs. Operations

(And, why you really need to know some engineering to do physics of computing!)

A	B	Out
0	0	1
0	1	1
1	0	1
1	1	0

Note that there is a crucially important distinction that needs to be made between physical logic ***gates*** (*i.e.*, hardware devices that can evaluate Boolean functions), versus ***gate operations***—*i.e.*, actual *transformations* of the computational state.

- A single physical hardware *device* can often be operated in multiple different ways!
  - *E.g.,* we can build a *single* hardware circuit that can evaluate Boolean functions in *either* a reversible or irreversible way, depending on how it's operated! *E.g.* a NAND gate in standard CMOS *and* in SCRL (see next slides for details) →
- The irreversibility of *e.g.* conventional gate operation protocols to compute the AND function does *not* come from the *function* being computed (AND), but on *how* it's being computed!



Therefore, in the physics of computing, it's critically important not to try to think about computational operations at a level that is *too* abstract (abstract CS + abstract physics), *i.e.*, at a level that's *completely divorced* from what concrete engineering implementations are actually doing in more detail!

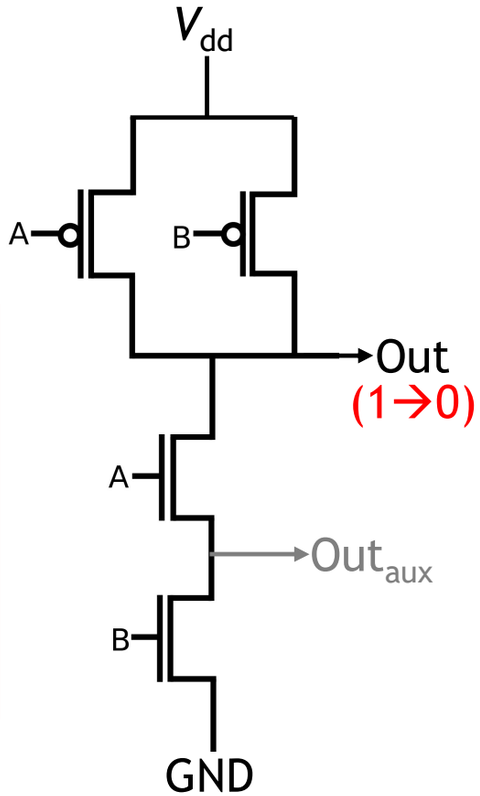
- That is an inadequate level of detail of analysis, and is unlikely to be very accurate/informative for doing detailed physics of computation research, or for developing innovative technologies.

Thus, it's essential to know *something* about electrical and computer engineering to really analyze the physics of computing technology (including reversible computing) in detail…

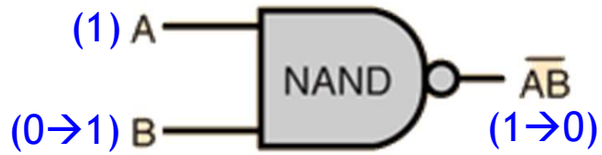
- **Subjects like:** Solid-state physics, semiconductor electronics, digital logic, VLSI design, computer architecture, *etc.*

Conventional/Irreversible vs. Adiabatic/Reversible Operation of the very same standard CMOS NAND gate circuit structure

Note: Neither of these operations ever consumes the gate's inputs!



Irreversible computational operation:
"After any change in AB, *destructively overwrite* the previous output value with the new value of $\overline{AB}$."

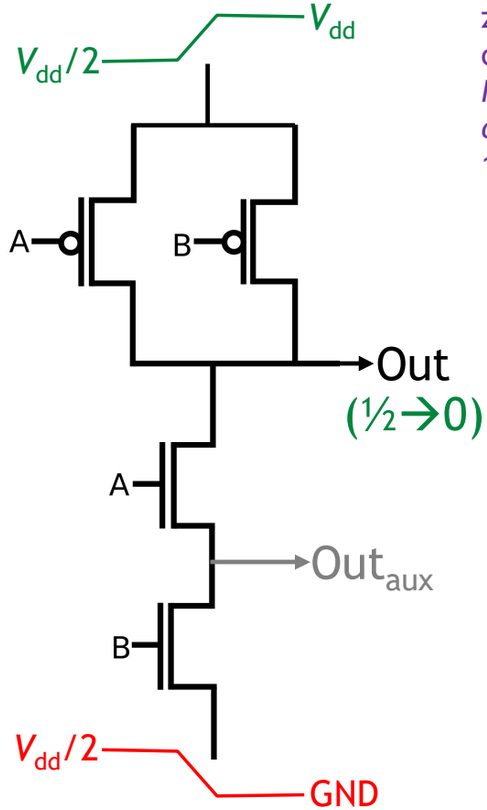


A	B	Out
0	0	1
0	1	1
1	0	1
1	1	0

$Out = \frac{1}{2}$

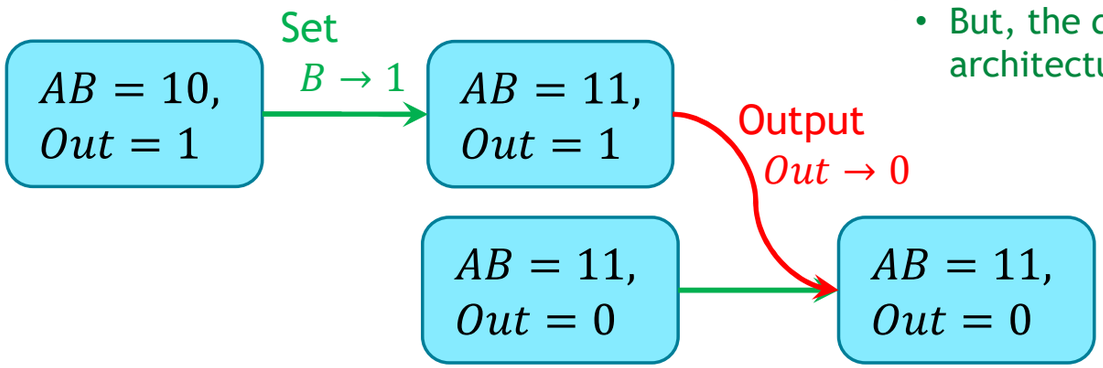
- Oftentimes, local state changes can be carried out either reversibly *or* irreversibly, depending on the detailed protocol of operations!
  - But, the difference has real architectural implications!

