FLUCTUATION-DISSIPATION RELATIONS

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1. LINEAR RESPONSE THEORY.

1.1. Linear response and susceptibilities.

General idea:

$$\text{Perturbation} \rightarrow \boxed{\text{System}} \rightarrow \text{Response}$$

The unperturbed system is in a reference state (equilibrium or stationary). A parameter λ takes on the value λ_0 in the reference state.

The perturbation consists in a small modification of the parameter:

$$\lambda(t) = \lambda_0 + \delta\lambda(t)$$

The response is the behavior of any observable B:

$$\langle B(t)\rangle = \langle B\rangle_{ref} + \langle \delta B(t)\rangle$$

time independent

The response $\langle \delta B(t)\rangle$ is a functional of the perturbation $\delta\lambda(t)$. Up to linear terms:

$$\langle \delta B(t)\rangle \simeq \int_{-\infty}^{\infty} dt'\; K(t,t')\,\delta\lambda(t')$$

Taylor expansion

For discrete time:

$$\langle \delta B(t_n)\rangle \simeq \sum_k K_{nk}\,\delta\lambda(t_k)$$

The kernel $K(t,t') = \left.\frac{\delta\langle B(t)\rangle}{\delta\lambda(t')}\right|_{\lambda(t')=\lambda_0}$ has two important properties:

i) Stationarity: $K(t,t') = K(t+\tau, t'+\tau)$

ii) Causality: $K(t,t')=0$ if $t'>t$

Then, we can write:

$$\boxed{\langle\delta B(t)\rangle = \int_{-\infty}^{t} dt' \, \underbrace{\phi_{\lambda B}(t-t')}_{\text{Response function}} \, \delta\lambda(t')} \qquad (1)$$

For discrete time:

$$\boxed{\langle\delta B(t_n)\rangle = \sum_{k=-\infty}^{n} \phi_{\lambda B}(t_n - t_k)\, \delta\lambda(t_k)}$$

These are the main expression of linear response theory. Fluctuation-dissipation theorems provide expressions for the response function $\phi_{\lambda B}(t-t')$.

However, from (1) we can extract important consequences.

Consider the perturbation:

$$\delta\lambda(t) = F e^{-i\omega t}$$

one can add a slow decay at $t\to-\infty$

Physical perturbations are real, but it is useful to consider complex perturbations as well. Due to the linear dependence of the response, we can obtain the response to, e.g., $\delta\lambda(t)\propto\cos\omega t$ by summing the response to $e^{i\omega t}$ and $e^{-i\omega t}$.

Inserting the perturbation into (1):

$$\langle \delta B(t) \rangle = \int_{-\infty}^{t} dt' \, \phi_{\lambda B}(t-t') \, F \, e^{-i\omega t'} = F e^{-i\omega t} \int_{-\infty}^{t} dt' \, \phi_{\lambda B}(t-t') e^{i\omega(t-t')}$$

$$\overset{\tau=t-t'}{=} F e^{-i\omega t} \int_0^{\infty} d\tau \, \phi_{\lambda B}(\tau) \, e^{i\omega\tau} = \chi_{\lambda B}(\omega) \, \delta\lambda(t)$$

where: $$\chi_{\lambda B}(\omega) = \int_0^{\infty} d\tau \, \phi_{\lambda B}(\tau) \, e^{i\omega\tau}$$

is the generalized susceptibility or susceptibility for an AC perturbation.

Properties of $\chi_{\lambda B}(\omega)$:

i) Since $\phi_{\lambda B}(\tau) \in \mathbb{R}$, we have:

$$\chi_{\lambda B}(-\omega) = \chi^{*}_{\lambda B}(\omega)$$

Consider now a constant perturbation switched on at time $t=0$:

$$\delta\lambda(t) = F \, \Theta(t) = \begin{cases} F & \text{if } t \geq 0 \\ 0 & \text{if } t < 0 \end{cases}$$

Inserting this perturbation in (1):

$$\langle \delta B(t) \rangle = \int_{-\infty}^{t} dt' \, \phi_{\lambda B}(t-t') \, F \, \Theta(t') = F \int_0^{t} dt' \, \phi_{\lambda B}(t-t')$$

$$\overset{\tau=t-t'}{=} F \int_0^{t} d\tau \, \phi_{\lambda B}(\tau) \Rightarrow \frac{d}{dt} \langle \delta B(t) \rangle = F \, \underbrace{\phi_{\lambda B}(t)}_{\leftarrow \text{Relaxation}}$$

and: $$\lim_{t\to\infty} \langle \delta B(t) \rangle = \underbrace{\chi_{\lambda B}(\omega=0)}_{\text{(static) susceptibility}} F = \underbrace{\chi_{\lambda B}}_{\text{(static) susceptibility}} F$$

1.2 Hamiltonian systems close to equilibrium

A classical system with Hamiltonian H_0 in equilibrium at temperature T is perturbed by a constant field F. The perturbed Hamiltonian is:

$$H(x) = H_0(x) - A(x)F$$

microstate

where $A(x)$ is the magnitude affected by the field (conjugated): center of charge, magnetization, ...

