DiVincenzo-like criteria for autonomous quantum machines

José Antonio Marín Guzmán,[1] Paul Erker,[2,3] Simone Gasparinetti,[4] Marcus Huber,[2,5] and Nicole Yunger Halpern[1,6,*]

[1]*Joint Center for Quantum Information and Computer Science, NIST and University of Maryland, College Park, MD 20742, USA*
[2]*Atominstitut, Technische Universität Wien, 1020 Vienna, Austria*
[3]*Institute for Quantum Optics and Quantum Information (IQOQI), Austrian Academy of Sciences, Boltzmanngasse 3, 1090 Vienna, Austria*
[4]*Department of Microtechnology and Nanoscience, Chalmers University of Technology, 412 96 Gothenburg, Sweden*
[5]*Institute for Quantum Optics and Quantum Information (IQOQI) Vienna, Austrian Academy of Sciences, Boltzmanngasse 3, 1090 Vienna, Austria*
[6]*Institute for Physical Science and Technology, University of Maryland, College Park, MD 20742, USA*

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Controlled quantum machines have matured significantly. A natural next step is to grant them autonomy, freeing them from timed external control. For example, autonomy could unfetter quantum computers from classical control wires that heat and decohere them; and an autonomous quantum refrigerator recently reset superconducting qubits to near their ground states, as is necessary before a computation. What conditions are necessary for realizing useful autonomous quantum machines? Inspired by recent quantum thermodynamics and chemistry, we posit conditions analogous to DiVincenzo's criteria for quantum computing. Our criteria are intended to foment and guide the development of useful autonomous quantum machines.

Automata are machines that operate independently of external control. In an early example, the ancient Greek mathematician Archytas of Tarentum supposedly built a wooden pigeon that spun around in a circle [1]. For centuries, automata served as curiosities for entertainment and for impressing visitors. Not until the 18th-century Industrial Revolution did engineers harness automata for practical purposes on large scales. (We use an expansive definition of *automaton*, not restricting the term to machines that resemble humans or animals.) Today, automata speed up manufacturing, deliver packages, drive car passengers, and even clean kitchen floors.

Autonomous quantum machines have embarked upon a trajectory that we hope will unfold analogously. Quantum thermodynamicists have designed autonomous engines [2–19], refrigerators [20**?** –47], clocks [48–54], and more [55–60] without external drives [61, 62]. Some of these machines do not even require thermodynamic-work inputs. Instead, the refrigerators and clocks siphon off heat flowing between different-temperature baths nearby. Nature, too, has designed autonomous quantum switches [63–66], energy transducers [67], and catalysts [68].

Experimentalists have just begun building autonomous quantum machines. For example, autonomous quantum refrigerators have been realized with trapped ions and superconducting qubits [37, 69]. Such experiments have initiated the bridge from theory to reality. Yet they largely resemble Archytas's pigeon: They are impressive curiosities, not practical tools. For example, a single-atom engine should extract only ≈ 1 eV of work per cycle. Cooling and trapping an atom costs far more work, so the engine cannot earn its keep. One exception was initiated recently: the autonomous quantum refrigerator formed from superconducting qubits [69]. The quantum refrigerator cooled a target qubit to below the temperatures realizable via passive thermalization with the dilution-refrigerator environment. This target qubit, reset to near its ground state, could serve in a later quantum computation. In such an application, the quantum refrigerator could draw energy from the temperature gradient between the dilution refrigerator's inner and outer plates. Cooling the autonomous refrigerator to the quantum regime would cost no extra work, the dilution refrigerator already being cold to support the upcoming computation.

One can envision other useful autonomous quantum machines.[1] First, an autonomous quantum computer would apply its own gates. Autonomy could pare down the control wires in superconducting-qubit architectures. Control wires limit the number of superconducting qubits that fit on a chip [75, App. C.4.I]. Also, being classical, control wires heat qubits up [76, Sec. 2.1]. Eliminating control wires could therefore benefit quantum computers' scalability and coherence times.[2]

To apply gates at the proper times, autonomous quantum computers would need autonomous quantum ma-

* nicoleyh@umd.edu

[1] Practicality has motivated the design of nonautonomous quantum thermal machines [70–74], too.

[2] One might object that qubits cannot rotate without external control—without experiencing classical fields. However, autonomous quantum computers could implement Brownian circuits [77]. Brownian circuits consist of gates effected only with qubit–qubit interactions.

chines of a second type: clocks. Theorists have designed autonomous quantum clocks that tick by emitting photons [48]. Such clocks differ from the quantum clocks used today, formed from ultracold atoms interacting with lasers [78]: Today's quantum clocks receive external feedback when the atoms are measured, the lasers are tuned, etc.

Third, autonomous quantum machines can detect, transduce, and transmit energy. *Photoisomers* are molecules operative across nature and technologies [63–66]. Examples include retinal, found in the protein rhodopsin in our eyes [79]. A photoisomer has one shape in thermal equilibrium at biological temperatures. Absorbing a photon—say, from the sun—enables the molecule to switch configurations. The switch can galvanize chemical reactions leading to the experience of sight. Photoisomers exhibit quantum phenomena including coherence relative to the energy eigenbasis, as well as nonadiabatic evolution. Beyond photoisomers, chemistry features other autonomous quantum machines: Photosynthetic complexes transform light into chemical energy [67], enzymes interconvert molecules with help from tunneling [68], etc.

