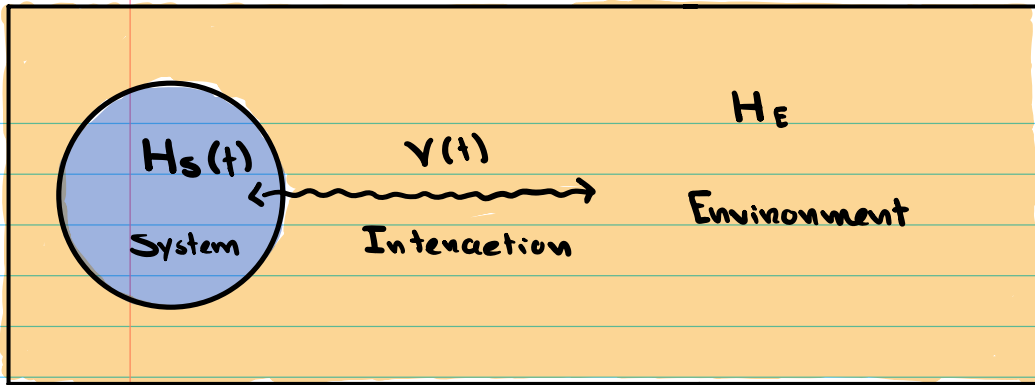


- It is impossible to extract energy from a (closed) thermal state using a finite driving.
- A finite driving, where the initial and final Hamiltonian are the same, is the quantum equivalent of a cyclic process. There is however a crucial distinction: the final state of the system  $\rho(t)$  is a non-equilibrium state!
- The energy change  $\Delta E$  induced by time-dependent driving is associated with work, since there is no reservoir present during the evolution (no entropy flow).

$W \equiv \Delta E > 0$  Impossible to extract work from a thermal state in a cyclic process.

## 2.2) Open Quantum Systems

- A quantum system is, in practice, open to its environment. The environment is usually too complicated to describe microscopically and we are only interested in the system.
- The theory of open quantum system describes how a quantum system evolves when it interacts w/ the environment. The evolution is not unitary, but is given by a quantum dynamical map.



- We split the Hilbert space of the full system into **system** (proper) and **environment**.

$$\mathcal{H} = \mathcal{H}_s \otimes \mathcal{H}_E$$

$$H(t) = H_s(t) \otimes \mathbb{1}_E + \mathbb{1}_s \otimes H_E + V(t).$$

$H_s(t) \equiv$  Hamiltonian of the system.

$H_E \equiv$  Hamiltonian of the environment.

$V(t) \equiv$  Interaction between them.

$\otimes \equiv$  Tensor product.

$\mathbb{1} \equiv$  Identity operator.

- The system and environment are assumed to be initially **uncorrelated** (statistically independent).

$$c(t_0) = c_s(t_0) \otimes c_E(t_0) \quad \text{Uncorrelated initial state of the whole.}$$

- For time  $t > t_0$ , the system and environment evolve unitarily:

$$c(t) = U(t, t_0) (c_s(t_0) \otimes c_E(t_0)) U^\dagger(t, t_0).$$

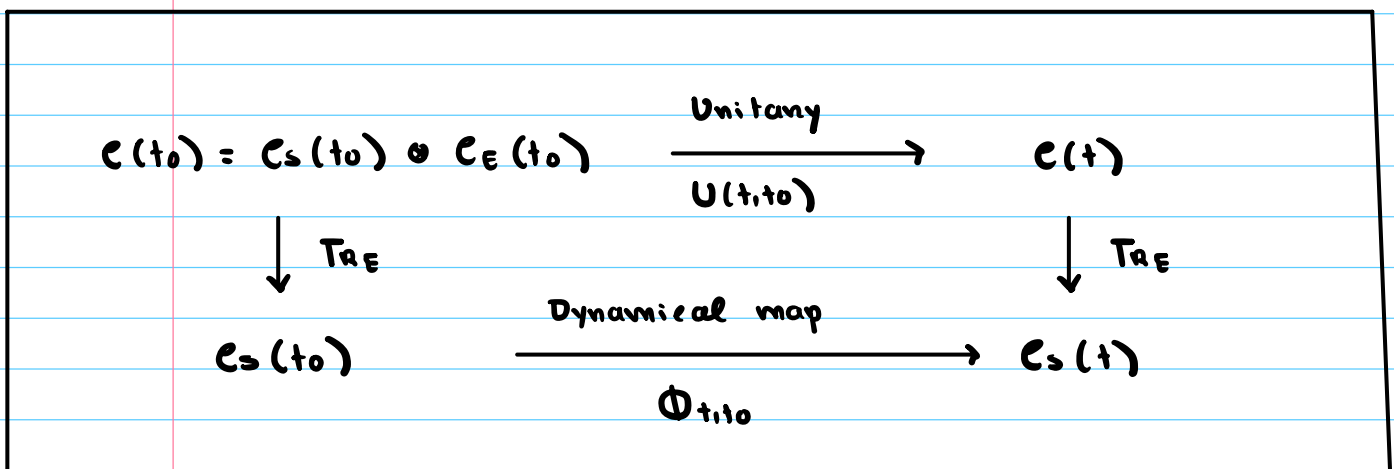
## Quantum dynamical map

- The quantum state of system or environment can be obtained by **tracing out (marginalizing)** the other system.

$$\rho_S(t) = \text{Tr}_E [\rho(t)] \equiv \Phi_{t,t_0} [\rho_S(t_0)].$$

$$\rho_E(t) = \text{Tr}_S [\rho(t)]$$

- The map  $\Phi_{t,t_0}$  is called a **quantum dynamical map**, or **completely positive trace-preserving map (CPTP map)**.



## Entropy change under dynamical maps

- The von Neumann entropy obeys the important inequality called **sub-additivity**.

## Sub-additivity of von Neumann entropy

Let  $\rho$  denote the density operator of the full system and  $\rho_S = \text{Tr}_E[\rho]$  and  $\rho_E = \text{Tr}_S[\rho]$  the density operators of the two subsystems. Then:

$$S[\rho_S \otimes \rho_E] = S[\rho_S] + S[\rho_E] \geq S[\rho],$$

with equality holding iff  $\rho = \rho_S \otimes \rho_E$ . ■

- It means that the full state  $\rho$ , which is generally a correlated state  $\rho \neq \rho_S \otimes \rho_E$ , contains more information than the individual systems that compose it. The full state has **correlations** which are not captured by looking at sub-systems.

- Consider then von Neumann entropy of the full evolution:

$$S[\rho(t_0)] = S[\rho_S(t_0) \otimes \rho_E(t_0)] = S[\rho_S(t_0)] + S[\rho_E(t_0)].$$

$$S[\rho(t)] \leq S[\rho_S(t)] + S[\rho_E(t)].$$

- Remarkably, we can write  $S[\rho(t)]$  as an equality!

$$S[\rho(t)] = -k_B \text{Tr}[\rho(t) \log \rho(t)]$$

$$= -k_B \text{Tr}[\rho(t) (\log \rho(t) - \log(\rho_S(t) \otimes \rho_E(t)) + \log(\rho_S(t) \otimes \rho_E(t)))]$$

$$= -D[\rho(t) | \rho_S(t) \otimes \rho_E(t)]$$

$$+ k_B \text{Tr}[\rho(t) \log \rho_S(t) \otimes \rho_E(t)]$$

Using: 
$$\begin{cases} \log(c \otimes \sigma) = \log c \otimes 11 + 11 \otimes \log \sigma \\ \text{Tr} [c(t) (A_S \otimes 11)] = \text{Tr}_A [c_S(t) A_S] \end{cases}, \text{ we have}$$

$$S[c(t)] = -D[c(t) | c_S(t) \otimes c_E(t)] + S[c_S(t)] + S[c_E(t)]$$

- The relative entropy appearing is a **measure of correlations** established **between system and environment**, sometimes called the **mutual information**.