If $B(x)$ is an arbitrary observable:

$$\langle B \rangle_{ref} = \langle B \rangle_0 = \int dx\, B(x) \frac{e^{-\beta H_0(x)}}{Z_0} \quad \text{with } Z_0 \equiv \int dx\, e^{-\beta H_0(x)}$$

partition function

When the perturbation is switched on, the system relaxes to:

$$\frac{e^{-\beta H(x)}}{Z_F} \quad \text{with } Z_F \equiv \int dx\, e^{-\beta(H_0 - AF)}$$

Therefore:

$$\lim_{t\to\infty} \langle B(t) \rangle = \int dx\, B(x) \frac{e^{-\beta(H_0 - AF)}}{Z_F} \simeq$$

$$\simeq \int dx\, B(x) \frac{e^{-\beta H_0}}{Z_0} \frac{1 + \beta AF}{1 + \left.\frac{\partial \ln Z_F}{\partial F}\right|_{F=0} F}$$

$$\simeq \int dx\, B(x) \frac{e^{-\beta H_0}}{Z_0} \left[1 + \beta AF - \left.\frac{\partial \ln Z_F}{\partial F}\right|_{F=0} F \right]$$

$$= \langle B \rangle_0 + \beta F \left[\langle BA \rangle_0 - \langle B \rangle_0 \frac{1}{\beta} \left.\frac{\partial \ln Z_F}{\partial F}\right|_{F=0} \right]$$

Then, the susceptibility reads:

$$\chi_{AB} = \beta \left[\langle BA \rangle_0 - \langle B \rangle_0 \frac{1}{\beta} \frac{\partial \ln Z_F}{\partial F}\bigg|_{F=0} \right]$$

notation change

We can go further by expressing the derivative of the partition function as:

$$\frac{1}{\beta} \frac{\partial \ln Z_F}{\partial F}\bigg|_{F=0} = \frac{1}{\beta} \frac{1}{Z_0} \int dx \frac{\partial}{\partial F}\bigg|_{F=0} e^{-\beta (H_0 - AF)} =$$

$$= \frac{1}{Z_0} \int dx\, A(x)\, e^{-\beta H_0(x)} = \langle A \rangle_0$$

Recalling that the free energy is:

$$\mathcal{F}(F) = -kT \ln Z_F = -\frac{1}{\beta} \ln Z_F$$

this is nothing but the well-known expression for thermodynamic conjugated variables:

$$\langle A \rangle_0 = -\frac{\partial \mathcal{F}(F)}{\partial F}\bigg|_{F=0}$$

Finally, the susceptibility is equal to a correlation at equilibrium:

$$\chi_{AB} = \beta \left[\langle AB \rangle_0 - \langle A \rangle_0 \langle B \rangle_0 \right]$$

This is the simplest form of a FDT.

Why dissipation? The perturbation changes the energy of the system as:

$$W = \langle H_0 - AF \rangle_0 - \langle H_0 \rangle_0 = -\langle A \rangle_0 F$$

which is the work needed to switch on the perturbation.

After the relaxation, the energy is:

$$\langle H_0 - AF \rangle_F = \langle H_0 \rangle_F - \langle A \rangle_F F \simeq$$

$$\simeq \langle H_0 \rangle_0 + \chi_{AH_0} F - \langle A \rangle_0 F$$

Then, the system dissipates a heat:

$$\underbrace{Q_{diss}}_{\text{Dissipation}} \simeq -\chi_{AH_0} F = -\beta \underbrace{\left[\langle AH_0 \rangle_0 - \langle A \rangle_0 \langle H_0 \rangle_0 \right]}_{\text{Fluctuation}} F$$

Let us consider now a periodic perturbation:

$$F(t) = F \cos \omega t = \frac{F}{2} \left[e^{i\omega t} + e^{-i\omega t} \right]$$

Using the generalized susceptibility:

$$\langle \delta B(t) \rangle = \frac{F}{2} \left[\chi_{AB}(-\omega) e^{i\omega t} + \chi_{AB}(\omega) e^{-i\omega t} \right]$$

$$= \frac{F}{2} \left[\chi^*_{AB}(\omega) e^{i\omega t} + \chi_{AB}(\omega) e^{-i\omega t} \right]$$

$$= F \, \mathrm{Re} \left[\chi_{AB}(\omega) e^{-i\omega t} \right]$$

If $\chi_{AB}(\omega) = \chi'_{AB}(\omega) + i\,\chi''_{AB}(\omega)$

not a derivative. Just a notation for the real and imaginary parts of the generalized susceptibility

we have:

$$\langle \delta B(t)\rangle = F\left[\chi'_{AB}(\omega)\cos\omega t + \chi''_{AB}(\omega)\sin\omega t\right]$$

Consider the work done on the system by the perturbation per unit time or power:

$$\mathcal{P}(t) = \dot{W}(t) = \left\langle \frac{\partial H(t)}{\partial t}\right\rangle = -\langle A(t)\rangle \dot{F}(t) = \langle A(t)\rangle F\omega \sin\omega t$$

Up to 2^{nd} order on F:

$$\mathcal{P}(t) = \langle A\rangle_0 F\omega\sin\omega t + F^2\omega\left[\chi'_{AA}(\omega)\cos\omega t\sin\omega t + \chi''_{AA}(\omega)\sin^2\omega t\right]$$

Averaging over a period $2\pi/\omega$:

$$\mathcal{P}_{av} \equiv \frac{\omega}{2\pi}\int_0^{2\pi/\omega}\mathcal{P}(t)\,dt = \frac{\omega}{2\pi}F^2\omega\,\chi''_{AA}(\omega)\int_0^{2\pi/\omega} dt\,\sin^2\omega t$$

$$\Rightarrow \quad \mathcal{P}_{av} = \frac{\omega F^2}{2}\chi''_{AA}(\omega)$$

The imaginary part of the generalized susceptibility tells us how much energy the system absorbs from the perturbation. Consequently, the imaginary part $\chi''_{AA}(\omega)$ of the susceptibility is called absorptive part or absorptive susceptibility.

The generalized susceptibility is crucial to analyze wave propagation in media (Jackson).

1.3. Fourier transforms and Green functions.

The relationship between the response function and the generalized susceptibility can be interpreted as a Fourier transform.