Third, autonomy could benefit quantum sensors [80]. Quantum sensors detect small magnetic fields and temperature gradients. External control includes microwave pulses and placement near the to-be-detected source. For instance, experimentalists have injected nanodiamond sensors into embryo tissues whose temperatures need measuring [81, 82]. One can envision quantum sensors that reach and report about sources autonomously.

More fancifully, one can imagine autonomous quantum machines assembling bespoke molecules, servicing quantum computers, delivering atoms as drones, or building other quantum devices. Such machines may seem like castles in the air. But so did controlled quantum computers, decades ago; and quantum computers have been built and are being scaled up. DiVincenzo's criteria have guided quantum computers from castle-in-the-air status to reality [83]. He posited five criteria necessary for building a quantum computer, plus two optional criteria necessary for information transmission. Analogously, we posit eight criteria necessary for building a useful autonomous quantum machine. Two optional criteria concern transportation and information transmission. We hope that these criteria, analogously to DiVincenzo's, guide experimentalists in realizing useful autonomous machines.

First, we stipulate what we mean by *machine*, *autonomous*, and *quantum*. Alternative definitions may exist, as the terms are broad. Still, we believe our definitions to be reasonable. Specifying them will clarify our criteria:

(a) ***Machine:*** *A physical device, potentially formed from components working together, that harnesses energy to accomplish a task.*

(b) ***Autonomous:*** *A machine is autonomous if its microscopic Hamiltonian remains constant in time.* Microscopic Hamiltonians contrast with effective Hamiltonians. An effective Hamiltonian can result from shifting a microscopic Hamiltonian into a rotating reference frame, then dropping small terms. A microscopic Hamiltonian remains constant in the absence of time-dependent external drives.

(c) ***Quantum:*** *A system is quantum if the axioms of quantum theory describe the system usefully.* Quantum systems can, but need not, exhibit quantum phenomena such as entanglement, coherence relative to relevant bases, discretized spectra, measurement disturbance, contextuality [84–86], and the quantum-computational resource called magic [87]. Classical systems can approximate discretized spectra, and classical waves exhibit coherence. Quantum theory's axioms describe classical systems, but not usefully; classical theories offer greater calculational efficiency and physical insight. We do not mean *nonclassical* by *quantum*. We call a phenomenon *nonclassical* if no classical theory (technically, no noncontextual ontological model [84–86]) reproduces the phenomenon.

I. CRITERIA

This section contains our DiVincenzo-like criteria for realizing useful autonomous quantum machines. Table I summarizes the criteria. We denote by σ_a the Pauli-a operator, for $a = x, y, z$; by $|1\rangle$, the eigenvalue-1 eigenstate of σ_z; and by $|0\rangle$, the eigenvalue-(-1) eigenstate.

A. Access to useful energy

Useful energy enables one to perform thermodynamic work. Work empowers a machine to direct its motion—to overcome its momentum and random buffets from its environment. Free energy, or a nonequilibrium generalization thereof, offers the capacity to perform work. A machine can access this energy directly or indirectly, as we now discuss.

We label as a *battery* any system that reliably stores (the capacity to perform) work and from which work can reliably be retrieved. Small-scale batteries include adenosine triphosphate (ATP), a molecule that powers chemical reactions in cells. Autonomous classical nanowalkers leverage ATP, as discussed under criterion I. Quantum thermodynamics features multiple battery models (e.g., [88–94]), many idealized. Examples include a *work bit*, a two-level system governed by a Hamiltonian $\Delta\sigma_z$, for $\Delta > 0$ [88, 89]. A work bit charges during $|0\rangle \mapsto |1\rangle$ and provides work during $|1\rangle \mapsto |0\rangle$.

Other energy sources do not provide work directly; they are nonequilibrium systems from which the machine harvests free energy (or a generalization thereof). Often,

Subsection	Criterion
A	Access to useful energy
B	Processing unit or target
C	Interactions among the machine's components
D	Timekeeping mechanism
E	Structural integrity
F	Sufficient purity
G	Output worth the input
H	Ability to switch off after completing assignment
I	Mobility (optional)
J	Interoperability (optional)

TABLE I: Summary: DiVincenzo-like criteria for autonomous quantum machines.

such sources have gradients of temperature, chemical potential, or other thermodynamic forces. The commonest example consists of two heat baths. One, at a temperature $T_{\mathcal{C}}$, is out of equilibrium with a heat bath at a temperature $T_{\mathcal{H}} > T_{\mathcal{C}}$. Heat flows between the baths. A machine can siphon off part of the current via a three-body interaction (discussed under criterion C). Such machines are called *absorption machines* [62]. Despite providing energy, baths can threaten the purity of a machine's state. Yet as discussed under criterion F, non-Markovian baths, which retain memories, can revive lost purity.

