Beyond Quantum Theory
Open Systems and Deterministic Representations
Mathematical Modeling of Processes in Physics

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bcgs intensive week course, july 2020

Content

1. Introduction

Processes: Variables change with time

- quasi-electron velocity in a conducting wire
- a car position in traffic
- a number of radioactive atoms in a substance
- a number of photons per unit time on a screen
- a stock index

We treat processes by appropriate mathematical tools.
In models of **generated dynamics causality and time homogeniety** are build in from start.

Modeling by generated dynamics relies on knowledge about

- set of relevant variables
- reversibility/irreversibility of motions
- stability of properties
- short and/or long time behavior
- role of fluctuations
- role of memory

Aim of the course

Overview and training to model systems with prognostic power in relevant variables.
We focus on the aspect of "equation of motion" and not so much on the aspect "theory of matter".
We use a systematic approach to equations of motion by **generated dynamics** to capture and better understand the antipodes

- reversible – irreversible
- deterministic – stochastic
- microscopic – macroscopic
- discrete - continuous

We go **beyond quantum theory**, which is "just" a theory of reversible stochastic processes.

- The general time reversible, deterministic, generated dynamics of discrete facts is a **permutation dynamics**. We argue that it is **the deterministic representation of quantum processes** which - like other processes - emerge from permutation dynamics by laws of large numbers in the sense of Phil Anderson's "More is different". This approach is - apart from different wording and reasoning- already known as the **cellular automaton interpretation of quantum mechanics** by Gerard 't Hooft.
- **Open systems** have few relevant system variables in contact with a huge number of irrelevant (environmental) variables. They **show irreversible stochastic behavior with a memory**.

Reversible Processes

Reversibility of relevant variables in idealized closed isolated systems

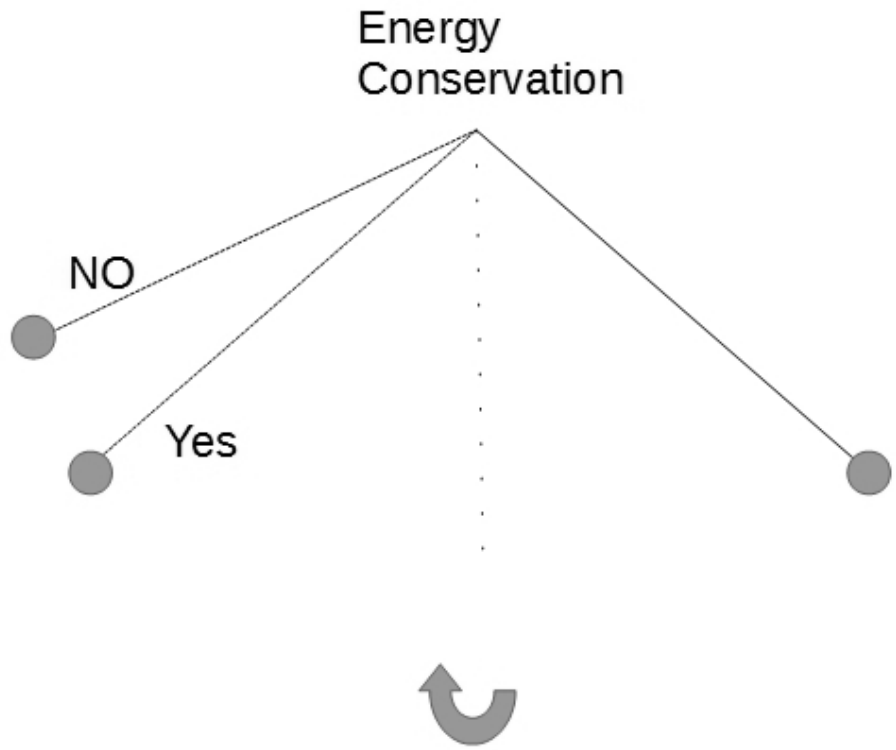

Figure: Energy Conservation

A reversed movie is not funny.

Instability of Reversibility

Reversibility is unstable against "environmental contact".
A huge number of variables of my body (external) and within the sheet of paper (internal) influence in an uncontrolled manner the two "relevant" variables of the manifold describing the sheet of paper. The huge number of uncontrolled variables, external and internal, are denoted as "environment".

