EchoKey Asks — Correlated Quantum Engine (exact-stroke demo): Mathematical Notes & Bookkeeping

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Purpose and scope

These notes accompany the script `ek_correlated_engine.py`. They provide a concise, math-first description of the microscopic engine and the exact bookkeeping used in the code. No dynamical approximations (Born/Markov/secular/Trotter) are employed; each stroke has a constant Hamiltonian with an exact propagator. Work is computed via quench identities. Entropic-resource accounting follows the spirit of Aguilar–Lutz's framework, specialized to quantities we compute exactly in the toy model.

State conventions. Total system is closed (unitary) and finite-dimensional. We use natural logarithms, $k_B = \hbar = 1$. For any density operator ρ, the von Neumann entropy is $S(\rho) = -\operatorname{Tr}[\rho \log \rho]$ and the quantum relative entropy is $D(\rho\|\sigma) = \operatorname{Tr}[\rho(\log \rho - \log \sigma)]$.

1 Hilbert space and indexing

We model six qubits:

$$S = \{S_h, S_c\} = \{0, 1\}, \quad B_h = \{2, 3\}, \quad B_c = \{4, 5\}.$$

Total Hilbert space: $\mathcal{H} = \bigotimes_{k=0}^{5} \mathbb{C}^2$. Reduced states are obtained by partial trace over complements of the indicated sets.

2 Hamiltonians

Single-qubit splittings

$$H_S = \frac{\omega_h}{2} Z_0 + \frac{\omega_c}{2} Z_1, \tag{1}$$

$$H_{B_h} = \sum_{i \in B_h} \frac{\omega_{bh,i}}{2} Z_i, \qquad H_{B_c} = \sum_{i \in B_c} \frac{\omega_{bc,i}}{2} Z_i, \tag{2}$$

$$H_B = H_{B_h} + H_{B_c}. \tag{3}$$

Couplings

$$H_g = \tfrac{1}{2} (X_0 X_1 + Y_0 Y_1), \tag{4}$$

$$H_{SB}^{(h)} = \sum_{i \in B_h} X_0 X_i, \qquad H_{SB}^{(c)} = \sum_{i \in B_c} X_1 X_i. \tag{5}$$

Piecewise-constant stroke Hamiltonians (durations $t_{\rm th}, t_{\rm work}, t_{\rm rlx}$):

$$H_{\rm th} = H_S + H_B + \kappa_h H_{SB}^{(h)} + \kappa_c H_{SB}^{(c)}, \tag{6}$$

$$H_{\rm work} = H_S + H_B + g_{\rm on} H_g + \chi\big(H_{SB}^{(h)} + H_{SB}^{(c)}\big), \tag{7}$$

$$H_{\rm rlx} = H_S + H_B + \tfrac{\kappa_h}{2} H_{SB}^{(h)} + \tfrac{\kappa_c}{2} H_{SB}^{(c)}. \tag{8}$$

Here $g_{\rm on}$ drives work exchange within S, while a small χ term during work provides a joint S–bath "power takeoff" that allows mutual information to decrease (spending correlations).

3 Initial state and thermal references

We initialize a *product* of Gibbs states at (T_h, T_c):

$$\rho_0 = \rho_{S_h}^{\rm th}(T_h) \otimes \rho_{S_c}^{\rm th}(T_c) \otimes \rho_{B_h}^{\rm th}(T_h) \otimes \rho_{B_c}^{\rm th}(T_c). \tag{9}$$

We also fix bath reference states $\rho_{B_h}^{\rm th}(T_h)$ and $\rho_{B_c}^{\rm th}(T_c)$ used in relative-entropy terms below. (This choice is explicit and auditable in code.)

4 Exact cycle protocol and quench work

Let $\rho_{\rm in}$ be the input to a cycle. For a constant Hamiltonian H applied for time Δt, the exact propagator is $U = \exp(-iH\Delta t)$.

$$\textbf{Stroke 1 (pre-thermalize):} \quad \rho_1 = U_{\rm th}\,\rho_{\rm in}\,U_{\rm th}^\dagger, \qquad U_{\rm th} = e^{-iH_{\rm th}t_{\rm th}}. \tag{10}$$

$$\textbf{Quench 1:}\ H_{\rm th} \to H_{\rm work}, \quad W_{q1} = \mathrm{Tr}[\rho_1\,(H_{\rm work} - H_{\rm th})]\,. \tag{11}$$

$$\textbf{Stroke 2 (work):} \quad \rho_2 = U_{\rm work}\,\rho_1\,U_{\rm work}^\dagger, \qquad U_{\rm work} = e^{-iH_{\rm work}t_{\rm work}}. \tag{12}$$

$$\textbf{Quench 2:}\ H_{\rm work} \to H_{\rm rlx}, \quad W_{q2} = \mathrm{Tr}[\rho_2\,(H_{\rm rlx} - H_{\rm work})]\,. \tag{13}$$

$$\textbf{Stroke 3 (relax):} \quad \rho_3 = U_{\rm rlx}\,\rho_2\,U_{\rm rlx}^\dagger, \qquad U_{\rm rlx} = e^{-iH_{\rm rlx}t_{\rm rlx}}. \tag{14}$$

$$\textbf{Quench 3:}\ H_{\rm rlx} \to H_{\rm th}, \quad W_{q3} = \mathrm{Tr}[\rho_3\,(H_{\rm th} - H_{\rm rlx})]\,. \tag{15}$$