B. Processing unit or target

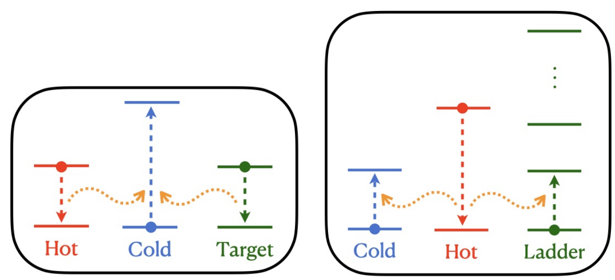
A processing unit receives and uses the energy accessed by the machine (criterion A). For example, a quantum computer's processing units are qubits that store quantum information that undergoes logic gates. In an autonomous quantum clock (described under criterion D), a processing unit ticks, emitting excitations.

A machine's purpose can be to operate on a target. For instance, a refrigerator's target is the system that undergoes cooling. An engine's target may be a battery that stores the energy extracted by the engine. A drone's target is the package to be delivered.

C. Interactions among the machine's components

The interacting components can include the energy source (criterion A), a processing unit (criterion B), a target (criterion B), and a timekeeping device (criterion D). We illustrate interactions with two examples: a quantum absorption refrigerator and a switch.

A simple quantum absorption refrigerator consists of three qubits: a hot, a cold, and a target qubit (Fig. 1a) [20, 62]. The hot qubit, $\mathcal{H}$, evolves under a Hamiltonian $H_{\mathcal{H}} = \Delta_{\mathcal{H}}\, \sigma_z$, wherein $\Delta_{\mathcal{H}} > 0$. This qubit exchanges heat with a thermal bath at a temperature $T_{\mathcal{H}} = 1/\beta_{\mathcal{H}}$. (We set Boltzmann's constant to $k_{\rm B} = 1$.) Hence $\mathcal{H}$ begins in the thermal state $e^{-\beta_{\mathcal{H}} H_{\mathcal{H}}}/Z_{\mathcal{H}}$. The partition function is $Z_{\mathcal{H}} := \text{Tr}(e^{-\beta_{\mathcal{H}} H_{\mathcal{H}}})$. The cold qubit, $\mathcal{C}$, evolves under a Hamiltonian $H_{\mathcal{C}} = \Delta_{\mathcal{C}}\, \sigma_z$ with a larger gap: $\Delta_{\mathcal{C}} > \Delta_{\mathcal{H}}$. $\mathcal{C}$ thermalizes with a bath at the lower temperature $T_{\mathcal{C}} < T_{\mathcal{H}}$, to the state $e^{-\beta_{\mathcal{C}} H_{\mathcal{C}}}/Z_{\mathcal{C}}$. The refrigerator cools the target qubit, $\mathcal{T}$, which evolves under the Hamiltonian $H_{\mathcal{T}} = \Delta_{\mathcal{T}}\, \sigma_z$, wherein $\Delta_{\mathcal{T}} > 0$.



(a) Quantum absorption refrigerator. **(b) Autonomous quantum clock.**

FIG. 1: Interactions amongst components: The quantum absorption refrigerator and clock evolve under similar Hamiltonians. However, the machines' qudits have different energy gaps: the refrigerator's $\Delta_{\mathcal{H}} < \Delta_{\mathcal{C}}$, whereas the clock's $\Delta_{\mathcal{H}} > \Delta_{\mathcal{C}}$. Also, the number of the target's energy gaps can differ between machines. The gaps, with the baths' temperatures ($T_{\mathcal{H}}$ and $T_{\mathcal{C}}$), determine the directions in which energy flows.

To analyze the absorption refrigerator, we invoke the density operator's statistical interpretation: We can imagine running the refrigerator many times. Each time, $\mathcal{H}$ begins in an energy eigenstate, $|1\rangle$ or $|0\rangle$, selected according to the Boltzmann distribution $\{e^{-\beta_{\mathcal{H}}\Delta_{\mathcal{H}}}/Z_{\mathcal{H}},\, e^{\beta_{\mathcal{H}}\Delta_{\mathcal{H}}}/Z_{\mathcal{H}}\}$. The cold qubit begins in an energy eigenstate selected analogously. In an illustrative "trial," $\mathcal{H}$ begins excited (in $|1\rangle$), while $\mathcal{C}$ and $\mathcal{T}$ begin de-excited (in $|0\rangle$). The hot and target qubits emit their excitations into $\mathcal{C}$, via the three-body interaction

$$|1\rangle_{\mathcal{H}}|0\rangle_{\mathcal{C}}|1\rangle_{\mathcal{H}} \leftrightarrow |0\rangle_{\mathcal{H}}|1\rangle_{\mathcal{C}}|0\rangle_{\mathcal{H}}. \tag{1}$$

Three-body interactions are necessary for autonomous cooling [20]. They can be effected perturbatively with simultaneous two-body interactions [27, 29, 69**?**]. The exchange (1) occurs only if $\Delta_{\mathcal{H}} + \Delta_{\mathcal{T}} = \Delta_{\mathcal{C}}$—only upon satisfying the first law of thermodynamics. The thermal qubits' gaps and temperatures bias the interaction (1) to the right. Ending in its ground state, $\mathcal{T}$ has undergone cooling by the refrigerator.