Figure: Real Live

Relaxation to Stationarity

Irreversibility leads to stationary states

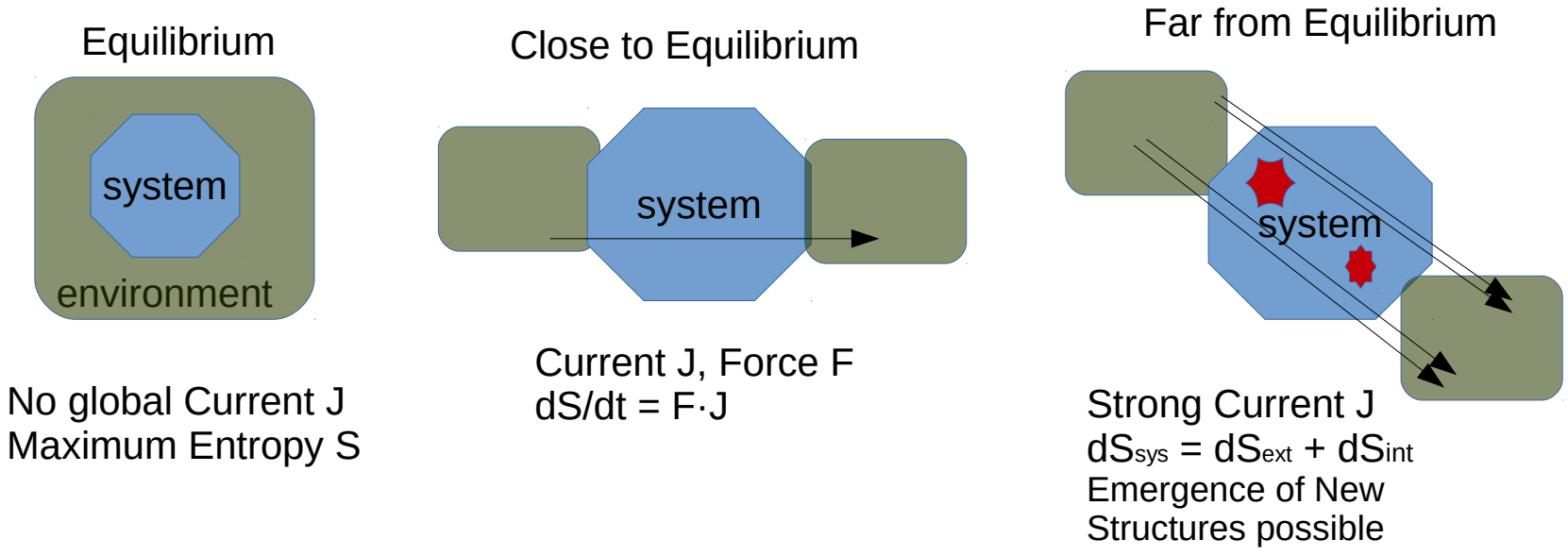

Figure: Equilibrium and Non-Equilibrium

Fluctuations - Reversible

Distinguishing between typical behavior and fluctuations we need a stochastic process description: quantum means reversible

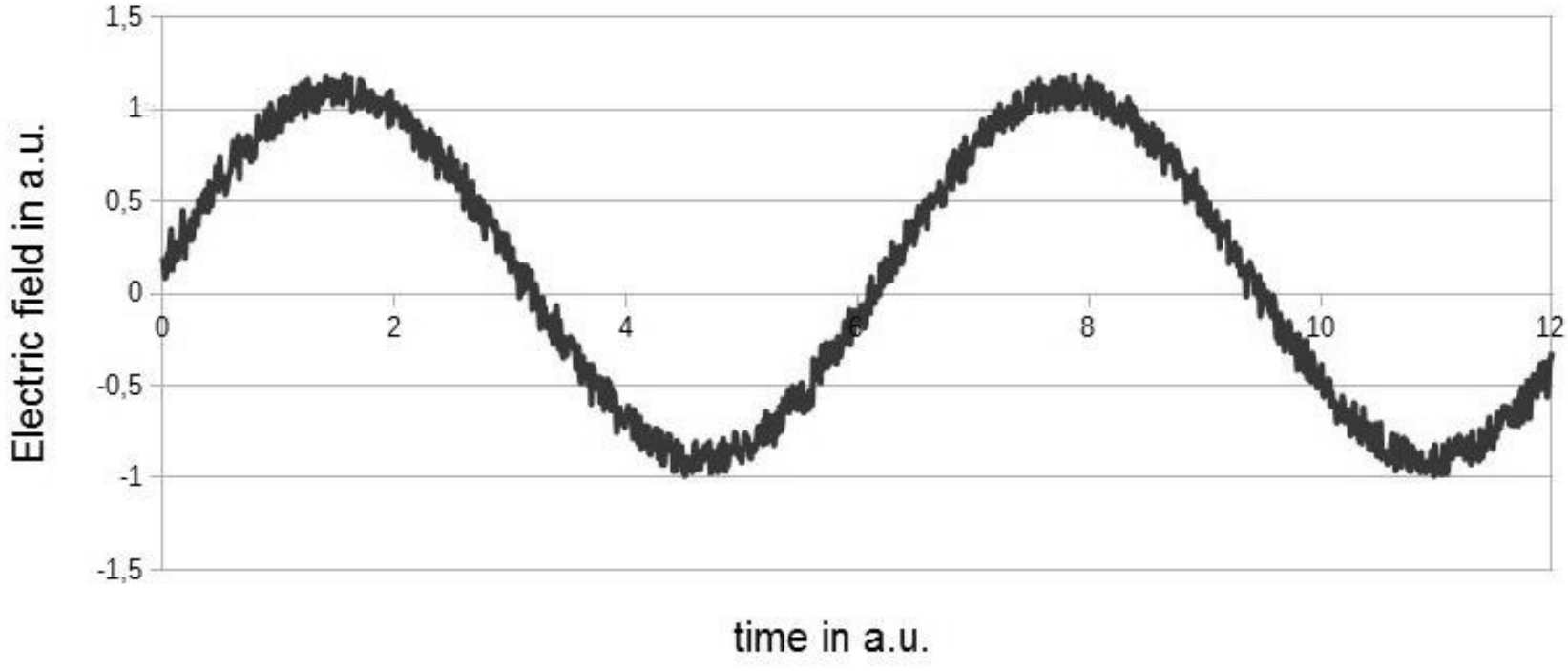

Figure: Qualitative sketch of the fluctuating field amplitude of a coherent laser light source