### Mutual Information

$$I_{S:E}(t) \equiv D[c(t) | c_S(t) \otimes c_E(t)] \geq 0 \quad \blacksquare$$

- We can now write the change in entropy from unitary evolution as:

$$S[c(t)] - S[c(t_0)] =$$

$$S[c_S(t)] + S[c_E(t)] - I_{S:E}(t) - S[c_S(t_0)] - S[c_E(t_0)]$$

$$= 0 \Leftrightarrow \Delta S_S(t) \equiv S[c_S(t)] - S[c_S(t_0)]$$

$$= I_{S:E}(t) - \Delta S_E(t), \text{ in other words:}$$

$$\Delta S_s(t) = I_{s:\epsilon}(t) - \Delta S_\epsilon(t)$$

- This provides an expression for the **entropy change of an open quantum system**. We can go one step further and split:

$$\begin{aligned} \Delta S_\epsilon(t) &= S[\rho_\epsilon(t)] - S[\rho_\epsilon(t_0)] \\ &= -D[\rho_\epsilon(t) | \rho_\epsilon(t_0)] - k_B \text{Tr}[(\rho_\epsilon(t) - \rho_\epsilon(t_0)) \log \rho_\epsilon(t_0)]. \end{aligned}$$

We finally arrive at our main result:

### Entropy change of an open quantum system

$$\Delta S_s(t) = \Sigma(t) + \mathcal{J}(t), \text{ where}$$

#### Entropy production

$$\Sigma(t) \equiv I_{s:\epsilon}(t) + D[\rho_\epsilon(t) | \rho_\epsilon(t_0)] \geq 0$$

#### Entropy Flow

$$\mathcal{J}(t) \equiv k_B \text{Tr}[(\rho_\epsilon(t) - \rho_\epsilon(t_0)) \log \rho_\epsilon(t_0)] \quad \blacksquare$$

- The **entropy production** has two contributions: **correlations** between system and environment and information about the **state of the environment** after interaction.
- The **entropy flow** can be positive or negative, depending on the environment.
- The expression is valid regardless of the state of the environment or its size: it is a **purely informational** expression, which **will become the second law of thermodynamics** when the environment is thermal.

### 2.3) Laws of Thermodynamics for Quantum systems

- We now consider that the initial state of the **environment** is the **thermal state**:

$$\rho_E(t_0) = \frac{e^{-\beta H_E}}{Z} \quad (\text{Initially thermal environment}).$$

- The (**informational**) entropy flow now becomes associated to the energy change in the environment (**heat**).

$$\begin{aligned} J(t) &= k_B \text{Tr} [(\rho_E(t) - \rho_E(t_0)) \log \rho_E(t_0)] \\ &= -k_B \text{Tr} [(\rho_E(t) - \rho_E(t_0)) H_E] \\ &= -\frac{1}{T} \Delta E_E(t) \equiv \frac{Q(t)}{T}. \end{aligned}$$

## Second law of thermodynamics for quantum systems

$$\Delta S_s(t) = \Sigma(t) + \frac{Q(t)}{T} . \quad \blacksquare$$

- In order to recover the **first law of thermodynamics**, we have to do an energy balance.
- **Work** is that part of the energy injected in the full system through a **time-dependent Hamiltonian**. The time-dependence represents some external degrees of freedom over which we have full control and can be used to manipulate in a deterministic fashion.

$$W(t) \equiv \text{Tr} [ H(t) \rho(t) - H(t_0) \rho(t_0) ] .$$

- Note that  $W(t) = 0$  if the Hamiltonian is time-independent, since then:

$$\begin{aligned} W(t) &= \text{Tr} [ H U(t, t_0) \rho(t_0) U(t, t_0)^\dagger - H \rho(t_0) ] \\ &= \text{Tr} [ U^\dagger(t, t_0) H U(t, t_0) \rho(t_0) ] - \text{Tr} [ H \rho(t_0) ] . \\ &= \text{Tr} [ U^\dagger(t, t_0) U(t, t_0) H \rho(t_0) ] - \text{Tr} [ H \rho(t_0) ] \\ &= \text{Tr} [ H \rho(t_0) - H \rho(t_0) ] = 0 , \end{aligned}$$

which follows from the cyclic property of the trace and  $[U, H] = 0$  and  $U^\dagger U = U U^\dagger = \mathbb{1}$ .