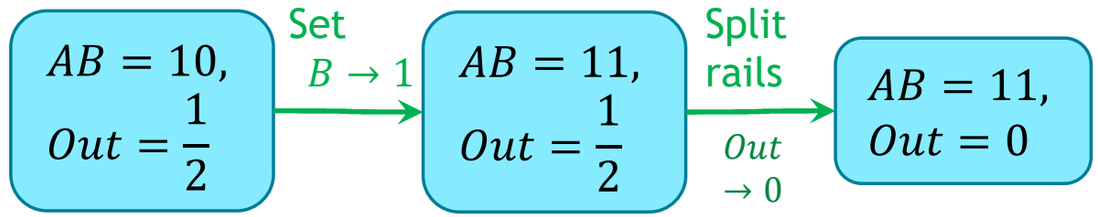
SCRL



Younis, Saed G., and T. F. Knight. "Asymptotically zero energy split-level charge recovery logic." In *International Workshop on Low Power Design*, pp. 177-182. Apr. 1994.

Reversible computational operation:
"After any change in AB, reversibly modify the output from ½ to the new value of $\overline{AB}$ (and undo this change later, before the next operation)."





An Important Remark on Landauer's Principle

Some authors identify the *Fundamental Theorem of the Thermodynamics of Computing* (described earlier) with Landauer's Principle, but I would argue that to make that identification is, properly speaking, a misleading misapprehension, which misses certain key points gained through a *proper* understanding of Landauer.

- The *Fundamental Theorem* merely has to do with how we happen to group physical states into computational states, and how total entropy can always be expressed as a sum of computational and non-computational entropies.
  - Merely changing the grouping (e.g. merging or unmerging computational states) does not inherently *increase* total entropy!
    - It only moves it (potentially reversibly) between nominally computational versus non-computational forms.
      - E.g. raise/lower a potential energy barrier separating two degenerate states
- But I would argue that the statement that is more *properly* called ***Landauer's Principle*** is actually a very *different* kind of statement, about a somewhat more complicated theoretical setup, namely this:
  - If we take (all, or part of) a (fully or partially) *known* computational state, or (as a special case of this) an unknown local state that has *known correlations to another system*, and we *obliviously allow some of the previously-known information to thermalize*, that is, to become *more uncertain*, then this *uncertainty increase* represents (quite immediately, by definition!) a net increase in absolute entropy.
    - The prototypical case, namely, oblivious erasure of a deterministically computed (and therefore, correlated) computational bit, is then just a trivial special case of this—since a correlated bit lost to a thermal environment is quickly thermalized.
  - To make the above statement mathematically precise and rigorous takes just a little bit more work (and some information theory), but is straightforward.

Proof of Landauer's Principle (example for correlated-subsystems case)

Let X, Y be state variables corresponding to *any two* disjoint computational subsystems $\mathfrak{X}, \mathfrak{Y}$ within a larger computer $\mathfrak{C}$.

- There is a joint probability distribution $P(X,Y)$, and a corresponding joint entropy $H(X,Y)$.
- Reduced entropies $H(X), H(Y)$ of the individual subsystems are defined in the usual way.

The mutual information between $\mathfrak{X}$ and $\mathfrak{Y}$ is defined as:

$$I(X;Y) \stackrel{\text{def}}{=} H(X) + H(Y) - H(X,Y).$$

Now, define the *independent entropy in* $\mathfrak{Y}$ as the *rest* of $\mathfrak{Y}$'s (reduced subsystem) entropy, *besides* the mutual information I that $\mathfrak{Y}$ has with $\mathfrak{X}$:

$$S_{\text{ind}}(Y) \stackrel{\text{def}}{=} H(Y) - I(X;Y) = H(Y|X),$$

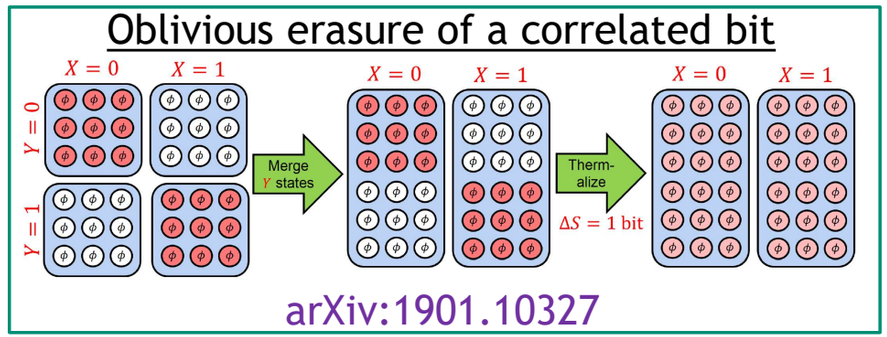
- Same thing as the conditional entropy of $\mathfrak{Y}$, conditioned on $\mathfrak{X}$.

Now, consider *erasing* $\mathfrak{Y}$ via *any* oblivious physical mechanism…

- Meaning, set $H(Y) = 0$ *unconditionally*, without reference to X *or to any other information we may have* about Y.
  - *E.g.*, remove an energy barrier separating $Y = 0$ and $Y = 1$ computational states, and call the merged state $Y = 0$.

And assume, in general, *non-computational information will fairly rapidly thermalize*. (If not, then why even consider it non-computational?)

- This thermalization process is when/where the absolute entropy increase happens in Landauer!
  - By assumption, environment evolution is not tracked, ergo $\mathfrak{C}$-$\mathfrak{E}$ correlation is lost.



Note that we could try to "reverse" the whole erasure process to restore the original reduced entropy $H(Y)$ of the $\mathfrak{Y}$ subsystem…

But now, $I(X;Y)_{\text{new}} = 0$ (any correlations have become lost!)

- $\therefore S_{\text{ind}}(Y) = H(Y)$, $\therefore \Delta S_{\text{ind}}(Y) = I(X;Y)_{\text{orig}} = \Delta S_{\text{tot}}$.

If, originally, Y was (*deterministically*) computed from X, then:

- $H(Y|X)_{\text{orig}} = 0$, *i.e.*, $S_{\text{ind}}(Y) = 0$, so $H(Y) = I(X;Y)_{\text{orig}}$.
  - *Apparent* entropy of *all* computed bits is *actually* **entirely** mutual information!
    - a.k.a. "information-bearing entropy" in Anderson's terminology

Independent entropy (and total universe entropy!) has increased by

$$\Delta S_{\text{tot}} = \Delta S_{\text{ind}}(Y) = I(X;Y)_{\text{orig}} = H(Y).$$

∴ Erasing *computed* (as opposed to *random!*) bits turns their *digital* information into new *physical* entropy.