Fluctuations - Irreversible

Markov processes describe irreversible fluctuations

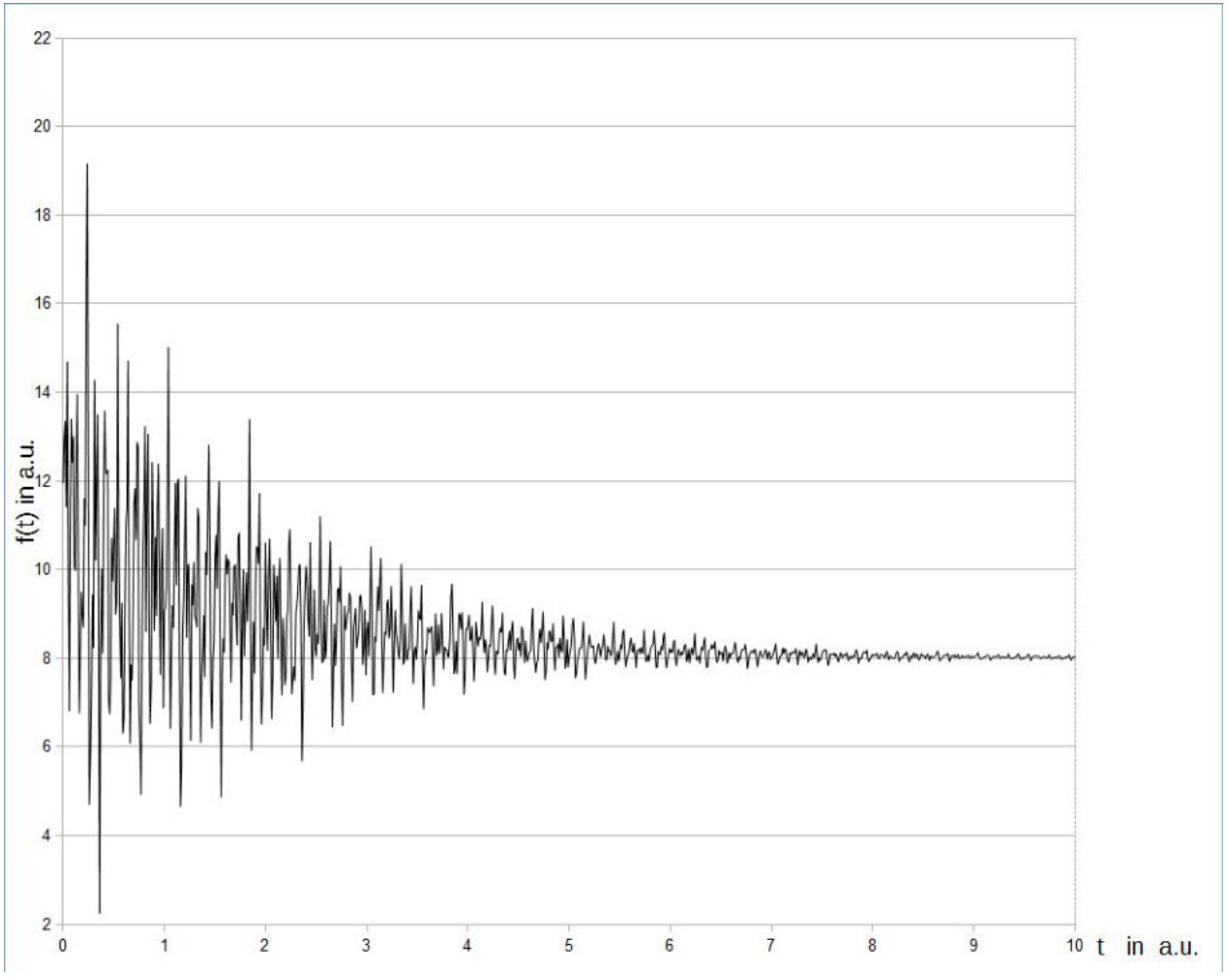

Figure: In the long time average of a signal its stationary value emerges

Discrete vs. Continuous

Facts: a discrete number of properties being the case at discrete instants of time.

More details take more variables into account.

We usually stop at some point:

(a) We cannot resolve more details.