Total *work on* the closed device is

$$W_{\rm on} = W_{q1} + W_{q2} + W_{q3}, \qquad W_{\rm out} = -W_{\rm on}. \tag{16}$$

This identity is exact for piecewise-constant $H(t)$: the continuous parts conserve the expectation of the active Hamiltonian; all energy changes come from quenches.

5 Heat attribution from bath bare energies

Although the global device is closed, we track energy changes of bath *bare* Hamiltonians as heat:

$$Q_h := -\big(\langle H_{B_h}\rangle_f - \langle H_{B_h}\rangle_i\big), \qquad Q_c := +\big(\langle H_{B_c}\rangle_f - \langle H_{B_c}\rangle_i\big). \tag{17}$$

Thus $Q_h > 0$ means energy flowed *from* the hot bath into the device; $Q_c > 0$ means energy flowed *to* the cold bath. We report $Q_{\rm in} = \max(0, Q_h)$ and an engine-style efficiency $\eta = W_{\rm out}/Q_{\rm in}$ when $Q_h > 0$. For comparison we print $\eta_C = 1 - T_c/T_h$.

6 Entropic resource bookkeeping

Define, for any state ρ at a cycle boundary (start i or finish f),

$$\rho_S = \mathrm{Tr}_{B_h B_c}\,\rho, \qquad \rho_{B_h} = \mathrm{Tr}_{SB_c}\,\rho, \qquad \rho_{B_c} = \mathrm{Tr}_{SB_h}\,\rho, \tag{18}$$

$$I(S\!:\!R)_\rho = S(\rho_S) + S(\rho_{B_h}\otimes\rho_{B_c}) - S(\rho), \tag{19}$$

$$\sigma(\rho) := I(S\!:\!R)_\rho + D\big(\rho_{B_h}\|\rho^{\mathrm{th}}_{B_h}\big) + D\big(\rho_{B_c}\|\rho^{\mathrm{th}}_{B_c}\big). \tag{20}$$

The *entropic resource change* over a cycle is

$$\Delta\sigma = \sigma_f - \sigma_i. \tag{21}$$

Interpretation: $\Delta\sigma < 0$ indicates net consumption of correlations/coherence/athermality ("entropic fuel") across the cycle; we tag such cycles ATHERMAL. Otherwise THERMAL. Our σ is a faithful subset of the full multi-part correlation balance in the general theory; it suffices to detect the sign change with quantities computed in the toy.

7 Energy bookkeeping checks

Let $E_H(\rho) = \mathrm{Tr}[\rho H]$. Because the Hamiltonian loop is closed at H_{th}:

$$E_{H_{\mathrm{th}}}(\rho_f) - E_{H_{\mathrm{th}}}(\rho_i) + W_{\mathrm{out}} = 0. \tag{22}$$

We print the residual

$$\mathrm{res}_{\mathrm{total}} := \big(E_{H_{\mathrm{th}}}(\rho_f) - E_{H_{\mathrm{th}}}(\rho_i)\big) + W_{\mathrm{out}} \approx 0, \tag{23}$$

which is at machine precision in the correlated (unitary) path.

We also split bare/interaction pieces at the same Hamiltonian H_{th}:

$$\Delta E_S := E_{H_S}(\rho_f) - E_{H_S}(\rho_i), \tag{24}$$

$$\Delta E_{\mathrm{int}} := E_{H_{\mathrm{th}}-H_S-H_B}(\rho_f) - E_{H_{\mathrm{th}}-H_S-H_B}(\rho_i). \tag{25}$$

With Q_h, Q_c defined above,

$$0 = W_{\mathrm{out}} - (Q_h - Q_c) + (\Delta E_S + \Delta E_{\mathrm{int}}), \tag{26}$$

whose residual we also report (`res_split`). In the decorrelated control path we *project* to a product of marginals (nonunitary), so residuals are expectedly nonzero.

8 Why $\chi \neq 0$ helps produce $\Delta\sigma < 0$

If H_{work} acts only on S ($\chi = 0$), then $U_{\mathrm{work}} = U_S \otimes I_R$ cannot reduce $I(S\!:\!R)$. With tiny baths, the contact strokes typically *increase* correlations and bath athermality, pushing $\Delta\sigma > 0$. A small χ provides a joint S–bath handle that can spend correlations while channeling energy via H_g.

9 Interpreting typical outputs

Cycles with $Q_h \leq 0$ are not heat-engine cycles under our sign convention (they can be refrigeration/heat-pump or correlation-driven). The demonstration target is a cycle with $W_{\mathrm{out}} > 0$ and $\Delta\sigma < 0$ (athermal burst). Residuals at $\mathcal{O}(10^{-15})$ confirm tight energy accounting in the correlated (unitary) path; $\mathcal{O}(10^{-2})$ residuals in the decorrelated control are expected.