Q.E.D.! ■

Basic Reversible Computing Theory

(For full proofs, see arxiv.org:1806.10183)

Fundamental theorem of traditional reversible computing:

- A deterministic computational operation is (unconditionally) non-entropy-ejecting if and only if it is *unconditionally* logically reversible (injective over its entire domain).

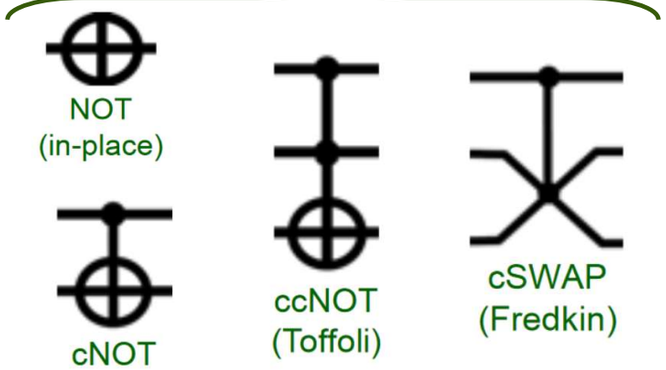
Fundamental theorem of generalized reversible computing:

- A *specific* (contextualized) deterministic computation is (specifically) non-entropy-ejecting if and only if it is *specifically* logically reversible (injective over the set of *nonzero-probability* initial states).
  - Also, for any deterministic computational operation, which is conditionally reversible under some assumed precondition, then the entropy required to be ejected by that operation approaches 0 as the probability that the precondition is satisfied approaches 1.

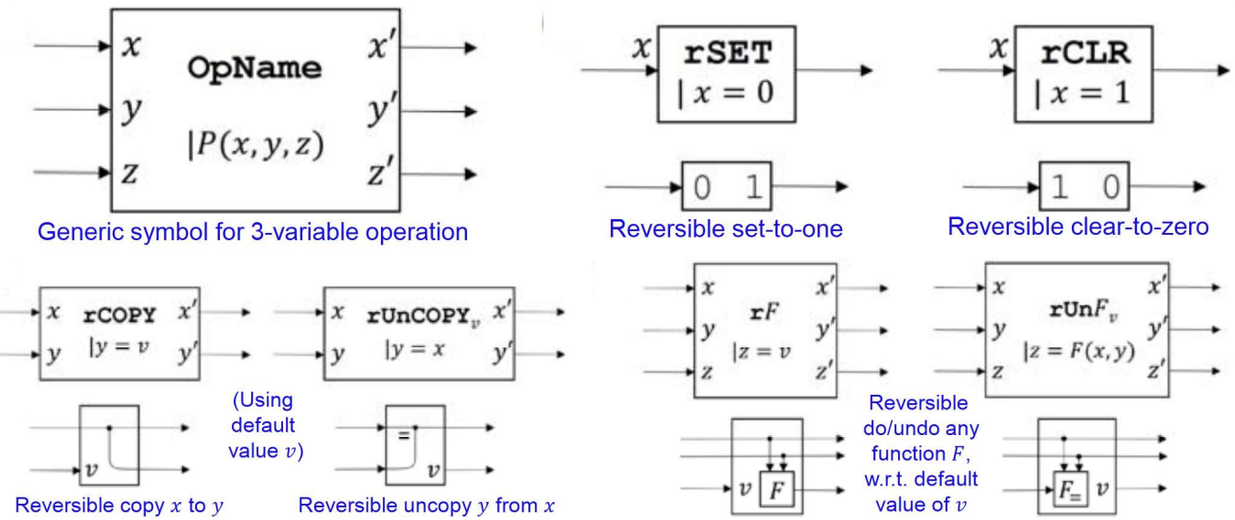
Bottom line: To avoid requiring Landauer costs, it is *sufficient just to have reversibility when some specified preconditions are satisfied.*

- Basis for practical engineering implementations.
  - We'll see some examples in tomorrow's talk.

Traditional *Unconditionally* Reversible "Gates" (Operations)



Generalized *Conditionally* Reversible Operations



Physical Implementation of Computational Operations

Consider the universe $\mathfrak{U}$.

- The computer system $\mathfrak{S}$ together with its surrounding environment $\mathfrak{E}$.
- Let the joint Hilbert space $\mathcal{H}_{\mathfrak{U}} = \mathcal{H}_{\mathfrak{E}} \otimes \mathcal{H}_{\mathfrak{S}}$.

Consider a computational operation O_s^t taking place within $\mathfrak{S}$.

- Between starting time $s \in \mathbb{R}$ and terminating time $s \in \mathbb{R}$, with $s < t$.

Assuming perfect knowledge of physics, the transformation of $\mathcal{H}_{\mathfrak{U}}$ from time s to t is described by some time evolution operator $U_s^t = U_s^t(\mathfrak{U})$ that applies for $\mathfrak{U}$ between those times.

- In general, the final density matrix $\rho_t = U_s^t \rho_s (U_s^t)^\dagger$.

Note that U_s^t describes the effect of *all* physical processes taking place within $\mathfrak{U}$, including:

- Dynamical evolution of the physical computational mechanisms in $\mathfrak{S}$.
- Delivery of needed free energy to the active computing elements in $\mathfrak{S}$.
- Thermal flows of dissipated energy out into the environment $\mathfrak{E}$.

We can call this the *open system case*.

Closed-System Variant

Simplified *vs.* open system model, but still physically realistic.

- A real computer *could* actually be operated as an *approximately* closed system for some limited period of time.
  - Until internal energy stores run out, and/or enclosure overheats.

So now, restrict our attention to the subspace of $\mathcal{H}_{\mathfrak{U}}$ that is the Hilbert space $\mathcal{H}_{\mathfrak{S}}$ of the computer sytem itself.

- Ignore, temporarily, any thermal flows across the $\mathfrak{S}$-$\mathfrak{E}$ boundary.
  - Imagine that $\mathfrak{S}$ is wrapped in a perfect thermal insulating barrier.
- Now model the effect of the dynamics within $\mathfrak{S}$ as being described by a *local* unitary time-evolution operator $U_s^t(\mathfrak{S})$ operating on $\mathcal{H}_{\mathfrak{S}}$.

Note, the change in the protocomputational basis $\boldsymbol{\mathcal{B}}$ between times s and t can also be modeled by a unitary matrix, ${}^{\boldsymbol{\mathcal{B}}(t)}_{\boldsymbol{\mathcal{B}}(s)}U$.

