III Time evolution of density matrices

III.1 Time evolution in closed quantum systems.

A observable, $\langle A \rangle = \mathrm{Tr}(\rho A)$.

Time evolution in Heisenberg picture

$$A(t) = e^{i\frac{t}{\hbar}H} A e^{-i\frac{t}{\hbar}H}$$

$H = H^*$ the Hamiltonian. More generally,

$$A(t) = U(t,t_0)^* A(t_0) U(t,t_0)$$

with $U(t,t_0) = e^{-\frac{i}{\hbar}(t-t_0)H}$ if H is time-independent, and

$$U(t,t_0) = \mathbb{T}\exp\left(-\tfrac{i}{\hbar}\int_{t_0}^{t} H(s)ds\right)$$

if H is time-dependent.

By cyclicity of the trace,

$$\langle A(t) \rangle = \mathrm{Tr}(\rho\, U^*(t) A\, U(t))$$

$$= \mathrm{Tr}(U(t)\rho\, U^*(t) A)$$

for all A. Thus the time evolution for ρ is

$$\rho(t) = U(t,t_0)\,\rho(t_0)\,U(t,t_0)^*.$$

(note: for ρ, U^* is on the right, opposite to the eq. for A)

The time evolution in commutator form is

$$\dot{A}(t) = \frac{i}{\hbar}[H(t), A(t)]$$

By the same cyclicity argument, get

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H(t), \rho(t)]$$

(von Neumann equation).

Example for Spin-$\frac{1}{2}$: Choose a basis such that H is diagonal, $H = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}$. Then

$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix}$ with $\rho_{11}, \rho_{22} \in \mathbb{R}$ and $\rho_{12} = \overline{\rho_{21}}$.

$\rho_D = \begin{pmatrix} \rho_{11} & 0 \\ 0 & \rho_{22} \end{pmatrix}$ commutes with H, so

ρ_{11} and ρ_{22} are time-independent.

The off-diagonal elements oscillate

$$\rho_{12}(t) = \rho_{12}(0) \cdot e^{-\frac{i}{\hbar}t(E_1 - E_2)}.$$

Assume H to be time-independent.

$$\dot{\rho} = 0 \quad \text{iff} \quad [H, \rho] = 0.$$

This is the case if ρ depends only on conserved quantities. Thus the question how many conserved quantities there are is essential. Integrable systems have many of them; large (thermodynamic) ones, very few.

If only H is conserved, $\rho = \rho(H)$. The <u>canonical</u> density matrix is

$$\rho = \frac{1}{Z_C} e^{-\beta H}$$

where $\beta = \frac{1}{k_B T}$ and $Z_C = \mathrm{Tr}\, e^{-\beta H}$.

Strictly speaking, one needs H to have discrete spectrum. This is the reason why one usually starts out in a finite volume or with a confining potential.

For the harmonic oscillator, $H = (a^\dagger a \cancel{+\frac{1}{2}})\hbar\omega$, (drop the $\frac{\hbar\omega}{2}$ by an energy shift),

$$Z_C = \frac{1}{1 - e^{-\beta\hbar\omega}}.$$

(32) For a system of harmonic oscillators,

$$H = \sum_{i=1}^{N} \frac{P_i^2}{2m} + \frac{m}{2}\omega_i^2 X_i^2$$

$$= \sum_{i=1}^{N} \hbar\omega_i \left(a_i^\dagger a_i + \frac{1}{2}\right)$$

with $[a_i, a_j^\dagger] = \delta_{ij}$ and $[a_i, a_j] = 0$,

$N = \sum_i a_i^\dagger a_i$ is conserved ($[N,H] = 0$).

Thus $\rho_{gc}(\beta, \mu) = \frac{1}{Z_{gc}} e^{-\beta(H - \mu N)}$

is stationary.

For a spin system, e.g.

$$H = -\sum_{x,y} J_{xy} \vec{S}_x \cdot \vec{S}_y$$

the total spin $\vec{S} = \sum_x \vec{S}_x$ commutes with H

hence it is natural to consider in general

a magnetic field B:

$$\rho_{J,\vec{B}} = \frac{1}{Z_{J,\vec{B}}} e^{-\beta(H - \vec{B}\cdot\vec{S})}$$

etc.

