

"Open" Quantum Systems

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Saturday Mornings of Theoretical Physics: "Quantum Amplitudes, Classical Ignorance & Quantum Information Processing", Oxford 30.06.2018

James: quantum systems are described by “pure states” $|\Psi(t)\rangle$

This is an oversimplification.

In practice, we could try to prepare a system in a pure state through a measurement → “collapse of the wave function”

In reality measurements are never perfect – because our experimental colleagues don’t get enough funding 😊 – so the best we can do is to assert that the system could be in any of the states $|\Psi_1\rangle, |\Psi_2\rangle, \dots, |\Psi_n\rangle$ with some probabilities p_1, p_2, \dots, p_n

How can we accommodate such “real-life” situations?

In the following I will use **Dirac notation**, which is the best way to deal with Heisenberg's way of doing QM.



If you find this outlandish, you are in good company

I knew of Heisenberg's theory, of course, but I felt discouraged, not to say repelled, by the methods of transcendental algebra, which appeared difficult to me, and by the lack of visualizability. (Schrödinger in 1926)



The feeling was mutual....

The more I think about the physical portion of Schrödinger's theory, the more repulsive I find it. What Schrödinger writes about the visualizability of his theory is probably not quite right, in other words it's crap. (Heisenberg, writing to Pauli in 1926)



Our workhorse: a single qubit

A qubit is simply a 2-state system:

Basis states $|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

General state = superposition $|\Psi\rangle = c_1|\uparrow\rangle + c_2|\downarrow\rangle = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$

Observables = Operators $\mathcal{O}|\Psi\rangle = |\Phi\rangle$ operators map states to other states

Operators
→ Matrices $\mathcal{O} = \begin{pmatrix} a & b \\ b^* & c \end{pmatrix}$, $a = a^*$, $c = c^*$

Operators in
ket-bra notation

$\mathcal{O} = |\Psi\rangle\langle\Psi|$ is an operator

$$\mathcal{O}|\Phi\rangle = |\Psi\rangle\langle\Psi|\Phi\rangle$$



bra-ket = complex number

Trace

$$\text{Tr}[\mathcal{O}] = \text{Tr} \begin{pmatrix} a & b \\ b^* & c \end{pmatrix} = a + c = \langle \uparrow | \mathcal{O} | \uparrow \rangle + \langle \downarrow | \mathcal{O} | \downarrow \rangle$$

Dynamics: TDSE

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H |\Psi(t)\rangle$$

H = Hamiltonian of the system

Manipulating a qubit

let it be a spin-1/2

Initial state

$$|\Psi(0)\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Act with a magnetic field for some time t_0
 $\omega \propto B$

$$H = \begin{cases} 2\omega S^x = \hbar\omega \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & \text{if } 0 \leq t \leq t_0 \\ 0 & \text{if } t > t_0 \end{cases}$$

State at time t

$$|\Psi(t)\rangle = c_1(t) |\uparrow\rangle + c_2(t) |\downarrow\rangle = \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}$$

Schrödinger eqn

$$i\hbar \frac{d}{dt} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = H |\Psi(t)\rangle = \hbar\omega \begin{pmatrix} c_2(t) \\ c_1(t) \end{pmatrix}$$

$$|\Psi(t > t_0)\rangle = \cos(\omega t_0) |\uparrow\rangle - i \sin(\omega t_0) |\downarrow\rangle$$

Can "rotate" the qubit.

QM in terms of Density Operators

Pure state $|\Psi(t)\rangle \Leftrightarrow$ density operator $\rho(t) = |\Psi(t)\rangle \langle\Psi(t)|$

$$\rho(t) |\Phi\rangle = \langle\Psi(t)|\Phi\rangle |\Psi(t)\rangle$$



“overlap”: how close is $|\Phi\rangle$ to $|\Psi(t)\rangle$

$\rho(t)$ encodes **all** measurable properties of the system, e.g.

Expectation value for any operator A

$$\langle\Psi(t)| A |\Psi(t)\rangle = \text{Tr}[\rho(t) A]$$

$$\text{Tr}(A) = \sum_n \langle n | A | n \rangle = \sum_n A_{nn}$$

Density operators can describe the more general situations where we don't know which pure state the system is in.