The second interaction example involves a *switch*, a component that keeps time and controls the rest of the machine. Denote by $\mathcal{S}$ a switch whose Hilbert space has an eigenbasis $\{|\varphi_j\rangle\}$ [95, Suppl. Note VIII]. If $\mathcal{S}$ is in state $|\varphi_j\rangle$, then a Hamiltonian H_j evolves the rest of the machine. Under different H_j's, the machine performs different tasks. For example, H_j can denote the j^{th} gate available to an autonomous quantum computer. A Hamiltonian $H_{\mathcal{S}}$ evolves the switch's state between $|j\rangle$'s. If the rest of the machine has a constant Hamiltonian $H_{\mathcal{R}}$, the total Hamiltonian is

$$H_{\text{tot}} = \sum_j \left(H_j \otimes |\varphi_j\rangle\!\langle\varphi_j|\right) + H_{\mathcal{S}} + H_{\mathcal{R}}. \tag{2}$$

Identity operators $\mathbb{1}$ are tensored on wherever necessary for each operator to act on the full Hilbert space.

Photoisomers were argued to contain switches [App. D][96].[3] A photoisomer has two degrees of freedom (DOFs), one nuclear and one electronic. The nuclear DOF, being heavy and slow, determines the electronic DOF's potential landscape. After photoexcitation, some nuclei rotate away from others under $H_{\mathcal{S}} = \ell_\varphi^2/(2I)$. ℓ_φ denotes the angular-momentum operator, and I denotes the moment of inertia. φ labels the nuclei's relative angular position (Fig. 2). The angles form a continuous set; so the sum in Eq. (2) becomes an integral, and H_j becomes $H(\varphi)$. $H_{\mathcal{S}}$ evolves the nuclear configuration from some initial angular position $|\varphi_0\rangle$ to other $|\varphi\rangle$'s. Rotating, the nuclear DOF changes the potential landscape and so the $H(\varphi)$ experienced by the electronic DOF, which forms the rest of the machine.

[3] Photoisomers are often called molecular switches. Molecular switches should not be confused with the switches described in the previous paragraph—timekeeping switches that control the rest of a machine. Molecular switches contain timekeeping switches, according to [96].

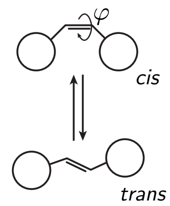


FIG. 2: Photoisomer: The molecule can switch between *cis* and *trans* configurations as some of its nuclei rotate. Reproduced from Fig. 1 of [96].

We have discussed switches under criterion C to elucidate their interactions with the rest of their machines. As timekeepers, though, switches belong also under the following criterion.

D. Timekeeping mechanism

Timekeeping devices include the switches introduced in the previous subsection; clocks, which tick regularly; and timers, which announce when programmable amounts of time have passed. Below, we review a simple autonomous quantum clock. Then, we discuss timekeeping mechanisms not formed from physical devices. Finally, we delineate three purposes of autonomous quantum machines' timekeeping mechanisms.

An autonomous quantum machine may carry an autonomous quantum clock to avoid decoherence by a classical clock. Reference [48] introduced a simple, idealized autonomous quantum clock (Fig. 1b). The clock contains a hot qubit $\mathcal{H}$ and a cold qubit $\mathcal{C}$, like the absorption refrigerator under criterion C. $\mathcal{H}$ has the larger gap here, however: $\Delta_{\mathcal{H}} > \Delta_{\mathcal{C}}$. The clock contains also a ladder $\mathcal{L}$ of d energy levels: $H_{\mathcal{L}} = \sum_{j=0}^{d-1} j\Delta\,|j\rangle\!\langle j|$. $\mathcal{L}$ begins in its ground state, $|0\rangle$. The qudits undergo a three-body interaction similar to the quantum absorption refrigerator's Eq. (1):

$$|1\rangle_{\mathcal{H}}|0\rangle_{\mathcal{C}}|0\rangle_{\mathcal{L}} \leftrightarrow |0\rangle_{\mathcal{H}}|1\rangle_{\mathcal{C}}|j\rangle_{\mathcal{L}}. \tag{3}$$

The ladder state $|j\rangle$ satisfies the first law through $\Delta_{\mathcal{H}} = \Delta_{\mathcal{C}} + j\Delta$. The condition $\Delta_{\mathcal{H}} > \Delta_{\mathcal{C}}$ biases the interaction (3) rightward. The hot qubit, de-exciting (undergoing $|1\rangle \mapsto |0\rangle$), drives the cold qubit upward in energy (through $|0\rangle \mapsto |1\rangle$) and drives the ladder system upward (through $|0\rangle \mapsto |j\rangle$). The baths reset $\mathcal{H}$ and $\mathcal{C}$, and the process repeats. Upon reaching its top rung, the ladder system ticks—emits an excitation—returning to $|0\rangle$.

Figures of this clock's merit include its *accuracy*, N [50]. Denote by $\bar{t}$ the average time interval between ticks; and by Δt, the standard deviation in that time interval. The accuracy is $N := (\bar{t}/\Delta t)^2$. To interpret it, we consider the limit as the number of ticks, assumed to be distributed independently and identically, approaches infinity. N equals the number of ticks that pass, on average, before the clock is off by one tick. One can improve N and other figures of merit by complicating the clockwork [50]. We discuss figures of merit further under criterion G.