Let $\rho_c = \frac{1}{Z_c} e^{-\beta H}$. Then

$$\ln \rho_c = -\ln Z_c - \beta H$$

so

$$S(\rho_c) = -\mathrm{Tr}(\rho_c \ln \rho_c) = +\ln Z_c + \beta \langle H \rangle_{\rho_c}$$

(where $\langle H \rangle_\rho = \mathrm{Tr}(\rho H)$). For any DM ρ,

$$\begin{aligned} S(\rho_c) - S(\rho) &= \mathrm{Tr}(\rho \ln \rho) - \mathrm{Tr}(\rho_c \ln \rho_c) \\ &= \underbrace{\mathrm{Tr}(\rho \ln \rho) - \mathrm{Tr}(\rho \ln \rho_c)}_{S(\rho|\rho_c) \geq 0} + \mathrm{Tr}(\rho \ln \rho_c) - \mathrm{Tr}(\rho_c \ln \rho_c) \\ &\geq \mathrm{Tr}(\rho \ln \rho_c) + S(\rho_c) \\ &= -\ln Z_c - \beta \langle H \rangle_\rho + \ln Z_c + \beta \langle H \rangle_{\rho_c} \\ &= \beta \left(\langle H \rangle_{\rho_c} - \langle H \rangle_\rho \right). \end{aligned}$$

This implies:

Theorem:

(i) Among all states ρ with fixed mean value of the energy, $E = \langle H \rangle_\rho$, the canonical state ρ_c has the largest entropy.

(ii) Let $F(\rho) = \langle H \rangle_\rho - \frac{1}{\beta} S(\rho)$.
Then $F(\rho) \geq F(\rho_c)$ for all DM ρ_c,
i.e. ρ_c minimizes the free energy.
(Gibbs variational principle).

Obviously, if $\dot{\rho} = 0$, then also

$$\frac{d}{dt} S(\rho) = 0 .$$

But even if $\dot{\rho} = \rho(t) = e^{-itH} \rho_0 \, e^{itH}$

$$S(\rho_t) = Tr(\rho(t) \ln \rho(t)) = S(\rho_0)$$

because the eigenvalues remain unchanged, $p_k(t) = p_k(0)$, and the trace can be taken in the time-dependent eigenbasis.

Thus unitary time evolution and von Neumann entropy tell us nothing about approach to a stationary state or even to a thermal equilibrium state (thermalization). To get dissipative phenomena and approach to some stationary state, one needs to take limits where unitarity is no longer true.

III.2 Time evolution in open quantum systems

An "open quantum system" consists of a system S and an environment R,[x)] which are coupled. The distinction is that only S is accessible to our measurements.

We assume that the total time evolution on $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_R$ is unitary. The question is what its reduction to $\mathcal{H}_S$ is like. That is, we are after

$$\mathbb{K}(t,\rho) = Tr_R(\rho(t))$$

$t \mapsto \mathbb{K}(t,\rho)$ is the time evolution of the reduced DM for S.

Let $(e_k)_k$ be an ONB for $\mathcal{H}_S$ and $(f_\ell)_\ell$ one for $\mathcal{H}_E$ then

$$(\mathbb{K}(t,\rho))_{kk'} = \sum_\ell \langle e_k \otimes f_\ell \,|\, U(t)(\rho \otimes P_{f_0})\, U(t)^* \, e_{k'} \otimes f_\ell \rangle$$

Here we have assumed that the environment is in a pure state; this is allowed, since we may purify it. Also, the joint state at initial time is $\rho \otimes P_{f_0}$, which means that the preparation removes correlations between S and R. Of course, the time evolution generates such

x) R from "reservoir"

correlations whenever there is a term in the Hamiltonian that couples $\mathcal{I}$ and $\mathcal{R}$.