"Mixed States"

Want to describe the situation where system could be in any of the states $|\Psi_1\rangle, |\Psi_2\rangle, \dots, |\Psi_n\rangle$ with some probabilities p_1, p_2, \dots, p_n

If $|\Psi_1\rangle$, expectation value of A would be

$$\langle A \rangle = \langle \Psi_1 | A | \Psi_1 \rangle$$



$$\langle A \rangle = \sum_i p_i \langle \Psi_i | A | \Psi_i \rangle$$

Corresponds to density op

$$\langle A \rangle = \text{Tr}[\rho A]$$

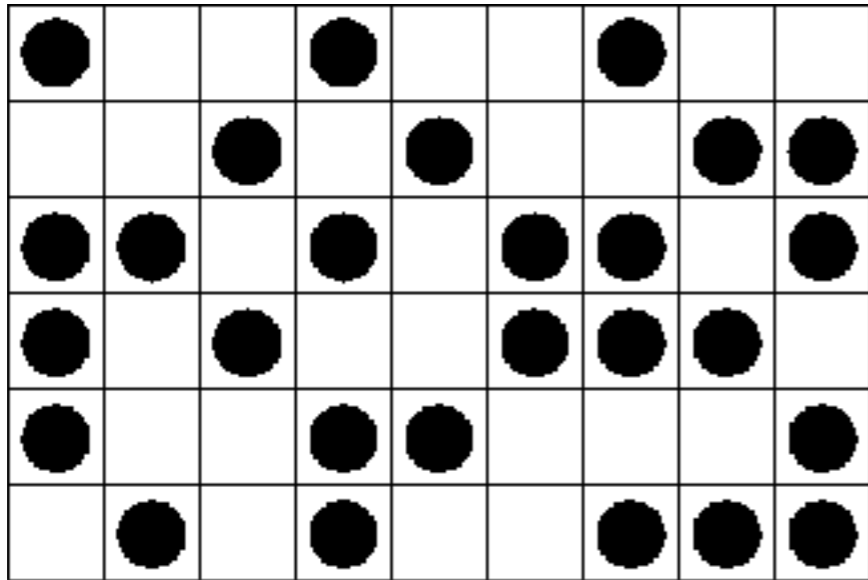
$$\rho = \sum_i p_i |\Psi_i\rangle\langle\Psi_i|$$

"Mixed state"

This cannot be written as $\rho = |\Phi\rangle\langle\Phi|$

Example: QM at finite temperature

Classical Stat. Mech.: configurations C , associated energy $E(C)$



thermal averages:

$$\langle\langle \mathcal{O} \rangle\rangle_T = \sum_{\text{configs } C} p(C) \mathcal{O}(C)$$

Probability of system being
in configuration C is

$$p(C) = \frac{e^{-E(C)/k_B T}}{\sum_{\text{configs } C} e^{-E(C)/k_B T}}$$

Example: QM at finite temperature

Quantum Mechanics: configurations \rightarrow energy eigenstates

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

thermal average
of observable \mathcal{O}

$$\langle \mathcal{O} \rangle_T = \sum_i p_i \langle \Psi_i | \mathcal{O} | \Psi_i \rangle$$