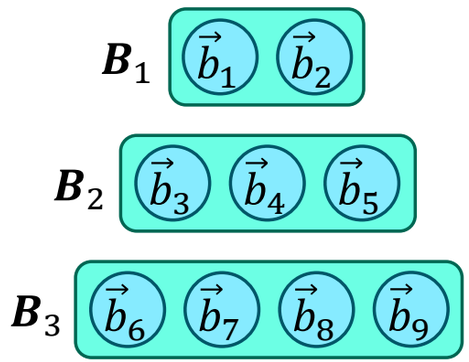
- Then denote a "basis-corrected" version of $U_s^t(\mathfrak{S})$ as:

$$U_s^t(\mathfrak{S}, \boldsymbol{\mathcal{B}}) = {}^{\boldsymbol{\mathcal{B}}(t)}_{\boldsymbol{\mathcal{B}}(s)}U \cdot U_s^t(\mathfrak{S}).$$

Quantum Statistical Operating Contexts

This generalizes the concept of a *statistical operating context* or initial probability distribution P that is needed to define a *statistically-contextualized* computational process.

Define as a mixed state ρ_s encompassing all of our uncertainty, as modelers, regarding the initial quantum state of the system at time s, prior to performing the computational operation O_s^t.



Also require that ρ_s is *block-diagonal* in the initial basis $\boldsymbol{\mathcal{B}}(s)$.

- And, the blocks need to correspond to the initial partition $\boldsymbol{C}(s)$.
  - I.e., no quantum coherences should exist between the different computational states.
    - Formally: ρ_s has no off-diagonal terms between basis states $\vec{b}_1, \vec{b}_2 \in \boldsymbol{\mathcal{B}}(s)$ where $\vec{b}_1 \in \boldsymbol{B}_i$ and $\vec{b}_2 \in \boldsymbol{B}_j$ for $c_i, c_j \in \boldsymbol{C}(s)$ where $i \neq j$.
  - This constraint is needed for modeling classical computation.
    - Can weaken when extending this framework to the quantum case.
  - There *can* be coherences *within* a computational state, though…
    - This could correspond, *e.g.*, to physical qubits that may exist within the machine (*e.g.*, long-lived nuclear spins in supporting materials) that are unrelated to the classical digital data being represented, or arbitrary changes of basis.

$$\rho_s = \begin{array}{c|ccccccccc} & |b_1\rangle & |b_2\rangle & |b_3\rangle & |b_4\rangle & |b_5\rangle & |b_6\rangle & |b_7\rangle & |b_8\rangle & |b_9\rangle \\ \hline \langle b_1| & r_{11} & r_{12} & & & & & & & \\ \langle b_2| & r_{21} & r_{22} & & & & & & & \\ \langle b_3| & & & r_{33} & r_{34} & r_{35} & & & & \\ \langle b_4| & & & r_{43} & r_{44} & r_{45} & & & & \\ \langle b_5| & & & r_{53} & r_{54} & r_{55} & & & & \\ \langle b_6| & & & & & & r_{66} & r_{67} & r_{68} & r_{69} \\ \langle b_7| & & & & & & r_{76} & r_{77} & r_{78} & r_{79} \\ \langle b_8| & & & & & & r_{86} & r_{87} & r_{88} & r_{89} \\ \langle b_9| & & & & & & r_{96} & r_{97} & r_{98} & r_{99} \end{array}$$

Quantum Contextualized Computations

This generalizes the concept of a *statistically* contextualized computation $\mathcal{C}(O,P)$ from the Generalized Reversible Computing paper (arxiv.org:1806.10183).

A *(quantum contextualized) computation* $\mathcal{C}_s^t(O_s^t,\rho_s)$ refers to the act of performing the computational operation O_s^t within the computer system $\mathfrak{S}$ when the initial mixed state of $\mathfrak{S}$ at time s is given by a quantum statistical operating context ρ_s.

- Must meet the conditions from the previous slide for $\boldsymbol{\mathcal{B}}(s)$ and $\boldsymbol{\mathcal{C}}(s)$.

What it means to physically implement a given (classical) computation

The basis-adjusted time-evolution operator $U_S^t(\mathfrak{S}, \boldsymbol{\mathcal{B}})$ *implements* the quantum contextualized computation $\mathcal{C}_S^t(O_S^t, \rho_S)$, written:

$$U_S^t(\mathfrak{S}, \boldsymbol{\mathcal{B}}) \Vdash \mathcal{C}_S^t(O_S^t, \rho_S),$$

- if and only if the density matrix $\rho_t = U_S^t(\mathfrak{S}, \boldsymbol{\mathcal{B}})\rho_S U_S^t(\mathfrak{S}, \boldsymbol{\mathcal{B}})^\dagger$ that results from applying the unitary $U_S^t(\mathfrak{S}, \boldsymbol{\mathcal{B}})$ to the initial mixed state ρ_S has the following property:
  - For any initial computational state $c_i(s) \in \boldsymbol{\mathcal{C}}(s)$ that has nonzero probability under ρ_S, if we zero out all elements of ρ_S outside the set of rows/columns corresponding to $c_i(s)$ and renormalize, and then apply $U_S^t(\mathfrak{C}, \boldsymbol{\mathcal{B}})$ to this restricted ρ_S', the resulting final mixed state ρ_t' implies the same probability distribution $P_i(t)$ over final computational states in $\boldsymbol{\mathcal{C}}(t)$ as is specified by applying the stochastic map O_S^t to the initial state, $O_S^t(c_i(s))$.

Note: It can OK, under this definition, if small coherences *temporarily* arise between different final computational states in $\boldsymbol{\mathcal{C}}(t)$,

- as long as the subsequent evolution causes them to decay very quickly.
  - That is, we don't want these "parasitic" coherences to impact the dynamics of subsequent operations.

Likharev's dissipation limits

International Journal of Theoretical Physics, Vol. 21, Nos. 3/4, 1982

Classical and Quantum Limitations on Energy Consumption in Computation

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Department of Physics, Moscow State University, Moscow 117234, U.S.S.R.

Received May 6, 1981

Likharev '81 analyzed limits of dissipation for his reversible JJ-based Parametric Quantron (PQ) technology concept.

- Based on analyzing rates of crossing a potential energy barrier through thermal excitation and quantum tunneling.

Main results:

- Limit due to classical thermal excitation over barrier (assuming underdamped junction):

$$W_C \approx \frac{k_B T}{\omega_c \tau} \ln \frac{1}{\omega_A \tau p}.$$

  - $\omega_c = \frac{k}{\eta} \approx \frac{2\Delta}{\hbar}$ with elasticity modulus $k = \frac{d^2 U}{dx^2}$ and effective viscosity η; and 2Δ is the superconducting gap energy;
  - ω_A approximates to the JJ plasma frequency $\omega = \sqrt{k/\eta} = \sqrt{2q_e I_c/\hbar C}$, and τ is the cycle period;
  - p is the tolerable error probability per operation.