Inserting $\mathbb{1} = \sum_{m,n} |\underbrace{e_m \otimes f_n}_{g_{mn}}\rangle\langle e_m \otimes f_n|$

we obtain

$$R(t,\rho)_{kk'} = \sum_{\ell} \sum_{\substack{m,n \\ m',n'}} \langle g_{k\ell} | U g_{mn} \rangle \langle g_{mn} | \rho \otimes P_{f_0} g_{m'n'} \rangle \cdot \langle g_{m'n'} | U^* g_{k'\ell} \rangle$$

$\delta_{n'0}\,\delta_{n0}$

$$= \sum_{\ell} \sum_{m,m'} \langle e_k \otimes f_\ell | U e_m \otimes f_0 \rangle \langle e_m | \rho e_{m'} \rangle \cdot \langle e_{m'} \otimes f_0 | U^* e_{k'} \otimes f_\ell \rangle$$

$$= \sum_{\ell} (K_\ell)_{km}\, \rho_{mm'}\, (K_\ell^*)_{m'k}$$

Thus

$$R(t,\rho) = \sum_{\ell} K_\ell \rho K_\ell^*$$

with "Kraus operators"

$$(K_\ell)_{kk'} = \langle e_k \otimes f_\ell | U (e_{k'} \otimes f_0) \rangle$$

The K_ℓ are often written by abuse of notation as $K_\ell = \langle f_\ell | U f_0 \rangle$.

They satisfy $\boxed{\sum_{\ell} K_\ell^* K_\ell = \mathbb{1}}$

Remarks.

1) If in some limit the K_ℓ become projections, we get back to von Neumann measurement in a limiting time evolution

2) The map $\rho \mapsto R(t,\rho)$ satisfies

(a) it is convex linear (i.e. linear on cones)

$$R(t, \sum p_i \rho_i) = \sum_i p_i R(t, \rho_i)$$

if $p_i \geq 0, \sum p_i = 1$.

(b) it conserves the trace

$$\mathrm{Tr}(R(t,\rho)) = \mathrm{Tr}(\rho)$$

(c) it is <u>completely positive</u>

i.e. the extension to $R(t,\cdot) \otimes \mathbb{1}_N$ is positive for all $N \in \mathbb{N}$

(c) is a stronger condition than just

$$R(t,\rho) \geq 0.$$

III.3 Markovian approximation and Lindblad dissipators.

The Kraus operators are ~~in general~~ time-dependent, and this dependence can be over long timescales, depending on the properties of the environment (ex. of conserved quantities, etc.).

The assumption that the environment has a dynamics on a much shorter timescale than the system motivates the Markovian approximation that $\dot{\rho}(t)$ is determined only by $\rho(t)$, irrespective of $\rho(t')$, $t'<t$, i.e.

$$\dot{\rho} = L(\rho)$$

(This assumption is in general untrue, there are memory effects, discussed later).

If it holds, we can find the form of $L(\rho)$. This was first done in a hallmark paper by Lindblad (1976) in a precise setting. Here, we give a heuristic argument. Consider a time δt which is small, but much larger than the R-scale of time, so that $\dot{\rho}$ can be calculated as

$$\dot{\rho}(0) = \frac{\rho(\delta t) - \rho(0)}{\delta t}.$$

Then

$$\rho(\delta t) = \rho(0) + \delta t \cdot L(\rho(0))$$

$$= \sum_{\ell} K_\ell \, \rho(0) K_\ell^*$$

with Kraus op's K_ℓ that depend on δt.

Then one of them, say, K_0 must be $\mathbb{1} + O(\delta t)$, and all the others $O(\sqrt{\delta t})$. So set

$$K_\ell = \sqrt{\delta t}\, R_\ell \qquad \ell \geq 1$$

and $\quad R_0 = \mathbb{1} + M \cdot \delta t$

We decompose M into its hermitian and antihermitian parts:

$$A = \frac{1}{2}(M + M^*) \qquad H = i\hbar \, \frac{M - M^*}{2}$$

so that $\quad M = -\frac{i}{\hbar} H + A$

(NB: H and A are operators on $\mathcal{H}_S$, i.e. for the effective system dynamics).