(b)The resolution destroys our ability to focus on "relevant variables" for the investigation

Figure: Wood of Trees

Discrete vs. Continuous

To (a): Nowadays Planck time ($5 \cdot 10^{-44}$ s) and Planck length ($2 \cdot 10^{-35}$ m) set limits of resolution because we have no understanding how matter behaves on smaller scales. There are intermediate levels of stability like grains, molecules, atoms, quarks. It may stop at some level or may go on.
To (b): Resolution of characteristics of processes sets the limit in choosing variables as relevant.

- We could always choose discrete variables and discrete time steps with appropriate resolution for a process at hand.
- When a smooth average drift with perhaps some fluctuations occurs we often use continuous variables and/or continuous time in order to have the powerful mathematics of calculus for analytic functions.
- Continuity is an appropriate view on nature when properties emerge that vary in small steps. Small step behavior helps in identifying relevant properties.

Micro vs. Macro

- When a distinction between relevant and irrelevant variables is appropriate with an effective dynamics for relevant variables we have a macroscopic description of a process.
- As long as we do not consider such effective dynamics we have a microscopic description.
- Sometimes we can identify more details and a formerly known microscopic description turns out to be macroscopic in view of the more detailed description with more variables.
- Separating microscopic from macroscopic has often to do with a limit of large numbers of irrelevant variables in comparison to the number of relevant variables, because with more details within higher resolution the total number of variables increase.
- Thermodynamics of a gas of atoms like He based on statistical physics is a good example for separating macroscopic from microscopic descriptions.

Examples of well known generated dynamics

Characterizing Processes

Reversible with Fluctuations	Irreversible with Fluctuations
Example: photons, atoms Name: **quantum process** Equation: Schrödinger/von Neumann equation $\dot{\rho} = -i[H, \rho]$ (1926-27)	Example: car in traffic, Brownian motion Name: **Markov process** Equation: master equation $\dot{P} = M P$ (1900 - 1931)
Reversible without Fluctuations	**Irreversible without Fluctuations**
Example: ~planets, ~pendulum Name: **Hamilton process** Equation: canonical equations $\dot{X} = \{H, X\}$ (1687 - 1847)	Example: skydiving, average population, running couplings Name: **„Aristotelian“ process** Equation: „Aristoteles“ equation $\dot{x} = v(x)$ (since „-330“)

Prerequisites for this course

- basic linear algebra and calculus $\vec{x}(t) = \vec{x}_0 e^{-2t}; \dot{\vec{x}}(t) = -2\vec{x}(t)$
- basic knowledge about Hamiltonian equations, Maxwell's equations $\dot{x} = \partial_p H(x,p) = \{H, x\}$; $\partial_t \vec{E}(\vec{x},t) = \mathrm{rot}\vec{B}(\vec{x},t) - \vec{j}(\vec{x},t)$
- basic knowledge of operators, states and expectation values in quantum theory $\dot{\psi} = -iH\psi$; $\psi_t = e^{-iHt}\psi_0$; $\dot{A} = i\,[H, A]$; $\langle A \rangle = \langle \psi \mid A \mid \psi \rangle$; $\langle A \rangle = \mathrm{Tr}\,\{P_\psi A\}$ with projector $P_\psi = \mid \psi \rangle \langle \psi \mid$
- basic knowledge of probability theory $P_{\mathrm{Gauss}}(x) = (2\pi\sigma^2)^{-1/2} \exp -(x - x_0)^2/(2\sigma^2)$
- basic knowledge of equilibrium statistical physics $\langle A \rangle = \mathrm{Tr}\,\{\rho A\}$; $\rho = \frac{e^{-H/T}}{\mathrm{Tr}\, e^{-H/T}}$
- basic knowledge of Fourier and Laplace transform $f(z) := \int_0^\infty dt\, e^{izt} f(t) = \frac{i}{z-\omega} f_0$ for $f(t) = f_0 e^{-i\omega t}$

Modeling Systems: I. Variables

Physical system are defined by a set of **relevant variables** x forming the **configuration manifold**.
Tangential vectors v serve as short time deviations.
∂_x is the generator of translations for any (analytic) function $f(x)$:

$$f(x+a) = e^{a\partial_x} f(x) = \sum_n \frac{a^n}{n!} \partial_x^n f(x) \tag{1}$$

Variable x is short hand for many alternative cases: discrete, multicomponent discrete or even multicomponent continuous, $x_k(\vec{s})$. Products as $x \cdot J$ are always meant as sums or integrals of products $\sum_k \int \mathrm{d}^n s \, x_k(\vec{s}) J_k(\vec{s})$. In usual nomenclature "external indices" denoted as $\vec{x}$, while the "internal indices" are discrete.

$$x_k(\vec{s}) \longrightarrow \varphi_k(\vec{x}) \tag{2}$$

Such variables $\varphi_k(\vec{x})$ are then called a **field**.

Modeling systems: II. Properties

Properties of a physical system are **functions on the configuration tangent bundle**

$$f(x, v) \tag{3}$$

or functions on the cotangent bundle

$$f(x, p)\,. \tag{4}$$

The tangent bundle contains (x, v) data and the cotangent bundle (x, p) data where a cotangent vector p is from the dual space (containing linear forms on the tangent vector space).