We adopt the following convention for the Fourier transform:

$$\tilde{f}(\omega) = \int_{-\infty}^{\infty} dt \; e^{i\omega t} f(t)$$

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \; e^{-i\omega t} \tilde{f}(\omega)$$

The susceptibility reads:

$$\chi_{\lambda B}(\omega) = \int_{0}^{\infty} dt \; e^{i\omega t} \phi_{\lambda B}(t) = \int_{-\infty}^{\infty} dt \; e^{i\omega t} \phi_{\lambda B}(t)\, \Theta(t)$$

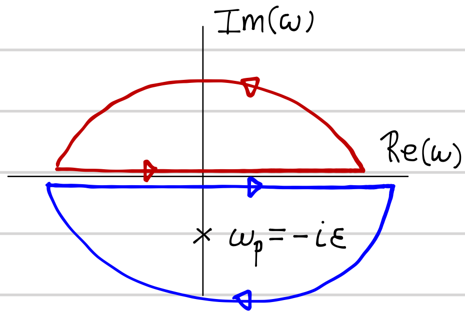
← step function

We define: $G_{\lambda B}(t) = \phi_{\lambda B}(t)\,\Theta(t)$ Green function.

Then $\chi_{\lambda B}(\omega) = \tilde{G}_{\lambda B}(\omega) \Rightarrow \langle \delta B(t) \rangle = \int_{-\infty}^{\infty} dt \; G_{\lambda B}(t-t')\, \delta\lambda(t')$

The step function $\Theta(t)$ does not have a well defined Fourier transform, but it can be expressed as:

$$\Theta(t) = \lim_{\varepsilon \to 0^+} -\frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega \; \frac{e^{-i\omega t}}{\omega + i\varepsilon}$$



Considering complex frequencies, the integrand has a simple pole at $\omega = -i\varepsilon$. For $t<0$, we use the red contour:

$$\oint d\omega \frac{e^{-i\omega t}}{\omega + i\varepsilon} = \int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega + i\varepsilon} + \int_{\frown} d\omega \frac{e^{-i\omega t}}{\omega + i\varepsilon}$$

The integral along the arc vanishes because:

$$e^{-i\omega t} = e^{-i\,\mathrm{Re}(\omega) t}\, e^{\mathrm{Im}(\omega) t} \to 0 \quad \text{for } \mathrm{Im}(\omega) \to +\infty \text{ and } t<0$$

Since there are no poles inside the contour:

$$\int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega + i\varepsilon} = 0 \quad \text{if } t<0$$

For $t>0$, we have to use the lower (blue) contour. The integral along the arc tends to zero

$$e^{-i\omega t} = e^{-i\,\mathrm{Re}(\omega) t}\, e^{\mathrm{Im}(\omega) t} \to 0 \quad \text{for } \mathrm{Im}(\omega) \to -\infty \text{ and } t<0$$

Then:

$$\oint d\omega \frac{e^{-i\omega t}}{\omega + i\varepsilon} = \int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega + i\varepsilon} = \underbrace{-}_{\text{clockwise contour}} 2\pi i \underbrace{e^{\varepsilon t}}_{\text{residue}} \xrightarrow[\varepsilon \to 0^+]{} -2\pi i$$

Interpreting: $\tilde{\Theta}(\omega) = \lim_{\varepsilon \to 0^+} \frac{i}{\omega + i\varepsilon}$ as the Fourier transform of the step function, the susceptibility can be written as a convolution in the frequency domain:

$$\chi_{\lambda B}(\omega) = \int_{-\infty}^{\infty} d\omega' \tilde{\phi}_{\lambda B}(\omega') \tilde{\Theta}(\omega - \omega') = \lim_{\varepsilon \to 0^+} \int_{-\infty}^{\infty} d\omega' \frac{i \tilde{\Phi}_{\lambda B}(\omega')}{\omega - \omega' + i\varepsilon}$$

1.4. The response of a classical harmonic oscillator

Consider a driven damped harmonic oscillator:

$$m\ddot{x}(t) = -m\omega_0^2 x(t) - \gamma\dot{x}(t) + F_{ext}(t)$$

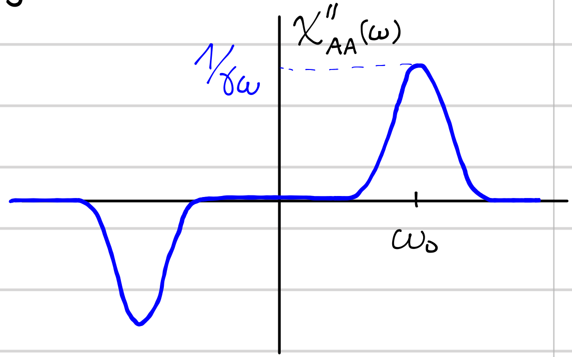
The Fourier transform: $\tilde{x}(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} x(t)$ verifies:

$$\left[-m\omega^2 + m\omega_0^2 - i\gamma\omega\right]\tilde{x}(\omega) = \tilde{F}_{ext}(\omega)$$

$$\Longrightarrow \quad \tilde{x}(\omega) = \frac{\tilde{F}_{ext}(\omega)}{m(\omega_0^2-\omega^2) - i\gamma\omega}$$

Then, the Green function/susceptibility reads:

$$\chi_{Fx}(\omega) = \tilde{G}_{Fx}(\omega) = \frac{1}{m(\omega_0^2-\omega^2) - i\gamma\omega}$$



$$\Rightarrow \chi''_{Fx}(\omega) = \frac{\gamma\omega}{m^2(\omega_0^2-\omega^2)^2 + \gamma^2\omega^2}$$

The poles are the roots of $\omega^2 + \frac{i\gamma}{m}\omega - \omega_0^2 = 0$

$$\omega_\pm = -\frac{i\gamma}{2m} \pm \omega_u \qquad \text{with } \omega_u \equiv \sqrt{\omega_0^2 - \frac{\gamma^2}{4m^2}}$$

The two poles are in the lower half of the complex plane since $\mathrm{Im}\,\omega_u < \frac{\gamma}{2m}$.