We have

$$(1 + M\delta t)\rho(1 + M^*\delta t) = \rho + (M\rho + \rho M^*)\delta t + O(\delta t)^2$$

$$= \rho + \left(-\frac{i}{\hbar}[H, \rho] + \{M, \rho\}\right)\delta t + O(\delta t)^2$$

and

$$\mathbb{1} = \sum_{\ell \geq 0} K_\ell^* K_\ell$$

$$= \mathbb{1} + (M^* + M)\,\delta t + O(\delta t)^2 + \sum_{\ell \geq 1} R_\ell^* R_\ell \,\delta t$$

so

$$A = -\frac{1}{2} \sum_{\ell \geq 1} R_\ell^* R_\ell .$$

In summary, we have Lindblad's master equation

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + D(\rho)$$

with the dissipator

$$D(\rho) = \{A, \rho\} + \sum_{\ell \geq 1} R_\ell \rho R_\ell^*$$

where $A = -\frac{1}{2} \sum_{\ell \geq 1} R_\ell^* R_\ell$

Let us define

$$\tilde{H} = H - \frac{i}{2} \sum_{\ell \geq 1} R_\ell^* R_\ell .$$

Then

$$\dot{\rho} = -\frac{i}{\hbar}\left(\tilde{H}\rho - \rho \tilde{H}^*\right) + \sum_{\ell \geq 1} R_\ell \rho R_\ell^*$$

$\tilde{H}$ is not selfadjoint; its antihermitian part is $-\frac{1}{2}\sum R_\ell^* R_\ell \leqslant 0$.

if $[H, \Gamma] = 0$,

$$e^{-it(H - i\Gamma)} = e^{-itH} e^{-t\Gamma}$$

which already suggests some damping.

The last part is necessary to ensure that $\mathrm{Tr}\,\dot{\rho} = 0$; this would not be the case if $\sum R_\ell \rho R_\ell^*$ were omitted (if any of the R_ℓ is nonzero).

The sol. of $\dot{\rho} = -\frac{i}{\hbar}(\tilde{H}\rho - \rho\tilde{H}^*)$ is of course

$$\rho(t) = e^{-\frac{i}{\hbar}t\tilde{H}} \rho(0) \left(e^{-\frac{i}{\hbar}t\tilde{H}}\right)^*$$

but $(\cdot)^*$ is now no longer equivalent to $(\cdot)^{-1}$

Remarks.

1. In general, the effective dynamics will not be Markovian, but there are interesting systems for which this has been proven (this is very hard) [Pulé, Davies]

2. Lindblad's result gives the most general form; can now consider examples.

Example: "spontaneous decay by emission"

We reduce an atom to a two-level system, which then has Hilbert space $\mathbb{C}^2$.
We assume the basis chosen such that the Hamiltonian is diagonal, and set the zero of energy such that

$$H = -\frac{\hbar\omega}{2}\,\sigma_3$$

Then $|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ is the groundstate, w. energy $-\frac{\hbar\omega}{2} = E_0$
and $|1\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ is an excited state, — " — $\frac{\hbar\omega}{2} = E_1$

A photon emitted in the transition from $|1\rangle$ to $|0\rangle$ will have energy

$$E_1 - E_0 = \hbar\omega.$$

The operator that sends $|1\rangle$ to $|0\rangle$ is $|0\rangle\langle 1|$,
which is $\sigma_+ = \frac{1}{2}(\sigma_1 + i\sigma_2) = \begin{pmatrix}0 & 1\\0 & 0\end{pmatrix}$

Define
$$R_1 := \sqrt{\Gamma}\,\sigma_+$$
where $\Gamma = \frac{1}{\tau} > 0$. Then $R_1^* = \sqrt{\Gamma}\,\sigma_-$.

(46)

$$\dot\rho(t) = -\frac{i}{\hbar}[H,\rho] - \frac{\Gamma}{2}(\sigma_-\sigma_+\rho + \rho\sigma_-\sigma_+) + \Gamma\sigma_+\rho\sigma_-$$

Write $\rho = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix}$. Then

$$\frac{d}{dt}\begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} = i\omega \begin{pmatrix} 0 & \rho_{01} \\ -\rho_{10} & 0 \end{pmatrix} + \Gamma \begin{pmatrix} \rho_{11} & -\frac{1}{2}\rho_{01} \\ -\frac{1}{2}\rho_{10} & -\rho_{11} \end{pmatrix}$$

$$\dot\rho_{11} = -\Gamma\rho_{11} \quad \Rightarrow \quad \rho_{11} = \rho_{11}(0)e^{-\Gamma t}$$