$$p_i = \frac{e^{-E_i/k_B T}}{\sum_i e^{-E_i/k_B T}}$$

Corresponding
density operator

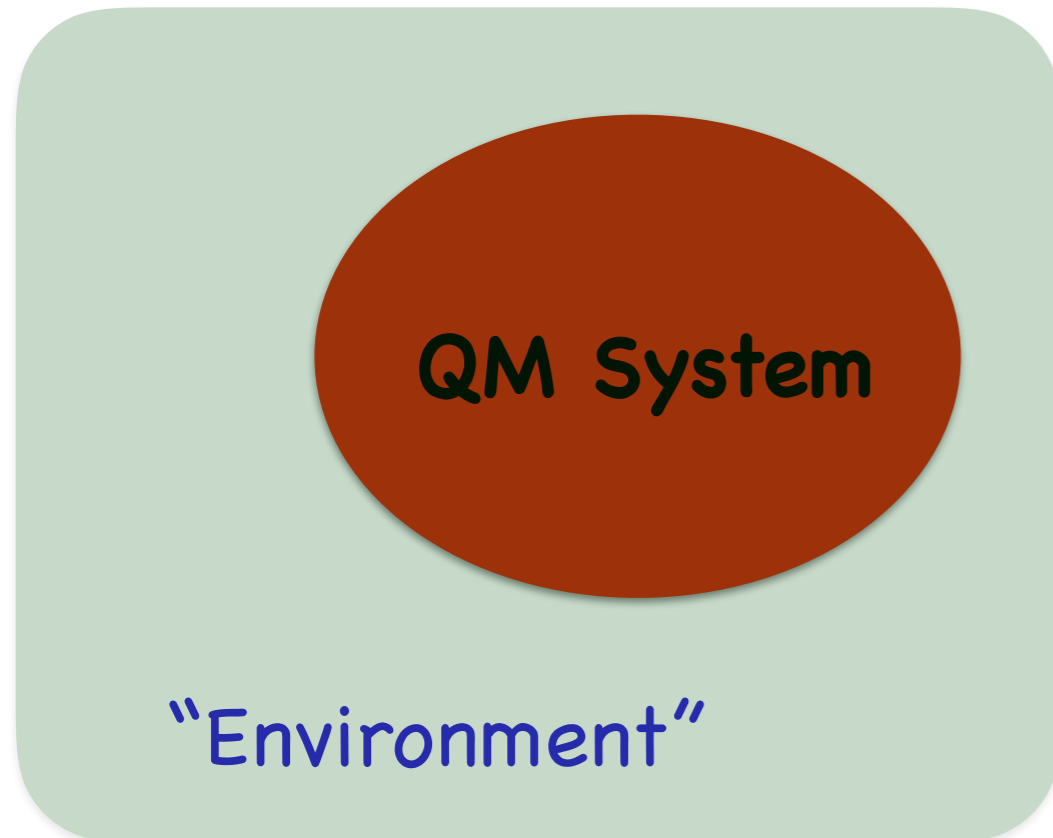
$$\langle \mathcal{O} \rangle_T = \text{Tr}[\rho(T)\mathcal{O}]$$

$$\rho(T) = \sum_i p_i |\Psi_i\rangle\langle\Psi_i|$$

mixed state

Reduced density operators

Mixed states arise from pure states upon “elimination” of some degrees of freedom:



- ρ = density operator of S&E
- ask questions only about S:

$$\text{Tr}[\rho \mathcal{O}_S]$$

acts only on S
degrees of freedom

- seek a “reduced” density operator involving only S degrees of freedom

$$\text{Tr}[\rho \mathcal{O}_S] \equiv \text{Tr}[\rho_S \mathcal{O}_S]$$

Solution

$$\rho_S = \text{Tr}_E[\rho]$$

Describes generically a mixed state.

Example: two spins 1/2 $|\Psi\rangle = \frac{1}{\sqrt{2}} [|\uparrow\rangle_1 |\downarrow\rangle_2 + |\downarrow\rangle_1 |\uparrow\rangle_2]$

Density operator

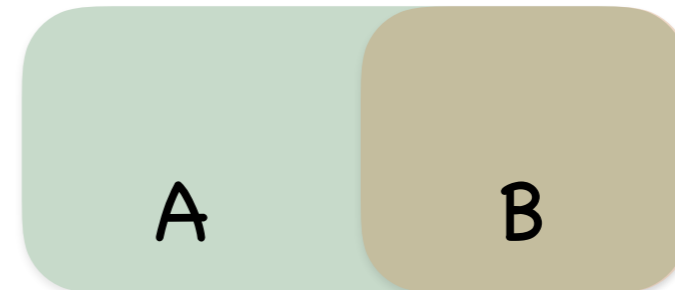
$$\rho = \frac{1}{2} [|\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\uparrow\downarrow\rangle\langle\downarrow\uparrow| + |\downarrow\uparrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|]$$

Reduced density operator

$$\rho_1 = \frac{1}{2} |\uparrow\rangle_1 \langle\uparrow| + \frac{1}{2} |\downarrow\rangle_1 \langle\downarrow| = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Application: Entanglement measures

Entanglement can be **quantified**



How strongly is A entangled with B ?