Limit due to quantum-mechanical tunneling through the barrier:

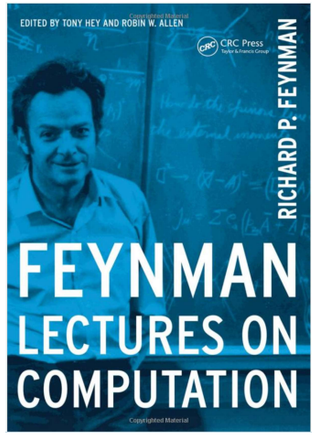
$$W_C \approx \frac{\hbar}{\tau} \ln \frac{1}{\omega_c \tau p}.$$

However! Likharev himself admits the limitations of this analysis:

- It is not a *fundamental*, technology-independent analysis.
- Alternative device concepts might do better!

> Our approach to the problem, of course, leaves open whether it is possible to invent some novel device providing lower power consumption. If we limit ourselves to the quasistatic devices, where the computation can be stopped at any moment, without inducing an error, one can hardly get away from the above estimates. In fact, the only role of the parametric quantron in our discussion has been to demonstrate how a flexible bistable potential well could be physically realized. (Of course, some numerical factors can appear in the estimates if peculiar well shapes are taken into account.)
>
> One can, however, argue that the above-mentioned condition of quasi-statics is by no means compulsory, and that the information can be processed by some "dynamical" devices, where the cycle period can be shorter than the relaxation time. This problem is left for further analysis.

Feynman's dissipation limits



In lectures for his 1983-1986 CalTech course, "Potentialities and Limitations of Computing Machines," Feynman derived a limit on energy dissipation per step for *Brownian machines* (*e.g.*, DNA copying) driven by chemical potentials.

- He concludes that an approximate formula for this is:

$$energy\ loss/step = kT\,\frac{minimum\ time\ taken/step}{time/step\ actually\ taken}$$

An example we gave of reversible computing was that of the chemical process of copying DNA. This involved a machine (if you like) that progressed in fits and starts, going forward a bit, then backwards, but more one than the other because of some driving force, and so ended up doing some computation (in this case, copying). We can take this as a model for more general considerations and will use this "Brownian" concept to derive a formula for the energy dissipation in such processes. This will not be a general formula for energy dissipation during computation but it should show you how we go about calculating these things. However, we will precede this discussion by first giving the general formula[7], and then what follows can be viewed as illustration.

[7]This rule is pretty general, but there will be exceptions, requiring slight corrections. We will discuss one such, a "ballistic" computer, in §5.5. [RPF]

However, he mentions in a footnote that a "slight correction" to this expression would be needed for *ballistic* machines, and later argues, quite informally, that in that case, the expression should be:

$$kT\,\frac{time\ to\ make\ collision}{speed\ [sic]\ at\ which\ it\ happens}$$

$$kT\,\frac{time\ to\ make\ collision}{speed\ at\ which\ it\ happens}. \qquad (5.37)$$

This expression has not been analyzed in any great detail for the billiard ball machine.

- An arguably very similar expression, *but*:
  - The whole argument in this part of the notes is *extremely* brief and informal ("hand-wavy")
  - The possible application of *e.g.* the Landauer-Zener formula for quantum-mechanical scattering processes is not considered at all
  - Modern STA (Shortcuts to Adiabaticity) techniques had not even been developed yet, and so of course are also not considered
  - *Asynchronous* ballistic models (e.g. ABRC) which avoid chaotic instabilities had also not been invented yet

Thus, we must conclude that Feynman's analysis of this problem is *not definitive*, nor the final word.

Section III: Looking Ahead

Fundamental Physics of Reversible Computing—An Introduction

Key Questions for the Physics of Reversible Computing

Are there fundamental (i.e., technology-independent) lower bounds (greater than zero) that follow from general non-equilibrium quantum thermodynamics on energy dissipation per reversible computational operation as a function of, say, the speed of the operation (and/or other fundamental physical parameters such as size, temperature, *etc.*)?

- And, if so, can such bounds be expressed via simple analytic scaling relations?

Can we deduce anything regarding *e.g.* exotic quantum phenomena, materials properties, *etc.*, that would need to be leveraged in order for a technology to saturate the bounds?

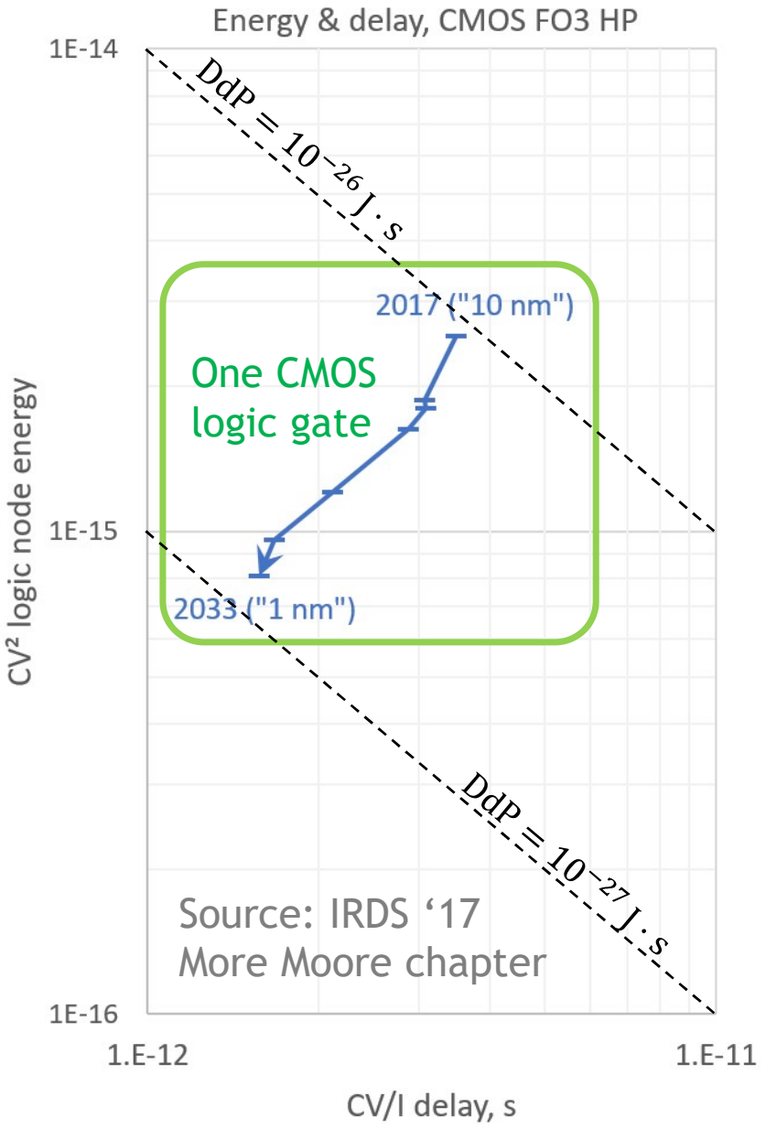
- Examples of quantum phenomena that are (or might be found to be) useful for this:
  - Decoherence-free subspaces (DFSs), Zurek pointer states
  - Topological invariants?
    - *e.g.*, signed flux charge threading a bounded planar superconducting circuit.
  - Dynamical versions of the *quantum Zeno effect* (QZE)?
  - …*others???*