The Green function in the time domain reads:

$$G_{Fx}(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t} \frac{-1}{m(\omega-\omega_+)(\omega-\omega_-)}$$

exercise

$$= \underbrace{\frac{1}{m\omega_u} e^{-\gamma t/2} \sin \omega_u t}_{\text{response function } \phi_{Fx}(t)}\ \theta(t)$$

1.5. Kramers-Kronig relations

Recall the definition of the generalized susceptibility:

$$\chi_{\lambda B}(\omega) = \int_0^\infty d\tau \, e^{i\omega\tau} \, \phi_{\lambda B}(\tau)$$

← we will omit these subscripts in this section.

If $\omega = \omega_1 + i\omega_2$:

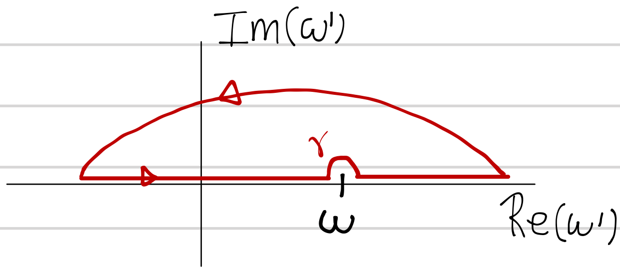
$$e^{i\omega\tau} = e^{i\omega_1\tau} \, e^{-\omega_2\tau}$$

↳ decreasing function if $\omega_2 > 0$.

We see that, if $\chi(\omega)$ exists for $\omega \in \mathbb{R}$, i.e., if the integral converges for $\omega \in \mathbb{R}$, the it converges for ω in the upper half of the complex plane.

Therefore $\chi(\omega)$ is an analytical function in the upper half plane $\Rightarrow$ all the poles of $\chi(\omega)$ are in the lower half.

Consider the following integral:



$$\oint \frac{\chi(\omega')}{\omega' - \omega} d\omega' = 0$$ ← no poles

and: $0 = \oint \frac{\chi(\omega')}{\omega'-\omega} d\omega' =$

$$= \int_{-\infty}^{\omega-\varepsilon} \frac{\chi(\omega')}{\omega'-\omega} d\omega' + \int_{\omega+\varepsilon}^{\infty} \frac{\chi(\omega')}{\omega'-\omega} d\omega' + \int_\gamma \frac{\chi(\omega')}{\omega'-\omega} d\omega' =$$

$$= \int_{-\infty}^{\omega-\varepsilon} \frac{\chi(\omega')}{\omega'-\omega} d\omega' + \int_{\omega+\varepsilon}^{\infty} \frac{\chi(\omega')}{\omega'-\omega} d\omega' + i \int_\pi^0 d\theta \, \frac{\cancel{\varepsilon e^{i\theta}} \, \chi(\omega + \varepsilon e^{i\theta})}{\cancel{\varepsilon e^{i\theta}}}$$

↑
$\omega' = \omega + \varepsilon e^{i\theta}$
$d\omega' = i\varepsilon e^{i\theta} d\theta$

In the limit $\varepsilon \to 0$:

$$P \int_{-\infty}^{\infty} \frac{\chi(\omega')}{\omega' - \omega} d\omega' = i\pi \chi(\omega)$$

where P is the Cauchy principal value.

Real part $\to$ $$\chi'(\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} d\omega' \frac{\chi''(\omega')}{\omega' - \omega}$$

Imaginary part $\to$ $$\chi''(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} d\omega' \frac{\chi'(\omega')}{\omega' - \omega}$$

Kramers-Kronig or dispersion relations.

It allows us to obtain the dispersive part $\chi'(\omega)$ from the absorptive part $\chi''(\omega)$.

2. MARKOVIAN DYNAMICS.

2.1. Classical Markovian chains

A Markovian chain is a system with a discrete number of states $i = 1, 2, \ldots$ that evolves in discrete time $t_n = n\tau$, $n = 0, \pm 1, \pm 2, \ldots$

The probability distribution at time t_n is a vector:

$$\vec{p}(t_n) = \left(p_1(t_n), p_2(t_n), \ldots \right)$$

where $p_i(t_n)$ is the probability to find the system in state i at time t_n.

Moreover, the conditional probabilities verify:

$$p(i, t_n | j_1, t_{n-1}; j_2, t_{n-2}; \ldots) = p(i, t_n | j_1, t_{n-1}).$$

← Markovianity

This means that the dynamics of the whole system is determined by the jump or transition probabilities:

$$P_{ij}^{(n)} = p(i, t_n | j, t_{n-1})$$

which verifies: $\sum_i P_{ij}^{(n)} = 1$ and $0 \leq P_{ij}^{(n)} \leq 1$ (stochastic matrix)

The evolution of the probability distribution is given by:

$$p_i(t_n) = \sum_j P_{ij}^{(n)} p_j(t_{n-1}) \Rightarrow \vec{p}(t_n) = \mathbb{P}^{(n)} \vec{p}(t_{n-1})$$

Therefore: $\vec{p}(t_n) = \mathbb{P}^{(n)}\,\mathbb{P}^{(n-1)} \cdots \mathbb{P}^{(1)}\,\vec{p}(0)$

For a stationary Markov chain ($\mathbb{P}^{(n)} = \mathbb{P}$), there exists at least a stationary solution $\vec{\pi}$, such that:

$$\mathbb{P}\,\vec{\pi} = \vec{\pi}$$

If the stationary distribution is unique, one can prove:

$$\vec{p}(t_n) \xrightarrow[n\to\infty]{} \vec{\pi} \qquad \forall \text{ initial condition } \vec{p}(0)$$