Modeling Systems: III. Random Variables

Random variables are the coordinates x of a random event.
We assume to know how to decide if an event has taken place and has become a **fact**. The registration of a fact is what we call a **measurement**, or in short a **trial**.
An improvable theory tells which documents are to be accepted to decide about facts.
Performing measurements under controlled conditions that could be met again later within some accepted range of validity is what we call an **experiment**.

Modeling Systems: IV Probability

Probability $P_j \geq 0$ of potential events in class Q_j is a prognostication for the relative frequencies h_j to be found when potential events have become facts. For a single experiment the outcome of h_j can be 1 or 0.
If measurements are done under "similar conditions", each time with probability P_j, one should find

$$\lim_{N\to\infty} h_j = P_j + \mathcal{O}(N^{-1/2})P_j \,. \tag{5}$$

For continuous random variables a **probability distribution**, with $P(\vec{x}) \geq 0$, yields **expectation values** for properties $A(x)$

$$\langle A \rangle := \int \mathrm{d}^f x \, P(\vec{x}) A(\vec{x}) \,. \tag{6}$$

It is linear in A and must fulfill the normalization

$$\langle 1 \rangle = \int \mathrm{d}^f x \, P(\vec{x}) = 1 \,. \tag{7}$$

Modeling Systems: V Probability Flux and Continuity

For continuous t and x a **continuity equation** with **probability flux** (probability current density) $j_t(x)$ must be fulfilled,

$$\boxed{\partial_t P_t(x) = -\partial_x j_t(x)}\,. \tag{8}$$

In discrete time steps δt and with discrete variables n the probability conservation is Kirchhoff's knot rule

$$\boxed{P_{t+\delta t}(n) - P_t(n) = \left[I_{\rm gain}(n) - I_{\rm loss}(n)\right]\delta t}\,, \tag{9}$$

Keep in mind (8),(9) cannot serve as equation of motion but as constraints on any equation of motion.

Example: Diffusion Equation

An equation of motion can result as soon as the flux j is specified as a functional of P.
In a phenomenological theory about ink in water the flux is proportional to the gradient of the density of ink particles but points in opposite direction (Fick's law).
It reflects to linear order in the gradient the observation of ink particle flow from regions of higher densities to regions of lower densities.
One has

$$j(x) = -D\partial_x P(x) \tag{10}$$

with the so-called diffusion constant D.
The resulting Master equation is a Fokker-Planck equation with diffusion only and is known as the diffusion equation or heat equation,

$$\boxed{\partial_t P_t(x) = D\partial_x^2 P_t(x)}\,. \tag{11}$$

Example: Diffusion Equation

The solution to an initial value of delta-peaked[1] ink at $x = x_0$ is an irreversible Gaussian distribution with variance increasing linear in time,

$$\boxed{P_t(x) = \frac{1}{\sqrt{4\pi D t}} \exp\left(-\frac{(x - x_0)^2}{4Dt}\right)}. \tag{12}$$

A variance increasing linear with time, $(\delta x)^2 = 2Dt$, is the signature of diffusive motion.

[1] so-called fundamental solution or Green's function of the linear differential equation

Exercise No. 1

1. Find examples for stochastic processes with fluctuations. Are they reversible or irreversible? How do you judge?
2. Where to put the classical Euler equations for rigid bodies in the overview of processes? Where to put Maxwell's equations? Where to put Quantum electrodynamics? Where to put General Relativity?
3. Solve the equation of motion $\dot{v} = -v/\tau$ with positive τ for an initial value v_0. Find the stationary solution.
4. Why can $\dot{x} = g(x)$ not describe a reversible process?
5. Show that the diffusion equation follows from Fick's law and the continuity equation. Show that the fundamental solution solves the corresponding initial value problem.
6. For every probability flux $j_t(x)$ being in balance with $P_t(x)$ we can define a velocity field $v_t(x)$ by

$$v_t(x) := j_t(x)/P_t(x)\,.$$

Show that the time derivative of the average value of coordinate x equals the average of the velocity field with respect to $P_t(x)$. Start by formulating the equation to show.

02. Generated Dynamics

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Content

I.1 Semi-Group and Group

We consider generated **semi-group or group dynamics** because they reflect **causality** and **time homogeneity**.

$$\boxed{T_{t_3-t_2} \cdot T_{t_2-t_1} = T_{t_3-t_1}} \tag{1}$$

with $T_0 = 1$. For continuous time t, the **generator** G is the derivative at $t = 0$,

$$\boxed{G = \partial_t T_t \mid_{t=0}}, \tag{2}$$

The full time evolution operator is

$$\boxed{T_t = e^{t \cdot G}} \, . \tag{3}$$

For discrete time t, the **generator** G is the logarithm of the one-step time evolution and can be expressed as

$$\boxed{G = \log\left(T_1\right) = \sum_{n=1}^{\infty} \frac{\left(T_1 - 1\right)^n}{n}}, \tag{4}$$

Time evolution is step by step and solving for short times allows to calculate for long times.