- We can then decompose **work** into:

$$\begin{aligned}
 W(t) &= \text{Tr} [H(t) c(t)] - \text{Tr} [H(t_0) c(t_0)] \\
 &= \text{Tr} [(H_S(t) \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E + V(t)) c(t)] - \\
 &\quad \text{Tr} [(H_S(t_0) \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E + V(t_0)) c(t_0)] \\
 &= \text{Tr} [H_S(t) c_S(t) - H_S(t_0) c_S(t_0)] \\
 &+ \text{Tr} [V(t) c(t) - V(t_0) c(t_0)] \\
 &+ \text{Tr} [H_E (c_E(t) - c_E(t_0))] \equiv \Delta E_S(t) - Q(t),
 \end{aligned}$$

Heat (energy associated with entropy flow)

$$Q(t) \equiv - \text{Tr} [H_E (c_E(t) - c_E(t_0))]$$

Energy change in the system (inc. interaction)

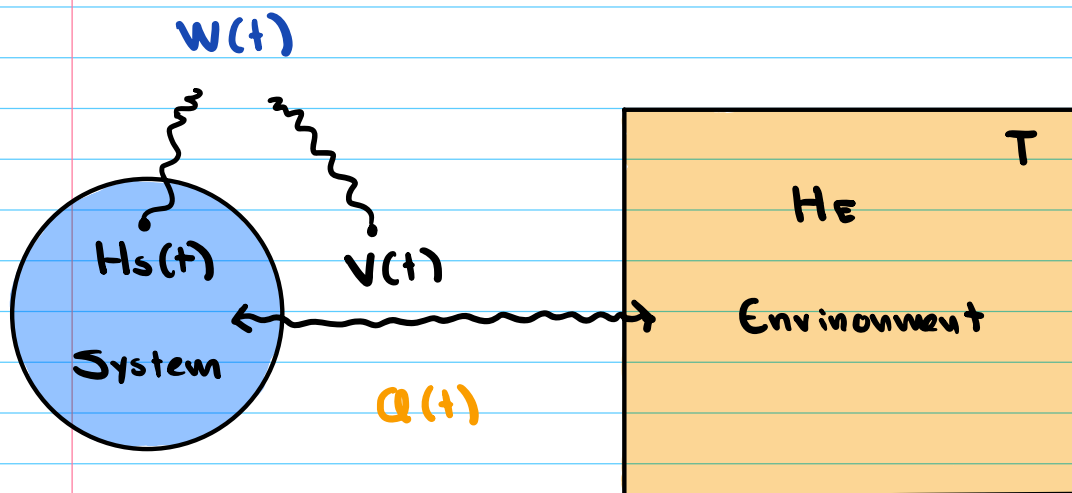
$$\begin{aligned}
 \Delta E_S(t) &\equiv \text{Tr} [H_S(t) c_S(t) - H_S(t_0) c_S(t_0)] \\
 &+ \text{Tr} [V(t) c(t) - V(t_0) c(t_0)]
 \end{aligned}$$

- Note that unless we include a finite (switch on-off) interaction  $V(t) = V(t_0) = 0$ , the **interaction** has to be included in the definition of energy belonging to the system.

## First law of thermodynamics for quantum systems

$$\Delta E_s(t) = W(t) + Q(t) \quad \blacksquare$$

## Summary and Take-away



- Quantum physics allow us to study the non-equilibrium thermodynamics of physical systems whose state is arbitrary: they can be as quantum as we want, provided that work and heat are still treated classically.
- The entropy production acquires a concrete meaning: irreversibility manifests itself as the build up of correlations between system and environment; and the non-equilibrium nature of the environment which is also affected by its interaction with the system.

- Even when the environment is not thermal, we can formulate a notion of entropy production that is purely informational in nature. However, there is no connection between entropy flow and energy: therefore, there is no heat in the usual sense.