12. Von Neumann Entropy vs. Thermodynamic Entropy

$$S_{\mathrm{vN}}(\rho) = -\mathrm{Tr}(\rho \ln \rho) = -\sum_i p_i \ln p_i$$

A measure of the degree to which the density operator state ρ is mixed.

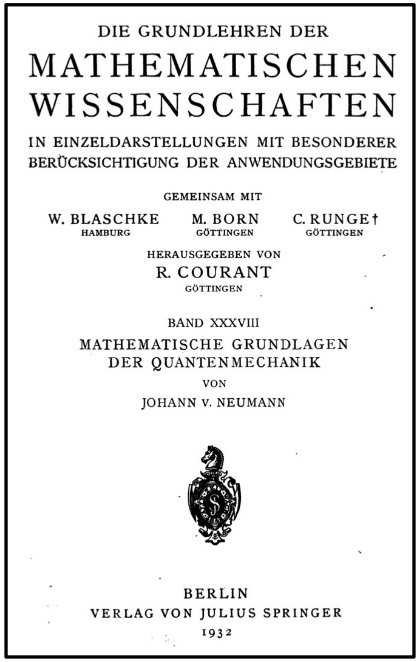
$$S_{\mathrm{TD}}(\sigma_2) \equiv \int_{\sigma_1}^{\sigma_2} \frac{\delta Q_R}{T} + S_0$$

The ratio of the change in heat to temperature of a reversible process that connects an initial state σ_1 to a final state σ_2.

- ***Claim***:

  S_{vN} is the quantum mechanical generalization of S_{TD}!

John von Neumann
(1903-1957)



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MATHEMATISCHE GRUNDLAGEN DER QUANTENMECHANIK
VON
JOHANN V. NEUMANN

BERLIN
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1932

<u>Set-Up In Brief</u>: A cyclic process involving

(a) A quantum gas in an initial pure state that transitions to a mixed state upon measurement, and hence undergoes an increase in S_{vN}.

(b) Gas then goes through a reversible expansion and compression process that brings it back to initial state, and produces a decrease in S_{TD}.

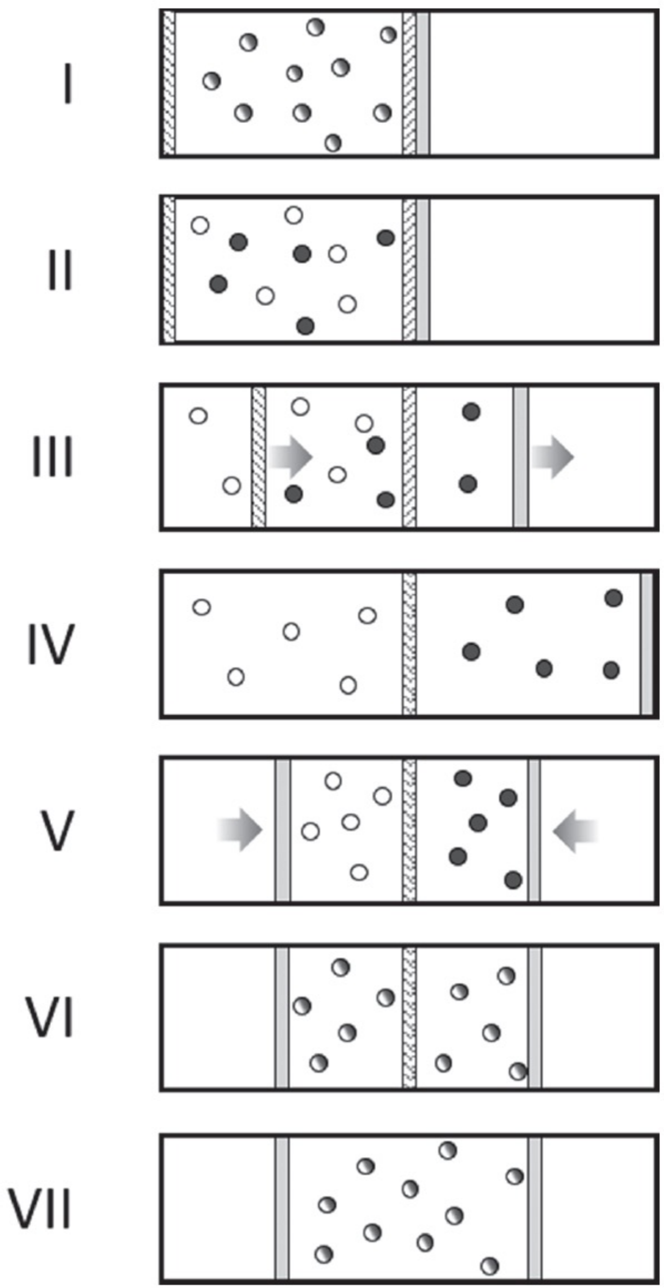
Claim: There must be a compensating increase in S_{TD} to offset (b), and this occurs in (a) if we equate S_{vN} with S_{TD}.