Inverse or Not Inverse

- In semi-groups not every element has an inverse within the semi-group. This is to be expected for effective dynamics of relevant variables when irrelevant variables cannot be followed in detail.
- With group dynamics the **principle of sufficient reason** is implemented. This is to be expected only when the time evolution of every variable can be followed in every detail.
- We call a system reversible, if for each transformation T_{t-t_0} an inverse transformation $T_{t-t_0}^{-1}$ exists, which also describes a possible time evolution of the system, otherwise irreversible.
- **Reversible systems** have a time evolution with **group dynamics** while **irreversible systems** have a time evolution with **semi-group dynamics** .

I.2 The Choice of State as Initial Condition

The defining feature of a **state** is that it can serve **as an initial condition** of the (semi-)group dynamics. The time evolution operator operates on states,

$$\boxed{\sigma_t = T_t \sigma_0 = e^{tG} \sigma_0} \,. \tag{5}$$

In continuous time we have a differential equation of motion

$$\boxed{\dot{\sigma}_t = G \sigma_t} \,, \tag{6}$$

which is the most popular version of the equation of motion in generated dynamics. In discrete time we have instead to the differential equation an iterative equation of motion

$$\boxed{\sigma_{t+1} = T_1 \sigma_t} \,. \tag{7}$$

As we will see, a **state** can consist of **properties** or of a **probability** or of a **pre-probability** or of **fact-states**.

I.3 The resolvent version of the equation of motion

The generated dynamics by (semi-)groups is characterized by (5). This amounts to calculate an exponential of a generator and typically cannot be done unless a spectral representation of the generator is known. A step forward prior to a full spectral representation is achieved by the Laplace transformed version of (5) and introduces the **resolvent** $(z - \mathcal{L})^{-1}$ associated to the generator, where z is a complex number.

$$\boxed{\sigma(z) = i\,[z - \mathcal{L}]^{-1}\,\sigma_0}\,, \tag{8}$$

where $\mathcal{L} := iG$ is called **the Liouville** of the dynamics.
Instead of an infinite exponential series expansion we only have to calculate the inverse of $(z - iG)$. In addition, the spectrum of $\mathcal{L}$ shows up in singular behavior of the resolvent when z comes close to a spectral value [1] of $\mathcal{L}$. Such form is widely exploited in signal processing, electrical engineering as well as in condensed matter and high energy physics.

[1] generalization of the notion of eigenvalue for matrices

I.3 On Spectral Theory for Operators

for reference see:

- Thirring: Quantum Mathematical Physics, Springer, 2013
- Markin: Elementary Operator Theory, de Gruyter, 2020

We consider **linear operators** like $\mathcal{L}$ acting on some linear space $\mathcal{X}$, equipped with a norm ("length") or a scalar product ("length and angel"). When the dimensionality is not finite, topological considerations are essential and we consider linear spaces where every Cauchy series has a limit within $\mathcal{X}$ (completeness). Such spaces are called Banach space (with a norm) or **Hilbert spaces** (with a scalar product). The set $spec(\mathcal{L})$ where the $z - \mathcal{L}$ is not bijective is called **spectrum of the resolvent**.

There are three disjoint subsets within the spectrum:

- The **point spectrum**: Here the resolvent does not exist.
- The **continuous spectrum**: Here the resolvent exists, surjectivity of $z - \mathcal{L}$ fails by missing closing points.
- The **residual spectrum**: Here the resolvent exists, the closure of the image of $z - \mathcal{L}$ does not give full X.
- Operators with only **point spectrum** are very similar to finite matrices and we may treat the points like **eigenvalues** (e.g. the harmonic oscillator Hamiltonian of quantum mechanics).
- The **continuous spectrum** corresponds to **quasi-eigenvalues** and non-normalizable eigenstates (e.g. plane waves or scattering states in quantum mechanics) in non-finite dimensional spaces. One can catch them in a N-dimensional discretization by studying the scaling of eigenstates and eigenvalues with dimension N.
- The residual spectrum can occur for non-surjective isometric operators like the right-shift operator $RS(x_1, x_2, x_3, \dots) = (0, x_1, x_2, x_3, \dots)$.

II.1 Continuous Aristotelian: Semi-Group

When the **state is just the configuration** (we call it **Aristotelian processes**), $\sigma = x$, the generator looks like

$$G = Ar = v(x)\partial_x \tag{9}$$

with some function $v(x)$, and by $\dot{x} = Gx$ and $\partial_x x = 1$ we arrive at

$$\dot{x} = v(x) \tag{10}$$

and more generally to an equation of motion for any property $\sigma = f(x)$,

$$\dot{f}(x) = f'(x) \cdot v(x)\,. \tag{11}$$

Such dynamics cannot be reversible, since at a given value of x there is only one value of $\dot{x}$ and the motion cannot be turned back.