Time correlations. Since the process is Markovian the conditional probability is:

$$p(i, t_n | j, 0) = (\mathbb{P}^n)_{ij} \quad \leftarrow \text{Evolution with } p_i(0) = \delta_{0,i}$$

and the joint distribution in the stationary regime is:

$$\pi(i, t_n; j, 0) = (\mathbb{P}^n)_{ij}\,\pi_j$$

Then, the two time average is:

$$\langle B(t_n) A(0)\rangle_{st} = \sum_{ij} B_i A_j\, \pi(i, t_n; j, 0) =$$

$$= \sum_{i,j} B_i A_j (\mathbb{P}^n)_{ij}\, \pi_j$$

whereas $\langle B\rangle_{st} = \sum_i B_i \pi_i$

From this expressions one can obtain correlations in the stationary regime:

$$\langle B(t_n) A(0)\rangle_{st} - \langle B\rangle_{st}\langle A\rangle_{st}$$

Continuous-time limit $\tau \to 0$: $\quad \mathbb{P} \simeq \mathbb{1} + \delta \mathbb{P} \tau$

$$P_{ij} = \Gamma_{ij} \tau \quad \text{for } i \neq j \quad \big(\underbrace{\Gamma_{ij}}_{} > 0, \; [\Gamma_{ij}] = \text{time}^{-1} \big)$$

$$P_{jj} = 1 - \sum_{i \neq j} \Gamma_{ij} \tau$$

↳ transition rates $\Gamma_{ii} = 0$

The evolution equation reads:

$$p_i(t+\tau) = \sum_j P_{ij}\, p_j(t) = \Big(1 - \sum_{j \neq i} \Gamma_{ji} \tau\Big) p_i(t) + \sum_{j \neq i} \Gamma_{ij} \tau\, p_j(t)$$

$$\Rightarrow \frac{d p_i(t)}{dt} = \boxed{\sum_j \big[\underbrace{\Gamma_{ij}\, p_j(t)}_{\text{incoming flow}} - \underbrace{\Gamma_{ji}\, p_i(t)}_{\text{outgoing flow}} \big]}$$

Master equation

incoming flow ↳ outgoing flow

Stationary distribution π_i: $\quad \sum_j \left[\Gamma_{ij} \pi_j - \Gamma_{ji} \pi_i \right] = 0 \quad \forall i$

If E_i is the energy of state i and

$$\frac{\Gamma_{ji}}{\Gamma_{ij}} = e^{-\beta (E_j - E_i)}$$

Detailed balance

Then the stationary distribution is the equilibrium state:

$$\pi_i = \frac{e^{-\beta E_i}}{Z} \quad \text{with} \quad Z = \sum_i e^{-\beta E_i}$$

2.2. Quantum maps.

The quantum analog of the transition matrix $\mathbb{P}$ are the so called completely positive trace preserving (CPTP) maps ξ acting on the density matrix ρ of a quantum system.

ξ transforms operators in a Hilbert space and has the following properties:

i) Trace preserving: $\mathrm{Tr}[\xi(\rho)] = \mathrm{Tr}[\rho]$

ii) Positiveness:

$$\rho \text{ positive} \Rightarrow \xi(\rho) \text{ positive.}$$

iii) Complete positiveness:

for any ancilla (auxilary sistem) of arbitrary finite dimension, the map

$$\mathbb{1} \otimes \xi \quad \text{is positive}$$

Every map ξ can be seen as the result of a unitary evolution of the system coupled to some environment E:

$$\xi(\rho) = \mathrm{Tr}_E (\mathcal{U} \, \sigma \otimes \rho \, \mathcal{U}^+) \qquad \text{(Dilation)}$$

environment state

system state

Kraus decomposition: for any CPTP map ξ there exists a set of operators K_m, such that:

$$\xi(\rho) = \sum_m K_m \rho K_m^+ \qquad \text{with} \quad \sum_m K_m^+ K_m = \mathbb{1}$$

The decomposition is not unique. In the case of a dilation where the state of the environment is:

$$\sigma = \sum_n p_n |n\rangle\langle n|$$

there is a Kraus decomposition with the family of operators:

$$K_{mn} = \sqrt{p_n}\, \langle m| U |n\rangle$$

This is an operator in the Hilbert space of the system.

The map ξ can be seen as a mixture of operations

$$\xi_m(\rho) = \frac{K_m \rho K_m^+}{Tr[K_m \rho K_m^+]} \quad \text{occurring with probability } Tr[K_m \rho K_m^+]$$

These operations act on pure states as:

$$|\psi\rangle \longrightarrow \xi_m(|\psi\rangle\langle\psi|) = \frac{K_m|\psi\rangle}{\| K_m|\psi\rangle\|} \quad \text{with probability } p_m(|\psi\rangle) = \| K_m|\psi\rangle\|^2$$

Special cases of CPTP maps are:

- Mixtures of unitary transformations: $K_m = \sqrt{p_m}\, U_m$
- Proyective measurements or dephasing: $K_m = |m\rangle\langle m|$ (projector).
- Shuffling an orthogonal basis $\{|i\rangle\}$: $K_{ji} = \sqrt{p_{ji}}\, |j\rangle\langle i|$

It maps $|i\rangle$ onto $|j\rangle$ with probability p_{ji} and kills the off diagonal terms.