Not all autonomous quantum machines need timekeeping devices as physical components. The finiteness of a machine's energy resources can induce a timer, as can the machine's coherence, we explain under criterion H. Furthermore, some autonomous quantum engines operate continuously: They undergo fixed dynamics, rather than cycles formed from discrete (timed) strokes [97].

An autonomous quantum machine's timekeeper fulfills three purposes. First, the timekeeper ensures that the machine initiates an action at the right time. For example, a quantum computer should begin each gate during the appropriate part of a computation. A Rydberg-atom computer [98] might autonomously perform a Rydberg-blockade entangling gate [99] as follows. Let the computer have an autonomous quantum clock that ticks by emitting an excitation. Two excitations can boost two atoms to their Rydberg (high-energy) states. The excited atoms will repel each other, entangling. Two more excitations may stimulate emissions from the atoms, which will return to their ground states.

Second, the timekeeper ensures that the machine performs an action for the desired amount of time. For example, a quantum computer implements a gate by effecting some Hamiltonian for the correct time interval. Xuereb *et al.* calculated the average fidelity $\bar{\mathcal{F}}$ of a CNOT gate U approximated with an autonomous quantum clock of accuracy N [100]. The evolution implemented is a channel $\mathcal{E}$. Denote by $d\psi$ the Haar measure (loosely speaking, the uniform measure) over the set of two-qubit pure states $|\psi\rangle$. The average fidelity is defined as $\bar{\mathcal{F}} := \int d\psi \langle\psi| U^\dagger \, \mathcal{E}(|\psi\rangle\langle\psi|) \, U |\psi\rangle$. According to [100], $\bar{\mathcal{F}} = (2 + e^{-\pi^2/(2N)})/3$. The clock accuracy N exponentially influences the correction to the constant $2/3$. Third, a timekeeper ensures that the machine turns off, satisfying criterion H, upon completing its task.

E. Structural integrity

Imagine placing three atoms beside each other, as with optical tweezers. If left unattended, the atoms will drift apart. A machine's components must not separate, lest they cease to satisfy the interaction criterion C. Denote by r the distance between two components. Any Coulombic interaction potential between them weakens as r^{-1}; and any Rydberg-blockade potential, as r^{-6} [98]. An autonomous quantum machine formed from multiple atoms, ions, etc. requires trapping, as by lasers. Laser light, forming a wave, provides a time-dependent external potential. Hence a laser-trapped machine can be autonomous only if the trapped spatial DOFs play no role in the machine's functioning. Those DOFs' Hamiltonian must commute with the microscopic Hamiltonian that governs the machine's operation.

Yet a machine need not consist of physically separated components. A photoisomer functions as an autonomous quantum energy transmitter, as explained in the introduction. The molecule contains an autonomous quantum clock, according to [96]. Similarly, photosynthetic complexes [67] and enzymes [68] are autonomous machines modeled usefully with quantum theory. A molecule can therefore form an autonomous quantum machine. So can an atom, arguably.[4] For example, three atomic energy levels can form an autonomous engine or refrigerator [2, 3, 20]. Not all self-contained autonomous quantum machines need be natural: Superconducting qubits cannot separate if printed on the same chip.

F. Sufficient purity

In this subsection, we define purity and compare it with coherence. Next, we explain the *sufficient* in the subsection's title. We then discuss the tradeoff between purity and accessible energy. Non-Markovianity may soften the tradeoff.

Purity is defined as follows. Denote by ρ an arbitrary quantum state (density operator) defined on a d-dimensional Hilbert space $\mathscr{H}$. ρ has an amount $\mathcal{P}(\rho) := \text{Tr}(\rho^2)$ of purity. If ρ is pure (if $\rho = |\psi\rangle\langle\psi|$ for some $|\psi\rangle \in \mathscr{H}$), then $\mathcal{P}(\rho) = 1$. If ρ is the maximally mixed state $\mathbb{1}/d$, then $\mathcal{P}(\rho) = 1/d$. A machine's processing unit, target, timekeeping device, and/or output might require purity at various times.

One might expect our criteria to include coherence, rather than purity. In quantum thermodynamics, coherence relative to the energy eigenbasis often serves as a resource (e.g., [49, 96, 102–110]). To quantify this coherence, we suppose that ρ evolves under a Hamiltonian $H = \sum_j E_j |j\rangle\langle j|$. For $j \neq k$, the off-diagonal element $\rho_{jk} := \langle j|\rho|k\rangle$ is a coherence. Denote the one-norm of an operator $\mathcal{O}$ by $||\mathcal{O}||_1 := \text{Tr}\big(\sqrt{\mathcal{O}\mathcal{O}^\dagger}\big)$. The mode-$\omega$ coherence can be quantified with $\sum_{j,k: E_j - E_k = \omega} ||\rho_{jk}||_1$ [104] (other measures exist). Despite its applications in timekeeping and work extraction, such coherence can be undesirable. For instance, qubits are often initialized to near their ground states, $|0\rangle$, before a quantum computation. Resetting computational qubits, an autonomous quantum refrigerator destroys coherences relative to the energy eigenbasis. Still, the refrigerator enhances the qubits' purities. Hence our criteria's including purity, rather than coherence.