II.2 Continuous Newton: (Mostly) Group

Reversible dynamics is possible with **states taken from the tangent bundle** $\sigma = (x, v = \dot{x})$. The historic invention of Newton corresponds to the following generator

$$G = N = \dot{x}\partial_x + a(x)\partial_{\dot{x}} \tag{12}$$

with some function $a(x)$ describing the acceleration as $\ddot{x} = \dot{v}(x) = a(x)$. Since the acceleration is of second order in time derivatives, at a given point, the velocity can be reversed and the motion can be turned back. The general equation of motion of **Newton processes** then reads for states $\sigma = f(x, \dot{x})$

$$\dot{f}(x, \dot{x}) = \partial_x f(x, \dot{x}) \cdot \dot{x} + \partial_{\dot{x}} f(x, \dot{x}) \cdot a(x)\,. \tag{13}$$

Remark: If $a = a(x, v, t)$ irreversible friction and environmental coupling can be described, too. The dependence on v breaks reversibility ("friction") and the dependence on t breaks time homogeneity, two features expected for environmental coupling.

II.2 Continuous Hamilton: Group

States taken from cotangential bundle $\sigma = (x, p)$ (phase space) allows further structure: the invariance of the volume element $\mathrm{d}x \wedge \mathrm{d}p$ (**Liouville's theorem**) under time evolution for proper counting of states in statistics. The processes are called **Hamilton processes**, where the generator has the form of Poisson's bracket

$$G = \{H(x,p), \cdot\} := (\partial_p H(x,p))\partial_x \cdot - (\partial_x H(x,p))\partial_p \cdot , \qquad (14)$$

with Hamilton function $H(x, p)$. The general equation of motion then reads for $\sigma = f(x, p)$

$$\dot{f}(x,p) = \partial_x f(x,p) \cdot \partial_p H(x,p) - \partial_p f(x,p) \cdot \partial_x H(x,p) . \qquad (15)$$

Interpreted as a property of the system conserved H is called **energy**. In many cases, since p and $\dot{x}$ are related, Newton and Hamilton lead to the same second order differential equation for x. By Legendre transformation an equivalent Lagrange formulation is possible.

II.3 Discrete: (Semi-) Group

A consequent discretization of configurations and time steps leads to an astonishing far reaching observation under the restriction of time homogeneous (semi-)group conditions:
There are only two different types of dynamics:

- (A) **Periodic** with all configurations involved (including stationarity as period $T = 0$).
- (B) **Relaxing** to stationarity in time τ.
- (B') **Relaxing** to periodicity with period T on reduced configurations in time τ.

In case (A) we have a dynamics by the **one-step generator taken from the group of permutations**.
As we will come back to this as a deterministic representation of quantum theory we will elucidate this observation in more detail now.

II.3 Discrete: - two value system

In system with N values of its configuration space, $x \in \{1, 2, \ldots, N\}$, **a time homogeneous evolution in discrete steps by (semi-)group dynamics is fixed by one-time-step.**
In case $N = 2$ we have only $N^2 = 4$ possibilities for the next step for each value: $1 \to 1$, $1 \to 2$, $2 \to 1$, $2 \to 2$ leading to $N^N = 4$ possible time evolutions, starting from an initial setting $\begin{pmatrix} 1 \\ 2 \end{pmatrix}$

$$\begin{pmatrix} 1 \\ 2 \end{pmatrix} \to \begin{pmatrix} 1 \\ 2 \end{pmatrix} \to \begin{pmatrix} 1 \\ 2 \end{pmatrix} \ldots \tag{16}$$

$$\begin{pmatrix} 1 \\ 2 \end{pmatrix} \to \begin{pmatrix} 2 \\ 1 \end{pmatrix} \to \begin{pmatrix} 1 \\ 2 \end{pmatrix} \ldots \tag{17}$$

$$\begin{pmatrix} 1 \\ 2 \end{pmatrix} \to \begin{pmatrix} 1 \\ 1 \end{pmatrix} \to \begin{pmatrix} 1 \\ 1 \end{pmatrix} \ldots \tag{18}$$

$$\begin{pmatrix} 1 \\ 2 \end{pmatrix} \to \begin{pmatrix} 2 \\ 2 \end{pmatrix} \to \begin{pmatrix} 2 \\ 2 \end{pmatrix} \ldots . \tag{19}$$

II.3 Discrete: - two value system

- Equations (16) and (17) show periodic dynamics, (16) with period $T = 0$ and (17) with period $T = 2$, and
- (17) and (18) show relaxation to a stationary state in one time step, $\tau = 1$.
- In the relaxation situation the one-step mapping is not invertible, since two values are mapped to the same value.