10 What is exact, what is simplified

Exact per stroke: unitary propagation with a single exponential per stroke; work from quench identities; start/end energies evaluated at the same Hamiltonian.
Simplified but faithful: we track $I(S:R)$ and two bath D terms. The general framework includes additional multi-part correlation terms inside S and inside R; our subset suffices to exhibit the operational sign of $\Delta\sigma$.

11 Reproduction tips

Gentle parameters that often yield an early ATHERMAL cycle:

```
--Th 2.2 --Tc 0.5 --kappa_h 0.30 --kappa_c 0.30 --t_th 2.6 --t_rlx 0.5 --g_on 0.24 --chi -0.1
```

12 Extensions (same bookkeeping)

- Larger baths for more realistic relaxation.
- Compare full $D(\rho\|\rho^{\mathrm{th}})$ vs diagonal $D(\rho^{\mathrm{diag}}\|\rho^{\mathrm{th}})$ to isolate coherence contributions.
- Shortcuts to adiabaticity in H_{work} to suppress friction.
- Non-Gibbs initial baths (squeezed), with references adapted accordingly.

13 Minimal derivations

Quench work identity (piecewise-constant H)

Let $H(t) = H_\alpha$ on $t \in [t_\alpha, t_{\alpha+1})$ with unitary $U_\alpha = e^{-iH_\alpha(t_{\alpha+1}-t_\alpha)}$ and instantaneous jumps $H_\alpha \to H_{\alpha+1}$ at $t_{\alpha+1}$. Since E_{H_α} is conserved during each stroke,

$$\Delta E = \sum_\alpha \mathrm{Tr}\big[\rho(t^-_{\alpha+1})\,(H_{\alpha+1} - H_\alpha)\big] = \sum_\alpha W_{q\alpha}. \tag{27}$$

Closing the Hamiltonian loop gives $\Delta E = 0$ for the closed device, hence $W_{\mathrm{on}} = \sum_\alpha W_{q\alpha}$ and $W_{\mathrm{out}} = -W_{\mathrm{on}}$.

Heat from bath bare energies

With $Q_h = -\Delta\langle H_{B_h}|H_{B_h}\rangle$, $Q_c = +\Delta\langle H_{B_c}|H_{B_c}\rangle$, positive Q_h corresponds to energy drawn from the hot bath, while positive Q_c corresponds to energy delivered to the cold bath.

Entropic resource change

For $\sigma(\rho) = I(S:R)_\rho + \sum_j D(\rho_{B_j}\|\rho^{\mathrm{th}}_{B_j})$, the per-cycle change is

$$\Delta\sigma = (I_f - I_i) + \sum_j \big(D(\rho_{B_j,f}\|\rho^{\mathrm{th}}_{B_j}) - D(\rho_{B_j,i}\|\rho^{\mathrm{th}}_{B_j})\big). \tag{28}$$

A negative $\Delta\sigma$ signals net consumption of information-theoretic resource over the cycle.

14 Mapping (code $\leftrightarrow$ symbols)

`H_th, H_work, H_rlx`	$H_{\mathrm{th}}, H_{\mathrm{work}}, H_{\mathrm{rlx}}$
`U_*`	$e^{-iH_*\Delta t}$
`W_out = -(Wq1+Wq2+Wq3)`	$W_{\mathrm{out}} = -\sum_\alpha W_{q\alpha}$
`Q_h = -(E_Bh_f - E_Bh_i)`	$Q_h = -(\langle H_{B_h}\rangle_f - \langle H_{B_h}\rangle_i)$
`Q_c = +(E_Bc_f - E_Bc_i)`	$Q_c = +(\langle H_{B_c}\rangle_f - \langle H_{B_c}\rangle_i)$
`I_SR`	$I(S\!:\!R)$
`D(Bh||th)`, `D(Bc||th)`	$D(\rho_{B_h}\\|\rho_{B_h}^{\mathrm{th}}),\ D(\rho_{B_c}\\|\rho_{B_c}^{\mathrm{th}})$
`Delta_sigma`	$\Delta\sigma$
`regime`	ATHERMAL if $\Delta\sigma < 0$, else THERMAL
`check_total_residual`	$(E_{H_{\mathrm{th}}}(\rho_f) - E_{H_{\mathrm{th}}}(\rho_i)) + W_{\mathrm{out}}$
`check_split_residual`	$W_{\mathrm{out}} - (Q_h - Q_c) + (\Delta E_S + \Delta E_{\mathrm{int}})$

Takeaway

This demo is exact per stroke with auditable energy/entropy ledgers. Retaining correlations ("paper" path) can outperform a decorrelated control and produce athermal cycles where $W_{\mathrm{out}} > 0$ while $\Delta\sigma < 0$. The residual checks validate the bookkeeping.