Our criteria include *sufficient* purity for two reasons: (i) Different machine components may require different amounts of purity. (ii) One component may require different amounts of purity at different times. We illustrate with the quantum absorption refrigerator described under criterion C. The hot and cold qubits, interacting with finite-temperature baths, are always mixed. The target

[4] The atom interacts with heat baths whose frequencies are filtered. One might count the filters as parts of the machine.

requires purity—closeness to $|0\rangle$—but only when the protocol ends. In contrast, suppose that an autonomous quantum clock's ladder (Fig. 1b) is mixed at any time. The clock's accuracy seems likely to suffer [48]. Similarly, a quantum computer must retain enough purity to meet the threshold for fault-tolerant quantum error correction throughout its computation [111–113]. The error rate is 0.6%–1% for the two-dimensional surface code [114, 115].

The sufficient-purity criterion trades off with the accessible-energy criterion A. As described below A, an autonomous quantum machine may extract energy from heat baths. The baths reduce the machine's $\mathcal{P}(\rho)$. However, non-Markovianity can revive a machine's purity [116]. A non-Markovian bath retains a memory; information, upon entering the bath from the machine, can recollect and act back on the machine. Non-Markovianity can arise from strong system–bath couplings, small baths, low temperatures, and initial system–environment couplings. One can engineer non-Markovianity from a Markovian environment: One would mediate machine–environment interactions through a memory-retaining interface [117]. Appendix A illustrates non-Markovianity's potential for reviving a machine's purity. Non-Markovianity, the appendix shows, can help baths achieve the energy criterion A without endangering the purity criterion F as much as thermal baths do.

G. Output worth the input

A machine's output is intended to fulfill the machine's purpose. How effectively the output fulfills the purpose depends on figures of merit. We illustrate with four examples. First, a refrigerator outputs a cooled target, $\mathcal{T}$, whose final temperature quantifies the refrigerator's effectiveness. So does the refrigerator's steady-state coefficient of performance (COP): Denote by $\dot{Q}_{\mathcal{T}}$ the current of heat extracted from $\mathcal{T}$ and by $\dot{Q}_{\mathcal{H}}$ the current of heat flowing from the hot bath. The steady-state COP is $\dot{Q}_{\mathcal{T}}/\dot{Q}_{\mathcal{H}}$ [62].

Second, an engine outputs work. Denote by $\dot{W}$ the power and by $\dot{Q}_{\mathcal{H}}$ the current of heat flowing from the engine's hot bath. Figures of merit include the steady-state efficiency, $\eta = \dot{W}/\dot{Q}_{\mathcal{H}}$; the power, $\dot{W}$; and the power at maximum efficiency, $\max_\eta\{\dot{W}\}$.

Third, a clock outputs ticks (emitted excitations). Its figures of merit include the accuracy, $N := (\bar{t}/\Delta t)^2$, described under criterion D. Another figure of merit is the resolution [48]. Recall that $\bar{t}$ denotes the average time between successive ticks. The resolution is $1/\bar{t}$.

Fourth, a quantum computer outputs a state σ that approximates an ideal ρ. Figures of merit can quantify the distance between the states. For example, the fidelity is $\left(\mathrm{Tr}\sqrt{\sqrt{\sigma}\,\rho\,\sqrt{\sigma}}\right)^2$.

Each figure of merit above measures an output's quality. Any agent running a machine can choose their threshold for an acceptable output figure of merit. Yet a more comprehensive figure of merit assesses not only the output, but also the input [118]. Inputs can include energy, time, control resources, and funding. As discussed in the introduction, one might expect from an autonomous atomic engine ≈ 1 eV per cycle. However, cooling the engine to the quantum regime and setting the engine up can cost orders of magnitude more energy. A useful autonomous quantum machine's output merits the input.

H. Ability to switch off after completing assignment

At least three mechanisms can spur an autonomous quantum machine to shut down. First, consider a machine that contains an autonomous quantum clock (criterion D). The clock can galvanize not only steps in the rest of the machine's operation (e.g., gates implemented at the right times), but also a halt. Second, the machine accesses only a finite amount of energy (criterion A)—for instance, finite-size hot and cold baths. Depleting the energy source winds the machine down.

Third, components of the machine can require varying degrees of purity to operate (criterion F). Hence the components' coherence times limit the operation time. We illustrate with a qubit with a ground state $|0\rangle$, excited state $|1\rangle$, and time-evolving density operator $\rho(t) = \sum_{j,k=0}^{1} \rho_{jk}(t)|j\rangle\langle k|$, for $t \geq 0$ [119]. Over the amplitude-damping time T_1, the excited-state weight $\rho_{11}(t)$ decays to $1/e$ of its initial value: $\rho_{11}(T_1) = \rho_{11}(0)/e$. Over the phase-damping time $T_2 < T_1$, the off-diagonal elements decay similarly: $\rho_{jk}(T_2) = \rho_{jk}(0)/e \;\forall j \neq k$.

I. Mobility (optional)

DiVincenzo listed two optional criteria necessary for transmitting information from place to place. Our optional criteria, I and J, concern the transmission of machines and of messages between machines. Mobility would benefit autonomous quantum machines including delivery drones, sensors that navigate to their targets, and machines that build molecules (or other machines). External potentials and accessible energy (criterion A) can help machines achieve directionality.