Answering the above questions can then become a starting point for innovation of breakthrough technologies for reversible computing that exhibit vastly improved engineering characteristics….

Existing Dissipation-Delay Products (DdP) —Non-reversible Semiconductor Circuits

Conventional (non-reversible) CMOS Technology:

- Recent roadmaps (*e.g.*, IRDS '17) show Dissipation-delay Product (DdP) decreasing by only <~10× from now to the end of the roadmap (~2033).
  - Note the typical dissipation (per logic bit) at end-of-roadmap is projected to be ~0.8 fJ = 800 aJ = ~5,000 eV.
- Optimistically, let's suppose that ways might be found to lower dissipation by an additional 10× beyond even that point.
  - That still puts us at 80 aJ = ~500 eV per bit.
- We need at least ~1 eV ≈ 40 kT electrostatic energy at a minimum-sized transistor gate to maintain reasonably low leakage despite thermal noise,
  - And, typical *structural* overhead factors *compounding* this within fast random logic circuits are roughly 500×,
  - so, ~500 eV is *indeed* probably about the practical limit.
    - At least, this is a reasonable order-of-magnitude estimate.



Existing Dissipation-Delay Products (DdP)—Adiabatic Reversible Superconducting Circuits

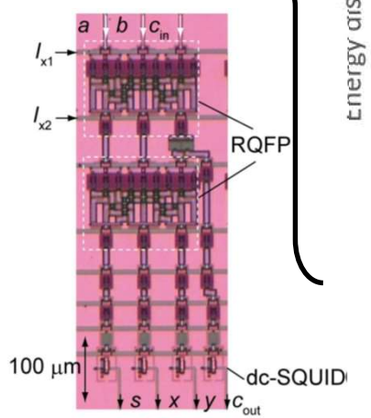
Reversible adiabatic superconductor logic:

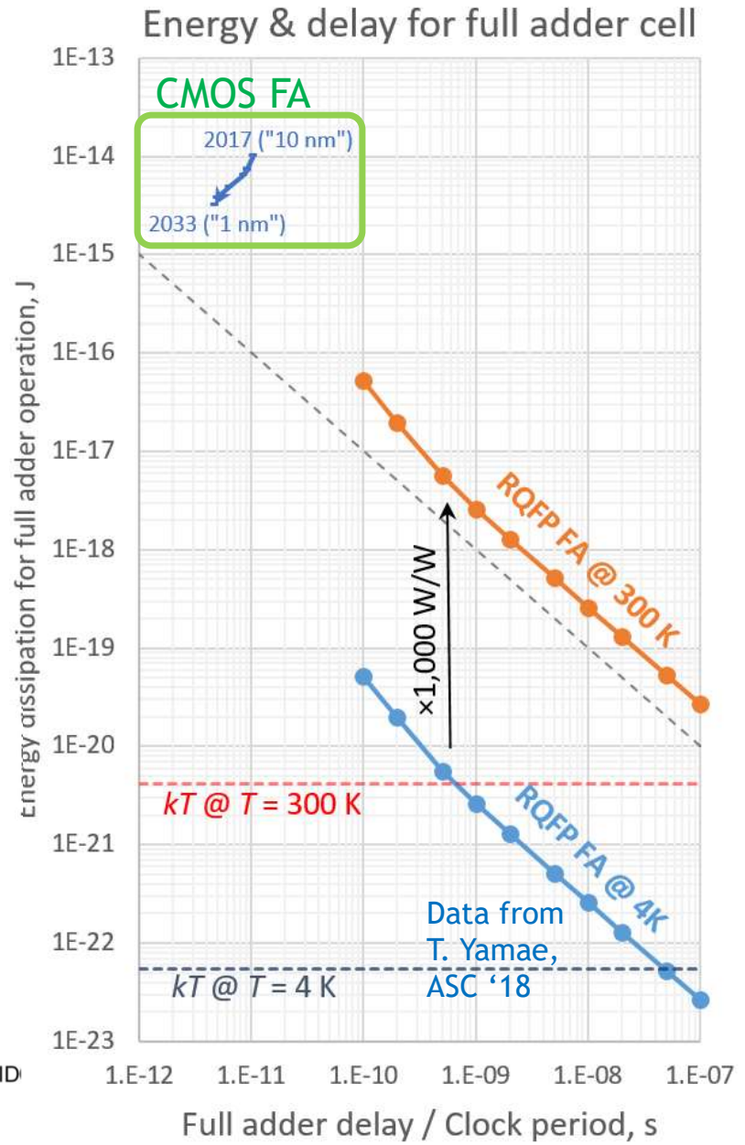
- State-of-the-art is the **RQFP** (Reversible Quantum Flux Parametron) technology from Yokohama National University in Japan.
  - Chips were fabricated, function validated.
- Circuit simulations predict DdP is >1,000× *lower* than even *end-of-roadmap* CMOS.
  - Dissipation extends *far below* the 300K Landauer limit (and even below the Landauer limit at 4K).
  - DdP is *still* better even after adjusting by a conservative factor for large-scale cooling overhead (1,000×).

Question: Could some *other* reversible technology do *even better* than this?

- We have a project at Sandia exploring one possible superductor-based avenue for this…
  - But, what are the *fundamental* (technology-independent) limits, if any?

RQFP = Reversible Quantum Flux Parametron (Yokohama U.)





Can dissipation scale better than linearly with speed?

Some observations from Pidaparthi & Lent (2018) suggest Yes!