A quantum Markov process $\rho(t_n)$ is the concatenation of CPTP maps:

$$\rho(t_n) = \xi^{(n)}(\rho(t_{n-1})) \Longrightarrow \rho_n = \xi^{(n)} \circ \xi^{(n-1)} \circ \dots \circ \xi^{(1)}(\rho(0))$$

If the process is stationary $\xi^{(n)} = \xi$ and: $\rho(t_n) = \xi^n(\rho(0))$

The stationary state verifies: $\xi(\pi) = \pi$

The stochastic evolution of a pure state is:

$$K_{m_n} K_{m_{n-1}} \cdots K_{m_1} |\psi\rangle = \underbrace{K_{\{m_i\}}}_{} |\psi\rangle$$

↳ Krauss operators of ξ^n

The sequence $\{m_i\}_{i=1}^n$ is a quantum trajectory that occurs with probability:

$$P_{\{m_i\}}(|\psi\rangle) = \| K_{\{m_i\}} |\psi\rangle \|$$

Heisenberg picture: we define the map ξ^+ as:

$$\mathrm{Tr}[B\,\xi(\rho)] = \mathrm{Tr}[\xi^+(B)\,\rho] \quad \forall B, \rho$$

Since $\mathrm{Tr}[B\,\xi(\rho)] = \sum_m \mathrm{Tr}[B K_m \rho K_m^+] = \sum_m \mathrm{Tr}[K_m^+ B K_m \rho]$

we have: $\xi^+(B) = \sum_m K_m^+ B K_m$ ← NOT trace preserving

For a Markov process:

$$\mathrm{Tr}[B\,\rho(t_n)] = \mathrm{Tr}[B(t_n)\,\rho]$$

with $\underbrace{\rho(t_n) = \xi^n(\rho)}_{\text{Schrödinger picture}}$ and $\underbrace{B(t_n) = \xi^{n+}(\rho)}_{\text{Heisenberg picture}}$

A standard definition of time correlation reads:

$$\langle A(0)B(t)\rangle = \mathrm{Tr}[A B(t) \rho]$$

$$\neq \langle B(t)A(0)\rangle = \mathrm{Tr}[B(t) A \rho]$$

Another possible definition is based on quantum measurements. Let:

projectors

$$A = \sum_i a_i |a_i\rangle\langle a_i| = \sum_i a_i \Pi_i^A \qquad B = \sum_j b_j |b_j\rangle\langle b_j| = \sum b_j \Pi_j^B$$

If we measure A on ρ, we get a_i with probability

$$p(a_i, 0) = \mathrm{Tr}[|a_i\rangle\langle a_i|\rho] = \mathrm{Tr}[\Pi_i^A \rho]$$

and the system colapses to $\rho' = |a_i\rangle\langle a_i| = \Pi_i^A$. If we measure B at time t_n, we get b_j with probability:

$$p(b_j, t_n | a_i, 0) = \mathrm{Tr}[\Pi_j^B \xi^n(\Pi_i^A)]$$

The joint probability reads:

$$p(b_j, t_n; a_i, 0) = \mathrm{Tr}[\Pi_i^A \rho] \sum_{\{m\}} \mathrm{Tr}[\Pi_j^B K_{\{m\}} \Pi_i^A K_{\{m\}}^+]$$

We can use it to calculate the two-time average:

$$\langle A(0) B(t_n)\rangle_{DM} = \sum_{i,j} a_i b_j \mathrm{Tr}[\Pi_i^A \rho] \sum_{\{m\}} \mathrm{Tr}[\Pi_j^B K_{\{m\}} \Pi_i^A K_{\{m\}}^+]$$

$$= \sum_i \sum_{\{m\}} a_i \mathrm{Tr}[\Pi_i^A \rho] \mathrm{Tr}[B K_{\{m\}} \Pi_i^A K_{\{m\}}^+]$$

$$= \sum_i a_i \mathrm{Tr}[\Pi_i^A \rho] \mathrm{Tr}[B(t_n) \Pi_i^A]$$

$$\Rightarrow \langle A(0)B(t)\rangle_{DM} = \langle B(t)A(0)\rangle_{DM} = \sum_i a_i \mathrm{Tr}[\rho \Pi_i^A B(t) \Pi_i^A]$$

It coincides with the standard correlation only if $[A, B(t)] = 0$ or $[A, \rho] = 0$.

Continuous limit $(\tau \to 0)$:

$$K_0 = \mathbb{1} - \tau(A + iH) \qquad (A, B \text{ self-adjoints})$$

$$K_m = \sqrt{\tau}\, L_m$$

Since: $[\mathbb{1} - \tau(A - iH)][\mathbb{1} - \tau(A + iH)] + \tau \sum_m L_m^\dagger L_m = \mathbb{1}$

$$\Rightarrow 2A = \sum_m L_m^\dagger L_m.$$

the Kraus operators are:

$$K_0 = \mathbb{1} - \tau\left[iH + \frac{1}{2}\sum_m L_m^\dagger L_m\right]$$

$$K_m = \sqrt{\tau}\, L_m$$

and the evolution equation reads:

$$\rho(t+\tau) = K_0 \rho(t) K_0^\dagger + \sum_m K_m \rho(t) K_m^\dagger$$

$$\Rightarrow \frac{d\rho(t)}{dt} = -i[H, \rho] + \frac{1}{2}\sum_m [2L_m \rho L_m^\dagger - L_m^\dagger L_m \rho - \rho L_m^\dagger L_m]$$

or $\boxed{\dfrac{d\rho(t)}{dt} = -i[H, \rho] + \sum_m \left[L_m \rho L_m^\dagger - \frac{1}{2}\{L_m^\dagger L_m, \rho\}\right]}$ Lindblad equation

anti-conmutator.

3. FLUCTUATION-DISSIPATION THEOREMS

In this lecture we will apply linear response theory to generic Markovian systems in which some parameter λ is perturbed as $\lambda = \lambda_0 + \delta\lambda(t)$.

3.1. Generalized classical FDT.

Consider a Markov chain whose transition probabilities depend on some parameter λ: $\mathbb{P}(\lambda)$.