We illustrate with autonomous classical nanowalkers, which may inspire builders of autonomous quantum walkers. Reference [120] reports on a nanowalker, formed from a DNA strip, walking along a track consisting of more DNA strips. The nanowalker burns ATP as fuel. Enzymes ensure the nanowalker's directionality: One enzyme ligates (joins together) the walker and the next site, and another enzyme cleaves the walker from the previous site.

J. Interoperability (optional)

Autonomous quantum machines may communicate with each other and work together. Communications may occur via (at least) two mechanisms.

First, machine $\mathcal{A}$ may emit a signal for machine $\mathcal{B}$ to absorb. For example, we envisioned an autonomous quantum clock emitting an excitation absorbed by an autonomous Rydberg-atom computer (under criterion D).[5] $\mathcal{A}$ and $\mathcal{B}$ must satisfy three requirements:

(1) $\mathcal{B}$ must be physically able to detect $\mathcal{A}$'s signal. For example, denote by $\hbar\omega$ the excitation's energy, by $\Omega_{\mathcal{B}}$ the bandwidth of $\mathcal{B}$, and by E_0 the center of $\mathcal{B}$'s energy spectrum. The energy must lie in the bandwidth: $\hbar\omega \in [E_0 - \Omega_{\mathcal{B}}/2,\, E_0 + \Omega_{\mathcal{B}}/2]$.

(2) The signal must, given condition (1), have a sufficiently high probability of affecting $\mathcal{B}$. The excitation's momentum should direct the signal toward $\mathcal{B}$, and no intervening medium should swallow the signal. Once the excitation arrives, $\mathcal{B}$ should have a high probability of absorbing it. Fermi's golden rule governs the rate $\Gamma_{\mathrm{i}\mapsto\mathrm{f}}$ at which $\mathcal{B}$ jumps from a state $|\mathrm{i}\rangle$ to any energy-E_{f} state $|\mathrm{f}\rangle$: $\Gamma_{\mathrm{i}\mapsto\mathrm{f}} = \frac{2\pi}{\hbar} |\langle \mathrm{f}|H'|\mathrm{i}\rangle|^2 \, \mu(E_{\mathrm{f}})$. H' denotes the excitation-induced perturbation to $\mathcal{B}$'s Hamiltonian. $\mu(E)$ denotes the density of $\mathcal{B}$'s energy-E states. If $\mathcal{B}$ absorbs the signal through a photodetector, the external efficiency quantifies how effectively $\mathcal{B}$ satisfies requirement (2).

(3) After absorbing a signal, $\mathcal{B}$ might take time to reset before being able to absorb another signal. Denote this *dead time* by τ_{D}. Suppose that $\mathcal{A}$ sends multiple signals. The time interval τ between them should be $\tau \geq \tau_{\mathrm{D}}$. Photodetectors have dead times. Also, consider a photoisomer that has absorbed a photon and rotated into a metastable configuration. The molecule must re-equilibrate before undergoing another photoexcitation. The metastable configuration can have a half-life of two days, in solution at room temperature, if the photoisomer is azobenzene [64].

Under the second signaling mechanism, machine $\mathcal{A}$ arrives near $\mathcal{B}$, changing the external potential experienced by $\mathcal{B}$. Again, we illustrate with a photoisomer. Some of its nuclei rotate through many $|\varphi\rangle$'s, in the notation under criterion C. Advancing so, the nuclei change the electronic DOF's potential landscape—change $H(\varphi)$.

In another example, a qubit and a bosonic mode undergo a dispersive interaction. Such an interaction is effective (approximate), and we omit the derivation [121]. During it, one attributes to the qubit an effective gap Δ; to the mode an effective frequency ω, a creation operator $a^\dagger$, and an annihilation operator a; and to the coupling a strength χ. We set $\hbar = 1$. The dispersive Hamiltonian is

$$\Delta\, \sigma_z + \omega a^\dagger a + \chi \sigma_z a^\dagger a. \tag{4}$$

If the qubit is excited (in $|1\rangle$), it effectively adds χ to the mode's frequency. Analogously, if the mode is occupied, it effectively adds χ to the qubit's gap. Each subsystem therefore affects the other's Hamiltonian.

[5] Under criterion D, we cast the clock as a part of the computer. Here, we cast the clock as separate but as aiding the computer.

II. OUTLOOK

We have proposed DiVincenzo-like criteria for autonomous quantum machines. Eight criteria, we regard as necessary for most autonomous machines' useful operation. Satisfying the remaining two criteria, machines can move and interface. We emphasize the *useful* in the penultimate sentence: The literature has demonstrated that autonomous quantum machines can be designed and, with effort, realized experimentally. Autonomous quantum machines should now progress from curiosities to tools, like their classical counterparts. We hope that these criteria guide the progression.

Certain autonomous quantum machines appear to call for another criterion: instructions. Instructions could guide an autonomous quantum drone to walk some distance forward, turn leftward, and then turn off. In another example, an autonomous quantum computer should implement one circuit, rather than another. Upon satisfying our criteria, however, one can effect instructions, which form a kind of emergent criterion. One could guide the drone with a track covered by the mobility criterion (I). The switching-off criterion (H) would enforce the final instruction. One can feed an autonomous quantum computer instructions by leveraging a clock (criterion D), interactions (criterion C), interoperability (criterion J), etc. Single-purpose machines, such as autonomous quantum engines, do not require such instructions.