$$\dot\rho_{00} = \Gamma\rho_{11} \quad \Rightarrow \quad \rho_{00} = \rho_{00}(0) + \rho_{11}(0)(1-e^{-\Gamma t})$$

$$\frac{d}{dt}\begin{pmatrix} 0 & \rho_{01} \\ \rho_{10} & 0 \end{pmatrix} = \begin{pmatrix} 0 & (i\omega - \frac{\Gamma}{2})\rho_{01} \\ (-i\omega-\frac{\Gamma}{2})\rho_{10} & 0 \end{pmatrix}$$

$$\rho_{01} = e^{it\omega} e^{-t\frac{\Gamma}{2}} \rho_{01}(0)$$

$$\rho_{10} = e^{-it\omega} e^{-t\frac{\Gamma}{2}} \rho_{10}(0)$$

decay of excited state on time scale $\frac{1}{\Gamma}$.

Decoherence with timescale $\frac{2}{\Gamma}$, twice as long.

A remark on Schrödinger's cat.

$$\psi = \frac{1}{\sqrt{2}} \left(|\text{dead}\rangle \otimes |0\rangle + |\text{alive}\rangle \otimes |1\rangle \right)$$

$$\rho_\psi = |\psi\rangle\langle\psi| = \frac{1}{2} \Big[|\text{alive},1\rangle\langle\text{alive},1| + |\text{dead},0\rangle\langle\text{dead},0|$$
$$+ |\text{alive},1\rangle\langle\text{dead},0| + |\text{dead},0\rangle\langle\text{alive},1| \Big]$$

The whole dilemma gets coupled to photons. Those little guys are like an environment of harmonic oscillators.

$\rightarrow$ decoherence, off-diagonals vanish fast

$\Rightarrow \rho_\psi \rightsquigarrow$ diagonal state.

[often-studied model: spin-boson model

$$H = \Delta\sigma_x + \sum_i a_i^\dagger a_i \hbar\omega_i + \sigma_x \otimes \sum_i (a_i + a_i^\dagger) f_i \quad]$$

In an ironic view, it is not the little atom that has the cat on its conscience, but all the photons that watched and went away without doing anything.

More generally

$$\rho = \frac{1}{2}(\mathbb{1} + \not{r}) \qquad \not{r} = r \cdot \sigma \qquad \text{so } \dot\rho = \frac{1}{2}\dot{\not{r}}$$

$$H = \not{h} \quad , \quad R_\ell = \alpha_\ell \sigma_\ell \quad , \alpha_\ell \in \mathbb{C}.$$

$$\sum_{\ell=1}^{3} R_\ell^* R_\ell = |\alpha|^2 \cdot \mathbb{1} \quad (= \not{\alpha}^2) \qquad |\alpha|^2 = |\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2$$

Lindblad

$$\dot\rho = -i[H,\rho] - \underbrace{\frac{1}{2}\{|\alpha|^2 \mathbb{1}, \rho\}}_{|\alpha|^2 \cdot \rho} + \sum_{\ell=1}^{3} \sigma_\ell \rho \sigma_\ell \cdot |\alpha_\ell|^2$$

$$-i[\not{h}, \not{r}] = (h \times r) \cdot \sigma$$

$$\dot\rho = \frac{1}{2}(h \times r) - \frac{|\alpha|^2}{2}(\mathbb{1} + \not{r}) + \frac{|\alpha|^2}{2}\mathbb{1} + \frac{1}{2}\left(|\alpha|^2 \not{r} - 2\sum_j |\alpha_j|^2 r_j \sigma_j\right)$$

$$\boxed{\dot r = h \times r - |\alpha_1|^2 e_1 \cdot r - |\alpha_2|^2 e_2 \cdot r - |\alpha_3|^2 e_3 \cdot r}$$

Bloch equations.

$$\sum_\ell |\alpha_\ell|^2 \sigma_\ell \not{r} \sigma_\ell = \sum_{\ell j} |\alpha_\ell|^2 r_j \sigma_j (-1)^{\delta_{\ell j}} = \sum_j r_j \sigma_j \left(|\alpha|^2 - 2|\alpha_j|^2\right)$$

$$= |\alpha|^2 \not{r} - 2\sum_j |\alpha_j|^2 r_j \sigma_j$$