The corresponding stationary distribution verifies:

$$\mathbb{P}(\lambda)\vec{\pi}(\lambda) = \vec{\pi}(\lambda)$$

For a small constant perturbation $\lambda = \lambda_0 + \delta\lambda$ we can expand:

$$\mathbb{P}(\lambda) \simeq \mathbb{P}_0 + \delta\lambda\,\mathbb{P}_1 \quad \text{where } \mathbb{P}_0 \equiv \mathbb{P}(\lambda_0).$$

$$\vec{\pi}(\lambda) \simeq \vec{\pi}_0 + \delta\lambda\,\vec{\pi}_1 \quad \text{with } \vec{\pi}_0 \equiv \vec{\pi}(\lambda_0) \text{ and } \vec{\pi}_1 = \left.\frac{d\vec{\pi}(\lambda)}{d\lambda}\right|_{\lambda=\lambda_0}$$

Up to first order, they verify:

$$(\mathbb{P}_0 + \delta\lambda\,\mathbb{P}_1)(\vec{\pi}_0 + \delta\lambda\,\vec{\pi}_1) = \vec{\pi}_0 + \delta\lambda\,\vec{\pi}_1 \Rightarrow \mathbb{P}_1\vec{\pi}_0 + \mathbb{P}_0\vec{\pi}_1 = \vec{\pi}_1$$

$$\Rightarrow \mathbb{P}_1\vec{\pi}_0 = (\mathbb{1} - \mathbb{P}_0)\,\vec{\pi}_1$$

We define the conjugate observable $A_\lambda = (A_{\lambda,1}, A_{\lambda,2}, \dots)$ as:

$$A_{\lambda,i} = \frac{\pi_{1,i}}{\pi_{0,i}} = \left.\frac{d\ln\pi_i(\lambda)}{d\lambda}\right|_{\lambda=\lambda_0}$$

Its average in the reference state $\vec{\pi}_0$ vanishes:

$$\langle A_\lambda\rangle_0 = \sum_i A_{\lambda,i}\,\pi_{0,i} = \sum_i \pi_{1,i} = \left.\frac{d}{d\lambda}\right|_{\lambda=\lambda_0} \overbrace{\sum_i \pi_i(\lambda)}^{=1\ \forall\lambda} = 0$$

This observable determines the static susceptibility.
For any observable $\vec{B}=(B_1, B_2, \dots)$:

$$\langle B\rangle_{\lambda_0+\delta\lambda} = \sum_i B_i\left[\pi_{0,i}+\delta\lambda\,\pi_{1,i}\right] = \langle B\rangle_0 + \delta\lambda \sum_i B_i A_{\lambda,i}\pi_{0,i}$$

$$= \langle B\rangle_0 + \delta\lambda\langle B A_\lambda\rangle_0$$

$$\Rightarrow \quad \chi_{\lambda B} = \langle A_\lambda B\rangle_0$$

which is a correlation since $\langle A_\lambda\rangle_0 = 0$

For a system in equilibrium with Hamiltonian $H_0(i) - FA_i$

$$\pi_{0,i}(F) = \frac{1}{Z_F} e^{-\beta H_0(i)+\beta F A_i}$$

and $\quad A_{F,i} = \left.\dfrac{d\ln \pi_{0,i}(F)}{dF}\right|_{F=0} = \beta A_i - \left.\dfrac{d\ln Z_F}{dF}\right|_{F=0} = \beta\left(A_i - \langle A\rangle_0\right)$

The susceptibility reads:

$$\chi_{AB} = \beta\left[\langle AB\rangle_0 - \langle A\rangle_0\langle B\rangle_0\right]$$

and coincides with the one calculated in section 1.2.

Let us focus now on a time-dependent perturbation $\lambda_n = \lambda_0 + \delta\lambda(t_n)$ $(n=1,2,\dots)$. The evolution is given by:

$$\vec{p}(t_n) = \mathbb{P}(\lambda_n)\,\mathbb{P}(\lambda_{n-1})\dots\mathbb{P}(\lambda_1)\,\vec{p}(0) =$$

$$= \left(\mathbb{P}_0 + \delta\lambda(t_n)\mathbb{P}_1\right)\dots\left(\mathbb{P}_0 + \delta\lambda(t_1)\mathbb{P}_1\right)\vec{p}(0)$$

If we keep the linear terms in the perturbation:

$$\vec{p}(t_n) \simeq \mathbb{P}_0^n\,\vec{p}(0) + \sum_{k=1}^{n} \mathbb{P}_0^{n-k}\,\mathbb{P}_1\,\mathbb{P}_0^{k-1}\,\vec{p}(0)\,\delta\lambda(t_k)$$

If the perturbation is switched on at $t=0$ and $\vec{p}(0)=\vec{\pi}_0$:

$$\vec{p}(t_n) \simeq \vec{\pi}_0 + \sum_{k=1}^{n} \mathbb{P}_0^{n-k} \mathbb{P}_1 \vec{\pi}_0 \, \delta\lambda(t_k)$$

$$= \vec{\pi}_0 + \sum_{k=1}^{n} \mathbb{P}_0^{n-k} (\mathbb{1} - \mathbb{P}_0) \vec{\pi}_1 \, \delta\lambda(t_k)$$

The average of an observable B_i is:

$$\langle B(t_n) \rangle = \sum_i p_i(t_n) B_i$$

$$= \langle B(0) \rangle_0 + \sum_{k=1}^{n} \underbrace{\sum_{i,j} B_i \left[(\mathbb{P}_0^{n-k})_{ij} - (\mathbb{P}_0^{n-k+1})_{ij} \right] \pi_{1,j}}_{\phi_{\lambda B}(t_n - t_k)} \, \delta\lambda(t_k)$$