Let ρ_A be the RDO of subsystem A and p_i its eigenvalues

$$\rho_A |p_i\rangle = p_i |p_i\rangle, \quad p_i \geq 0$$

“entanglement entropy”

$$S_A = - \sum_i p_i \ln(p_i)$$

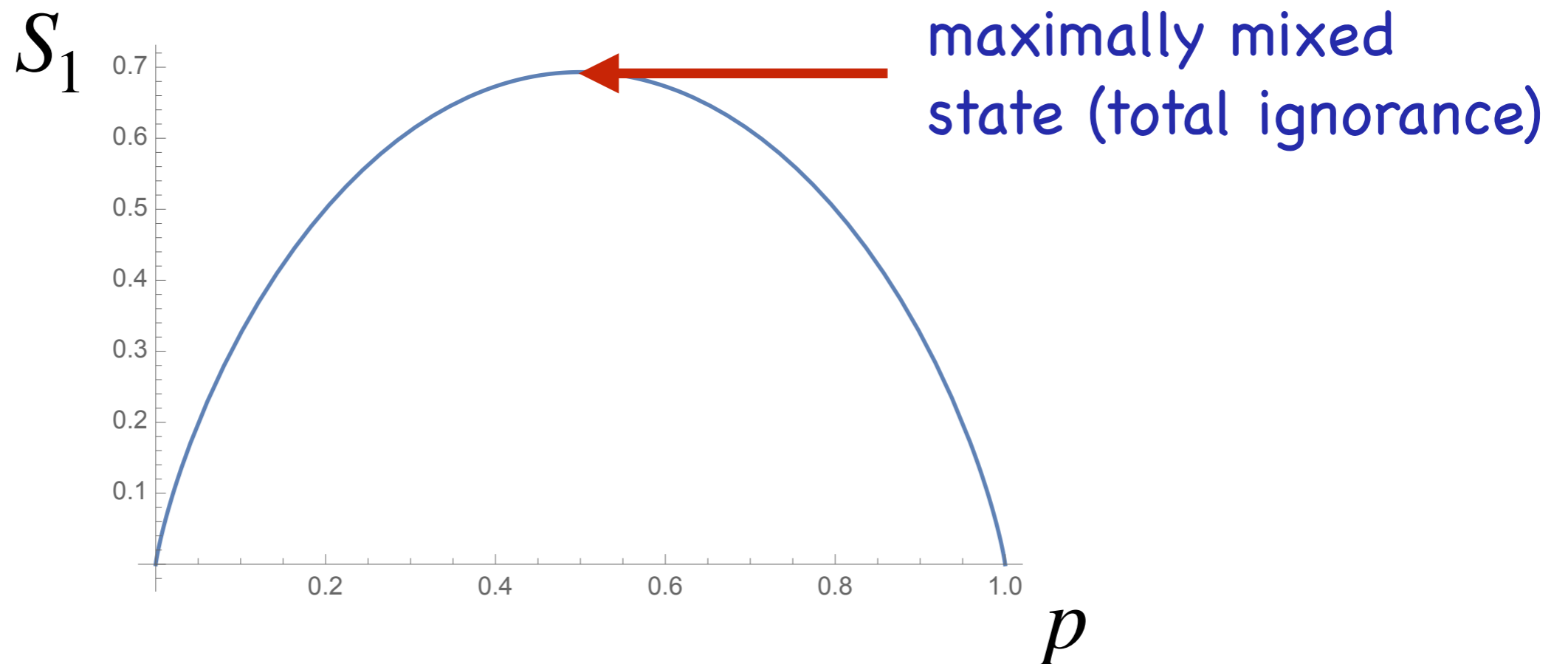
- very similar to definition of **thermodynamic entropy**
- measures how strongly mixed the RDO is, i.e. degree of ignorance about the state A is in

Example: $|\Psi\rangle = \sqrt{p} |\uparrow\rangle_1 |\downarrow\rangle_2 + \sqrt{1-p} |\downarrow\rangle_1 |\uparrow\rangle_2$, $0 \leq p \leq 1$

RDO: $\rho_1 = p |\uparrow\rangle_1 \langle \uparrow| + (1-p) |\downarrow\rangle_1 \langle \downarrow| = \begin{pmatrix} p & 0 \\ 0 & 1-p \end{pmatrix}$

eigenvalues $p, 1-p$

$$S_1 = -p \ln(p) - (1-p) \ln(1-p)$$



“Entanglement growth”

Consider a spin-1/2 (our qubit) in contact with a second spin-1/2 (environment)

Coupling described by $H = \frac{4J}{\hbar} S_1^x S_2^x$

Recall $S_j^x |\uparrow\rangle_j = \frac{\hbar}{2} |\downarrow\rangle_j$, $S_j^x |\downarrow\rangle_j = \frac{\hbar}{2} |\uparrow\rangle_j$

initially: $|\Psi(0)\rangle = |\uparrow\rangle_1 |\uparrow\rangle_2$ unentangled

later times: $|\Psi(t)\rangle = \cos(Jt) |\uparrow\rangle_1 |\uparrow\rangle_2 - i \sin(Jt) |\downarrow\rangle_1 |\downarrow\rangle_2$

is entangled! (measurement of spin 2 affects that of spin 1)

QM systems generically become **more entangled** under time evolution !