- Landau-Zener (1932) formula for quantum transitions in e.g. scattering processes with a missed level crossing…
  - Probability of exciting the high-energy state (which then decays dissipatively) scales down *exponentially* as a function of speed…

$$P_{\mathrm{D}} = \mathrm{e}^{-2\pi\Gamma}$$

    - This scaling is commonly seen in many quantum systems!
- Thus, dissipation-delay *product* may have *no lower bound* for quantum adiabatic transitions—***if*** this kind of scaling can actually be realized in practice.
  - *I.e.*, in the context of a complete engineered system.
- **Question:** Will unmodeled details (*e.g.*, in the driving system) fundamentally prevent this, or not?

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Open Access Article

Exponentially Adiabatic Switching in Quantum-Dot Cellular Automata

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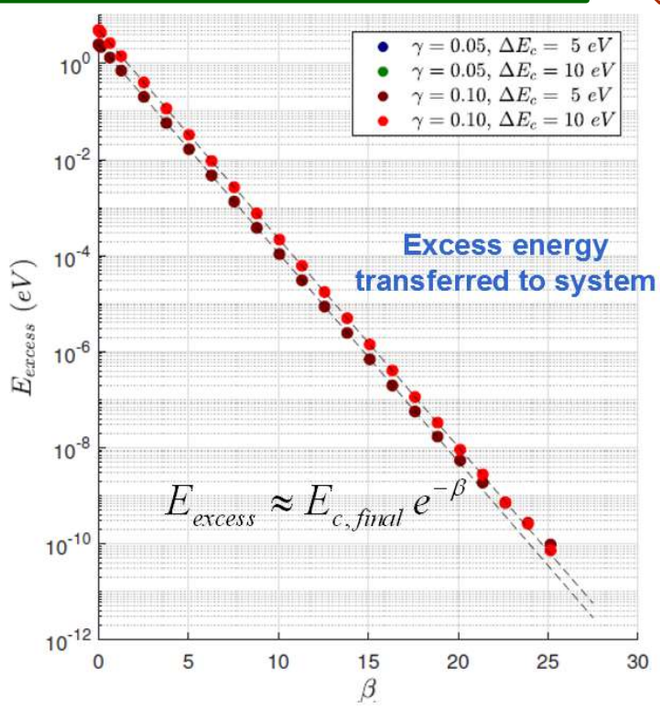

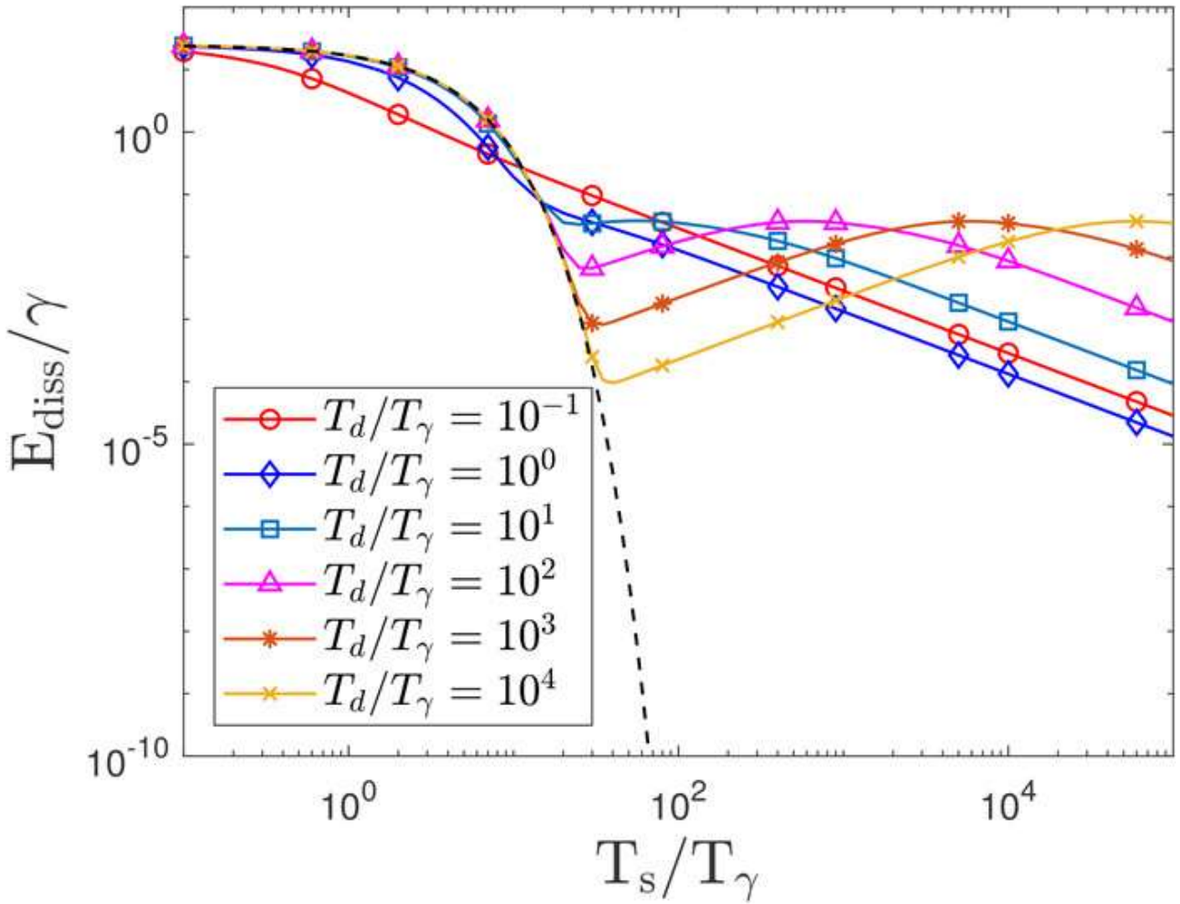

FIG. 10. Dissipated energy of an open system as a function of switching speed for different dissipation time constants. The dashed line is the excess energy of an isolated system. Here, the environmental temperature $k_BT / \gamma = 0.5$.