The response function can be written as:

$$\phi_{\lambda B}(t_n) = \sum_{i,j} B_i \left[(\mathbb{P}_0^{n})_{ij} - (\mathbb{P}_0^{n+1})_{ij} \right] A_{\lambda,j} \pi_{0,j}$$

$$= -\left[\langle B(t_{n+1}) A_\lambda(0) \rangle_0 - \langle B(t_n) A_\lambda(0) \rangle_0 \right]$$

$$= -\Delta_t \langle B(t_n) A_\lambda(0) \rangle_0$$

In the continuous limit: $\boxed{\phi_{\lambda B}(t) = -\langle \dot{B}(t) A(0) \rangle_0}$

For a Hamiltonian system $H = H_0 - AF(t)$

$$A_F = \beta (A - \langle A \rangle_0)$$

and $\phi_{AB}(t) = -\beta \frac{d}{dt} [\langle B(t) A(0) \rangle_0 - \langle A \rangle_0 \langle B \rangle_0$

3.2. Generalized quantum FDT

The proof is very similar to the classical case, but we have to account for non-commutativity.

Given an operator π_λ that depends on a parameter λ, we define the symmetric logarithmic derivative SLD, Λ_λ, as:

$$2\frac{d\pi_\lambda}{d\lambda} = \Lambda_\lambda \pi_\lambda + \pi_\lambda \Lambda_\lambda$$

If $\left[\frac{d\pi_\lambda}{d\lambda}, \pi_\lambda\right] = 0$ then: $\Lambda_\lambda = \pi_\lambda^{-1}\frac{d\pi_\lambda}{d\lambda} = \frac{d}{d\lambda}\ln \pi_\lambda$.

Consider now a quantum Markov process where the corresponding CPTP map depends on a parameter λ: ξ_λ

For a fixed value of λ, the stationary state verifies:

$$\xi_\lambda(\pi(\lambda)) = \pi(\lambda)$$

For a small constant perturbation $\lambda = \lambda_0 + \delta\lambda$:

$$\xi_\lambda(\rho) = \xi_0(\rho) + \delta\lambda\, \xi_1(\rho) \quad \text{where} \quad \xi_0 = \xi_{\lambda_0}$$

$$\pi(\lambda) = \pi_0 + \delta\lambda\, \pi_1 \quad \text{with} \quad \xi_0(\pi_0) = \pi_0 \quad \text{and} \quad \pi_1 = \left.\frac{d\pi(\lambda)}{d\lambda}\right|_{\lambda=\lambda_0}$$

Up to first order:

$$\xi_\lambda(\pi_0 + \delta\lambda\pi_1) = \xi_0(\pi_0) + \delta\lambda\left[\xi_0(\pi_1) + \xi_1(\pi_0)\right] = \pi_0 + \delta\lambda\pi_1$$

$$\Rightarrow \quad \xi_0(\pi_1) + \xi_1(\pi_0) = \pi_1 \Rightarrow \xi_1(\pi_0) = \pi_1 - \xi_0(\pi_1)$$

We define the conjugated observable as the SLD:

$$\Lambda_0 \equiv \Lambda_{\lambda_0} \Rightarrow 2\pi_1 = \Lambda_0\pi_0 + \pi_0\Lambda_0$$

Its expected value vanishes:

$$\mathrm{Tr}[\pi_0 \Lambda_0] = \mathrm{Tr}[\pi_1] = \frac{d}{d\lambda}\Big|_{\lambda=\lambda_0} \mathrm{Tr}[\pi_\lambda] = 0$$

We now consider the time dependent perturbation $\lambda_n = \lambda_0 + \delta\lambda(t_n)$ $(n = 1, 2, \dots)$ and π_0 as initial condition:

$$\pi(t_n) = \xi_{\lambda_n} \circ \xi_{\lambda_{n-1}} \circ \dots \circ \xi_{\lambda_1}(\pi_0)$$

Up to linear terms:

$$\pi(t_n) = \xi_0^n(\pi_0) + \sum_{k=1}^{n} \xi_0^{n-k} \circ \xi_1 \circ \xi_0^{k-1}(\pi_0)\, \delta\lambda(t_k)$$

$$= \pi_0 + \sum_{k=1}^{n} \xi_0^{n-k} \circ \xi_1(\pi_0)\, \delta\lambda(t_k)$$

For any observable B:

$$\langle B(t_n)\rangle = \mathrm{Tr}[B\,\pi(t_n)] = \langle B\rangle_0 + \sum_{k=1}^{n} \mathrm{Tr}\left[\xi_0^{n-k} \circ \xi_1(\pi_0)\, B\right] \delta\lambda(t_k)$$

$$\Rightarrow \phi_{\lambda B}(t_n) = \mathrm{Tr}\left[\xi_0^n \circ \xi_1(\pi_0) B\right] = \mathrm{Tr}\left[\xi_0^n(\pi_1) B - \xi_0^{n+1}(\pi_1) B\right]$$

$$= \mathrm{Tr}\left[\pi_1 \left(B(t_n) - B(t_{n+1})\right)\right]$$

$$= \frac{1}{2} \mathrm{Tr}\left[(\Lambda_0 \pi_0 + \pi_0 \Lambda_0)(B(t_n) - B(t_{n+1}))\right]$$

$$\Rightarrow \boxed{\phi_{\lambda B}(t_n) = -\frac{1}{2}\Delta_t \left[\langle B(t_n)\Lambda_0\rangle_0 + \langle \Lambda_0 B(t_n)\rangle_0\right]}$$

Continuous limit: $\phi_{\lambda B}(t) = -\frac{1}{2}\frac{d}{dt}\left[\langle B(t)\Lambda_0\rangle + \langle \Lambda_0 B(t)\rangle_0\right]$