Coupling to the environment is bad for applications

Reduced density operator of the qubit:

$$\rho_1(t) = \cos^2(Jt) |\uparrow\rangle\langle\uparrow| + \sin^2(Jt) |\downarrow\rangle\langle\downarrow|$$

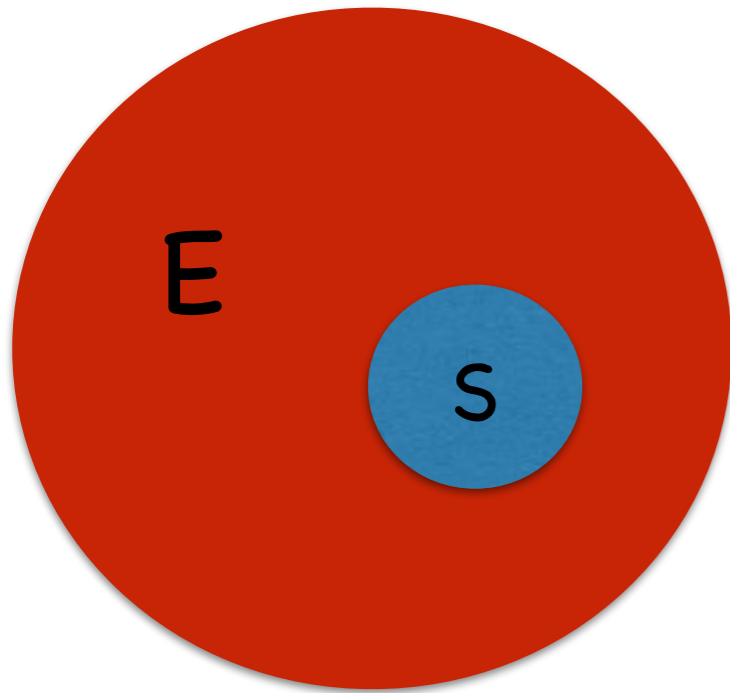
qubit changes its state with time.

In applications (e.g. ion traps) it is important to counter this effect and keep the qubit "alive".

→ ask this afternoon!

Entanglement growth and "thermalization"

Large QM System



Hamiltonian of S&E: H

density op of S&E: $\rho(t)$

energy: $E = \text{Tr}[H \rho]$

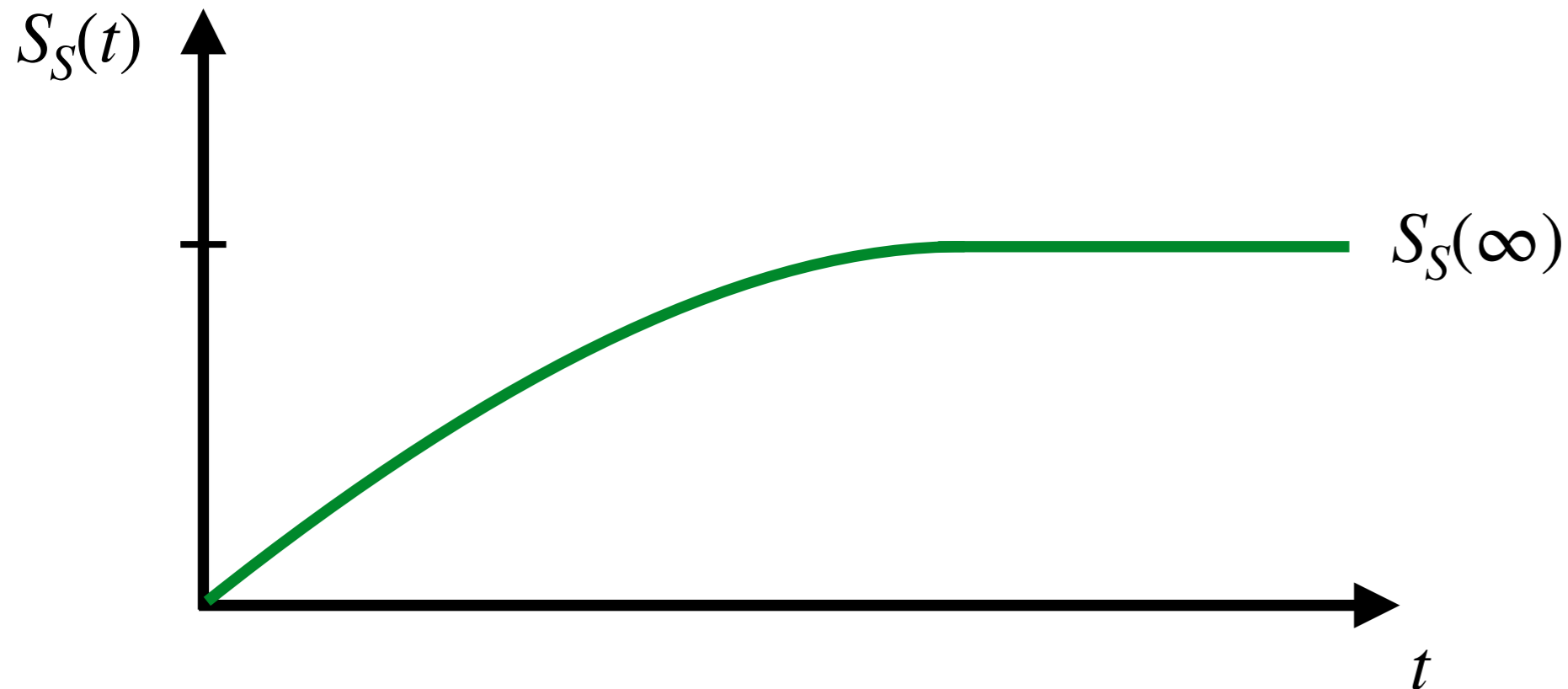
reduced density op
of the subsystem $\rho_S(t) = \text{Tr}_E[\rho(t)]$