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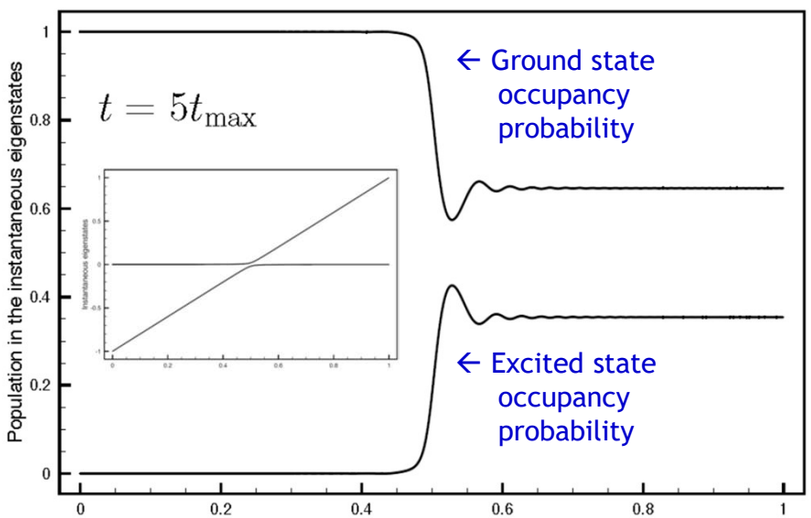
DOI: 10.1063/5.0033633

Shortcuts to Adiabaticity (STA)

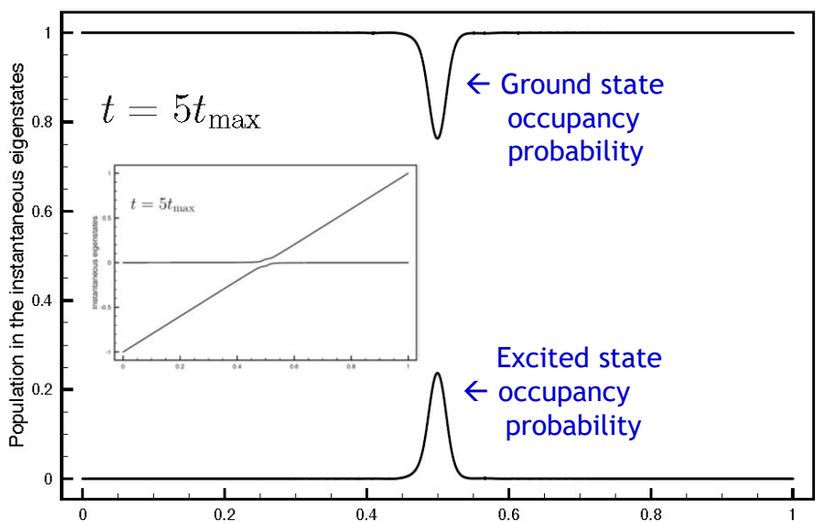
A line of theoretical physics research showing that, *in principle*, quantum state transformations can always be carried out with exactly *zero* dissipation, even at any given *finite* delay!

- Requires the introduction of a finely-tuned "counterdiabatic" perturbation to the system's time-dependent Hamiltonian.
- **Again, we ask:** Is this idealized prediction *actually achievable,* if fundamental thermodynamic limits that apply to the complete system are accounted for?



Normal quantum adiabatic process:
Substantial excitation/dissipation

Figure credit:
Collaborator
David Guéry-Odelin
(Université de Toulouse)

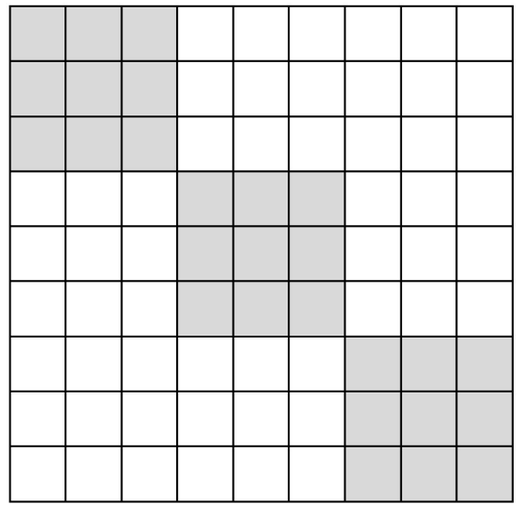


Using counterdiabatic protocol:
Zero net excitation/dissipation

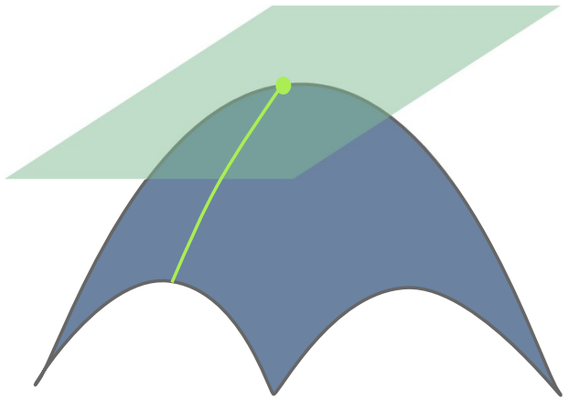
Limits to Reversible Computing?

—An approach from the theory of Open Quantum Systems

(Work with Karpur Shukla, Brown University, and Victor V. Albert, CalTech)



- Computational states modelled as *decoherence-free subspace blocks* (DFSB) of overall Hilbert space.
- Quantum Markov equation with multiple asymptotic states: admits subspace dynamics (including DFSB structures) for open systems under Markov evolution.
  - Induces geometric tensor for *manifold of asymptotic states*.
    - Similar to quantum geometric tensor / Berry curvature for closed systems.
- Current work: use multiple asymptotic state framework to derive thermodynamic quantities…
  - Uncertainty relations, dissipation and dissipation-delay product.



Conclusion

Some form of reversible computing is *absolutely required* in order for the energy efficiency (and thus, cost efficiency) of general digital computing to avoid asymptoting against *firm* thermal barriers in the foreseeable future.

- This follows directly from the proper *understanding* of Landauer's Principle (slide 21) that is substantiated by the (rigorous) arguments summarized in slides 22-23.
- Various researchers who have misapprehended Landauer are simply *missing the whole point.*
  - Various critics of Landauer & Bennett have simply failed to appreciate the essential, *unavoidable* role that information-theoretic *correlation* plays in computing, which is the ultimate origin of the *absolute entropy increase* that is rigorously caused by Landauer erasure…
    - …when the true *meaning* of Landauer's Principle is understood properly!
- All *conventional* (*i.e.*, non-reversible) digital circuit architectures rely *fundamentally* on frequent *oblivious erasure of correlated bits*, ergo, they can never surpass the Landauer limit (by the elementary proof on slide 22).
  - In contrast, properly-designed *reversible* architectures are designed to *avoid* such erasure, ergo are *not* subject to the Landauer limit.

The fundamental limits of *reversible* computing are still very far from being fully understood…

- There is a significant opportunity for physicists to develop fundamental new results in this area.

Leveraging of exotic quantum phenomena may be required to saturate the fundamental limits.

It seems likely that *breakthrough technologies for reversible computing remain to be discovered.*

- And this, in turn, would lead to incalculable increases in the value of computing, and civilization!