<u>Issues to consider</u>:

#1. Can a quantum measurement be characterized by a transition between a pure state and a mixed state?

#2. Can a quantum measurement be characterized by an increase in S_{TD}?

Set-Up In Detail: 7 stage cyclical process



$S_{\rm vN}$ increase of $N\ln 2$

Stage I:

- N-particle gas in left side of chamber with vol $2V_0$ in equilibrium with reservoir at temp T.
- Each particle in vector state:

$$|0\rangle = \sqrt{1/2}(|+\rangle + |-\rangle)$$

- *Pure* pre-measurement gas state:

$$\rho_{\rm pre} = |0_1 0_2 \cdots 0_N\rangle\langle 0_1 0_2 \cdots 0_N|$$

- So: $S_{\rm vN}(\rho_{\rm pre}) = 0$

Stage II:

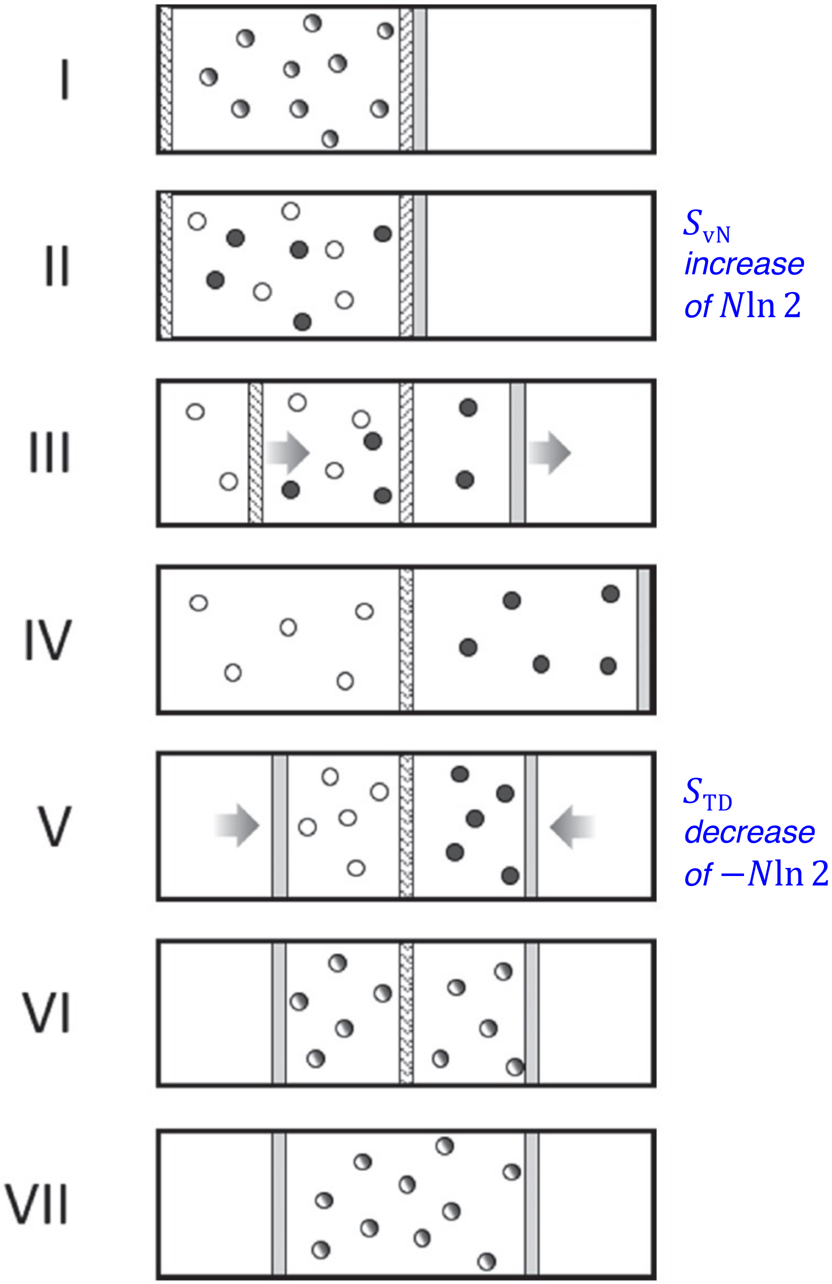
- Each particle is measured.
- *Maximally mixed* post measurement gas state:

$$\rho_{\rm post} = \frac{1}{2^N}\{|+_1 \cdots +_N\rangle\langle +_1 \cdots +_N| + |+_1 -_2 +_3 \cdots +_N\rangle\langle +_1 -_2 +_3 \cdots +_N| + \cdots + |-_1 \cdots -_N\rangle\langle -_1 \cdots -_N|\}$$

- So: $S_{\rm vN}(\rho_{\rm post}) = \ln 2^N = N\ln 2$

N-partite vector space $\mathcal{H}$ has dim $= 2^N$

Set-Up In Detail: 7 stage cyclical process



Stages III-IV:

- Particles are reversibly separated into left and right chambers by semi-permeable membrane.
- No work done, no heat exchanged.

Stage V:

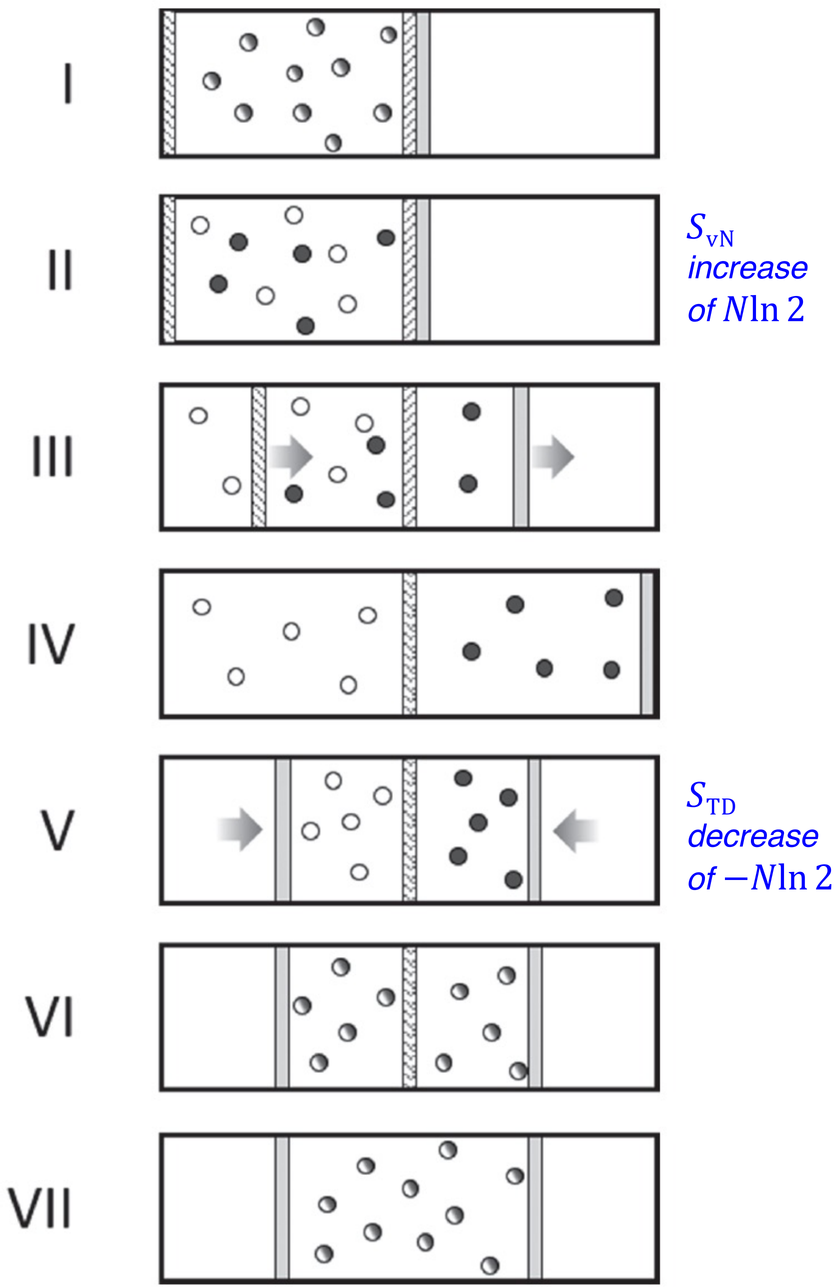
- Isothermal compression of left and right chambers from $2V_0$ to V_0.
- Work done on gas is:

$$W = -\int_{2V_0}^{V_0} \left(\frac{NT}{V}\right) dV = NT\ln 2$$

- Heat emitted by gas is $Q = -W = -NT\ln 2$
- TD entropy change in gas is:

$$\Delta S_{\mathrm{TD}} = \int_{\sigma_1}^{\sigma_2} \frac{\delta Q_R}{T} = \frac{-NT\ln 2}{T} - 0 = -N\ln 2$$

Set-Up In Detail: 7 stage cyclical process



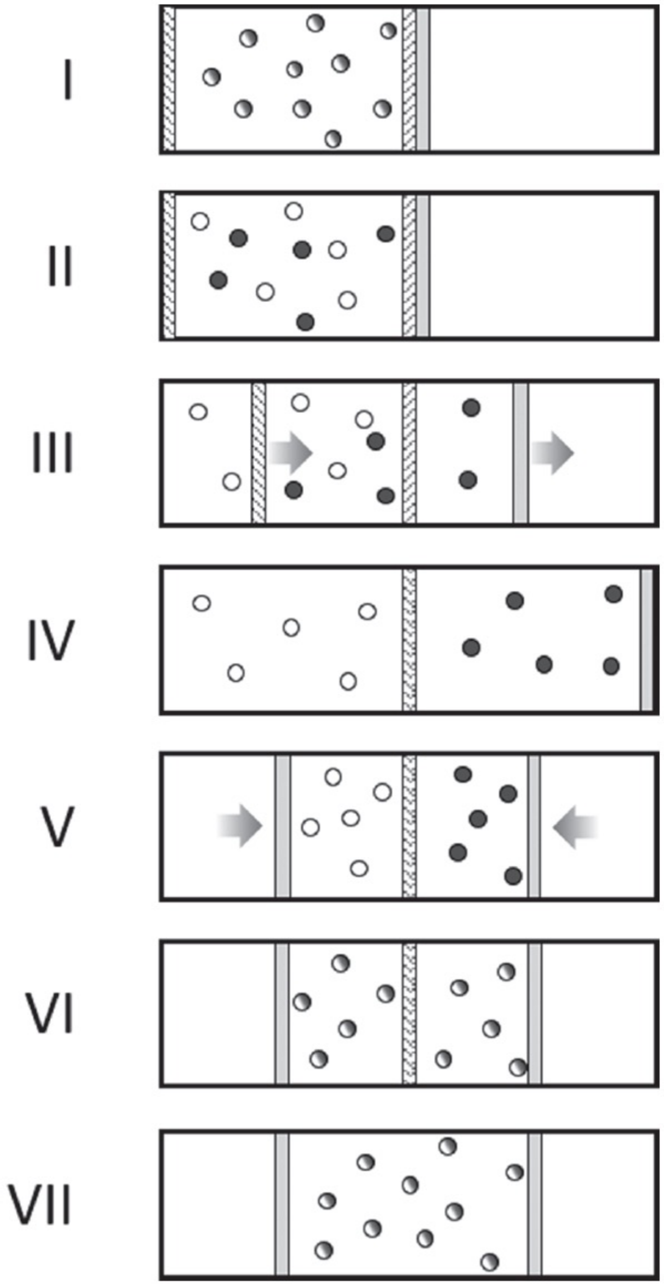
Stage VI:

- The $|+\rangle$ and $|-\rangle$ gases are reversibly transformed back into a $|0\rangle$ gas via unitary operations.

Stages VII:

- Partition is removed; gas returns to initial state.

Set-Up In Detail: *7 stage cyclical process*



S_{vN} *increase of* $N\ln 2$

S_{TD} *decrease of* $-N\ln 2$

von Neumann's Argument:

- All transitions between II and VII are reversible, so 2nd Law requires $\Delta S_{\mathrm{TD}} = 0$.
- There is a decrease in S_{TD} of $-N\ln 2$ during Stage V.
- So: There must be an increase in S_{TD} of $N\ln 2$ prior to Stage V.
- *And*: There is an increase in S_{vN} of $N\ln 2$ due to measurement at Stage II.
- So: If $S_{\mathrm{vN}} = S_{\mathrm{TD}}$, then no violation of 2nd law.

Issue #1: Can a quantum measurement be characterized by a transition between a pure state and a mixed state?

What is a quantum measurement?

- *According to von Neumann*:

$$|0\rangle = \sqrt{½}(|+\rangle + |-\rangle) \xrightarrow[\text{collapse}]{} \textit{either } |+\rangle \textit{ or } |-\rangle$$

pre-measurement vector state — *each with probability ½*

Or:

$$\rho_{\text{pre}} = |0\rangle\langle 0| \longrightarrow \rho_{\text{post}} = ½|+\rangle\langle +| + ½|-\rangle\langle -|$$

pure density operator state — *mixed density operator state*

- *But*: To the experimentalist, there is a definite result! ← *Her experience is that the post-measurement state is a definite (i.e., pure) state.*

- *Moreover*: The Schrödinger dynamics is unitary: it cannot transform a pure state to a mixed state.
  - *So if post-measurement states are mixed states, then we need an explanation of how the Projection Postulate "takes over" from the Schrödinger dynamics during a measurement.* ← *The "Measurement Problem"!*

Issue #2: Can a quantum measurement be characterized by an increase in S_{TD}?

- *This is Szilard's Principle*: *Gaining* information that allows us to discern between n ($= 2^N$) equally likely states is associated with a minimum increase in S_{TD} of $k \ln n$.
- What about Landauer's Principle?
  - *In general: What about the critique of information theoretic attempts to secure the 2nd Law?*

Issue #3: Did von Neumann really intend to equate S_{vN} with S_{TD}, or did he intend to equate S_{vN} with S_{Gibbs}?

- Sheridan (2020): In von Neumann's gas, each "molecule" is supposed to represent the state of an entire gas, as opposed to a single gas molecule.
  - *The "gas" is really an ensemble of quantum vector states (represented by a density operator).*
- *Thus*: The decrease in entropy in Stage V is a decrease in the Gibbs entropy S_{Gibbs} of a (classical) distribution that corresponds to the density operator state of the quantum system.