How entangled is the subsystem with its environment?

Time evolution of entanglement entropy

$$S_S(t) = - \text{Tr}_S \left[\rho_S(t) \ln(\rho_S(t)) \right]$$

Start with an unentangled state



- Entanglement grows linearly in time, then saturates
- $S_S(\infty)$ proportional to volume V_S of subsystem
- $S_S(\infty)$ related to **thermodynamic entropy** of system at

energy E
$$S_S(\infty) = \frac{V_S}{V} k_B \ln(\Omega(E))$$

As you may have anticipated, this is not a coincidence...

- RDO becomes indistinguishable from a Gibbs ensemble

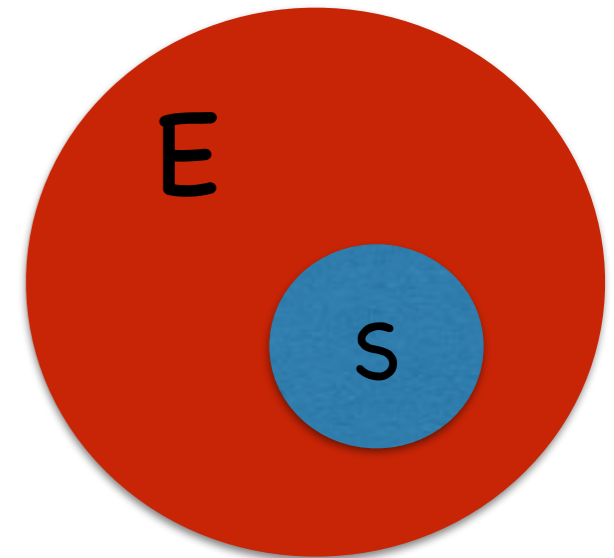
$$\rho_S(t) = \rho_S(T) \quad T \text{ fixed by total energy } E$$

“Environment” serves as a heat bath for S.

This is how QM gives rise to Stat. Mech. !

Ideas of “thermalization” go back to the early days of QM [v. Neumann (1929)], but the subject has become “hot” only in the last decade...

Edward Teller: “von Neumann would carry on a conversation with my 3-year-old son, and the two of them would talk as equals, and I sometimes wondered if he used the same principle when he talked to the rest of us...”



Summary

1. Need concept of **mixed states** to account for inaccessible information in QM systems.
2. These are described by **(reduced) density operators**.
3. RDOs give a way of **quantifying entanglement**.
4. **Entanglement grows** under time evolution.
5. Macroscopic systems become **locally thermal** over time:
Quantum Mechanics \Rightarrow Statistical Mechanics.

Thank you for your attention !