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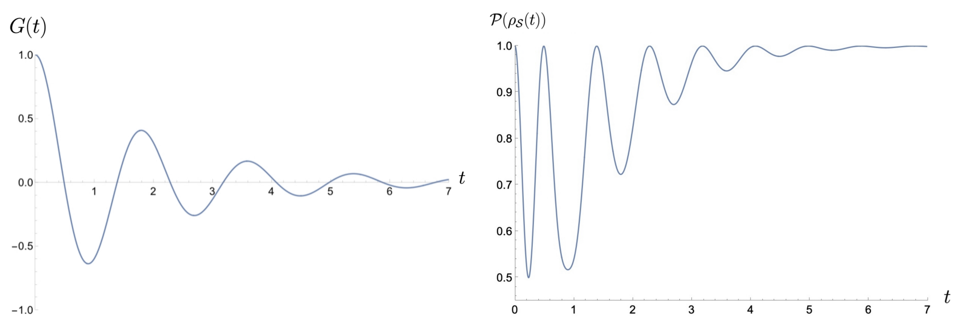
Appendix A NON-MARKOVIANITY'S POTENTIAL FOR REVIVING A MACHINE'S PURITY

We illustrate the title's claim by following [116]. That reference presents a setup common in cavity quantum electrodynamics: Consider a qubit $\mathcal{S}$ governed by a Hamiltonian $H_{\mathcal{S}} = \Delta\,\sigma_z$ with an energy splitting $\Delta > 0$. A bosonic environment $\mathcal{E}$ evolves under a Hamiltonian $H_{\mathcal{E}} = \sum_\ell \omega_\ell\, a_\ell^\dagger a_\ell$. Mode ℓ corresponds to energy ω_ℓ, to an annihilation operator a_ℓ, and to a creation operator $a_\ell^\dagger$. In the rotating-wave approximation, S couples to $\mathcal{E}$ via the Jaynes–Cummings Hamiltonian $H_{\text{int}} = \sum_\ell \left(g_\ell\, \sigma_+ a_\ell + g_\ell^* \sigma_- a_\ell^\dagger \right)$. The qubit has raising and lowering operators $\sigma_+ := |1\rangle\langle 0|$ and $\sigma_- := |0\rangle\langle 1|$, and the g_ℓ's denote coupling constants. Denote by $\rho_{\mathcal{S}/\mathcal{E}}(t)$ the time-t reduced state of $\mathcal{S}/\mathcal{E}$ in the interaction picture. Let $\mathcal{S}$ and $\mathcal{E}$ begin in a product state $\rho_{\mathcal{S}}(0) \otimes \rho_{\mathcal{E}}(0)$, $\rho_{\mathcal{E}}(0)$ being the bath's vacuum state.

$\mathcal{S}$ evolves under a linear, completely positive map Φ_t as $\rho_{\mathcal{S}}(t) = \Phi_t\, \rho_{\mathcal{S}}(0)$. The evolved state has off-diagonal coherences $\rho_{jk}(t) := \langle j|\rho_{\mathcal{S}}(t)|k\rangle$ determined by the complex *decoherence function* $G(t)$: $\rho_{jk}(t) = G(t)\rho_{jk}(0)\ \forall j \neq k$. To specify $G(t)$, we assume that $\mathcal{E}$ has a Lorentzian spectral density function (SDF) of width λ. Define the function $\lambda' := \sqrt{\lambda^2 - 2\gamma_0\lambda}$, whose γ_0 depends on the couplings g_ℓ. Suppose that the mode is on resonance with the qubit: The SDF is centered at Δ. The decoherence function becomes

$$G(t) = e^{-\lambda t/2} \left[\cosh\left(\frac{\lambda' t}{2}\right) + \frac{\lambda}{\lambda'} \sinh\left(\frac{\lambda' t}{2}\right) \right]. \tag{A1}$$

If $\gamma_0 < \lambda/2$, the coupling is weak, and the bath is Markovian. $G(t)$ is real and decreases monotonically with t. If $\gamma_0 > \lambda/2$, the coupling is strong, and the bath is non-Markovian. Figure 3 shows the implications for a qubit initialized to $|1\rangle$. The complex $G(t)$ has a magnitude that oscillates over time (Fig. 3a). The coherences $|\rho_{jk}|$ revive, and so does $\rho_S(t)$'s purity (Fig. 3b). Hence non-Markovianity can help baths achieve the energy criterion A without threatening the purity criterion F as much as thermal baths do.



(a) Decoherence function vs. time. **(b) Purity vs. time.**

FIG. 3: Coherence and purity at strong coupling: A bosonic mode decoheres a qubit initialized in $|1\rangle$. The Lorentzian width $\lambda = 1$. The coupling $\gamma_0 = 50\lambda/2$ is strong, so the bath is non-Markovian. For all t, the decoherence function $G(t) \in \mathbb{R}$. $G(t)$ and the purity, $P(\rho_S(t))$, oscillate. Hence non-Markovianity can revive the purity. (P eventually reaches 1 because the decoherence maps all states to $|0\rangle$.)

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