II.3 Discrete: $N = 3$ value system

In case $N = 3$ we have only $N^2 = 9$ possibilities for the next step for each value: $1 \to 1$, $1 \to 2$, ..., $3 \to 3$ leading to $N^N = 27$ possible time evolutions, starting from an initial setting 123 :

after step 1	after step 2	after step 3	type
111	111	111	B $\tau = 1$
112	111	111	B $\tau = 2$
113	113	113	B $\tau = 1$
121	121	121	B $\tau = 1$
122	122	122	B $\tau = 1$
123	123	123	A $T = 0$
131	111	111	B $\tau = 2$
132	123	132	A $T = 2$
133	133	133	B $\tau = 1$
211	122	211	B' $\tau = 1, T = 2$
212	121	212	B' $\tau = 1, T = 2$
213	123	213	A $T = 2$
221	222	222	B $\tau = 2$

II.3 Discrete: $N = 3$ value system

continued table

after step 1	after step 2	after step 3	type
222	222	222	B $\tau = 1$
223	223	223	B $\tau = 1$
231	312	123	A $T = 3$
232	323	232	B $\tau = 1$
233	122	122	B' $\tau = 1, T = 2$
311	133	311	B' $\tau = 1, T = 2$
312	231	123	A $T = 3$
313	333	333	B $\tau = 2$
321	123	321	A $T = 2$
322	222	222	B $\tau = 2$
323	323	323	B $\tau = 1$
331	113	331	B' $\tau = 1, T = 2$
332	223	332	B' $\tau = 1, T = 2$
333	333	333	B $\tau = 1$

II.3 Discrete: - N value system

From $N = 3$ we learn:

- There are $N!$ of N^N cases (A) with periodic dynamic involving all N variables. The corresponding one-time-steps are just the $N!$ invertible permutations of the permutation group S_N.
- There are cases (B') of relaxing dynamics to periodic motion, reduced to the configuration space of $N - 1$ or less values. The corresponding one-time-steps generate semi-groups on the N original values. The corresponding mappings are not invertible on all original values.
- All other cases (B) correspond to relaxation to stationarity within some relaxation time $\tau < N$.

II.3 Discrete: Reversible permutation dynamics on facts

The reversible permutation dynamics is a group dynamics, generated by a one-step time evolution operator $T^{[\pi]}$ corresponding to a permutation $\pi \in S_N$. It can be represented as a matrix acting on states which are indicator vectors. We like to call them **fact states** or just **facts**. Indicator vectors **indicate which of** N **possible exclusive values is a fact**. For example, let the 3rd value in a $4-$value system be a fact, then the corresponding fact reads as an indicator vector:

$$\phi^{[3]} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} . \tag{20}$$

The permutation $\pi : 1234 \to 2413$ is represented by

$$T^{[\pi]} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} . \tag{21}$$

II.3 Discrete: Reversible permutation dynamics on facts

You may check that $T^{[\pi]}\phi^{[k]} = \phi^{[\pi(k)]}$. In general, one-step evolution operators corresponding to permutations have in each row and in each column exactly one non-vanishing entry of 1. Thus, the sum of each column is 1 and the sum of each row is 1. Thus, **these matrices are** not only **stochastic**, but also **double-stochastic**. They are also **orthogonal** and also **unitary**. The matrix representation can be written for arbitrary N as

$$\boxed{T^{[\pi]}_{lm} = \delta_{l\pi(m)} \; ; \; \left(T^{[\pi]}\right)^{-1} = T^{[\pi]\dagger} \; ; \; T^{[\pi]\dagger}_{lm} = \delta_{m\pi(l)}} \, . \tag{22}$$

Facts can be written as

$$\boxed{\phi^{[k]}_m = \delta_{mk}} \tag{23}$$

such that it generates a permutation dynamics by π:

$$T^{[\pi]}\phi^{[k]} = \phi^{[\pi(k)]} \, . \tag{24}$$

III.1 Chapman-Kolmogorov and Master Equations

For **Markov processes**, the defining feature is that the probability distribution serves as the state of the time evolution, $\sigma = P$. The corresponding equation of motion is called **Master equation**

$$\boxed{\partial_t P_t = M P_t}\,, \tag{25}$$

where $G = M$ is a linear operator represented as an integral kernel $M(x', x)$ or matrix. The semi-group property of the time evolution operator $T = e^{Mt}$ (**stochastic matrix**) reads in kernel notation as so-called **Chapman-Kolmogorov** equation

$$T_{t_2-t_0}(x', x) = \int \mathrm{d}x''\, T_{t_2-t_1}(x', x'') T_{t_1-t_0}(x'', x) \tag{26}$$

Probability conservation requires

$$\int \mathrm{d}x'\, T(x', x) = 1\,, \tag{27}$$

$$\int \mathrm{d}x'\, M(x', x) = 0\,. \tag{28}$$

Inversion -if it works at all - does, in most cases, lead out of the stochastic matrices which must have non-negative elements.

Recall diffusion

The M-Operator can - under conditions to be discussed later - very often be approximated by linear differential operators with coefficient functions called **drift** and **diffusion**. The corresponding linear partial differential equation of second order in ∂_x is denoted as **Fokker-Planck equation**. It can be encoded in a stochastic differential equation called **Langevin equation**. The diffusion equation

$$\partial_t P_t(x) = D\partial_x^2 P_t(x) \tag{29}$$

is a special case with

$$M(x, x') = D\partial_x^2 \delta(x - x')\,. \tag{30}$$

III.2 Markov: Two Value System

The Master equation in continuous time

$$\dot{P}_t(+) = w_{+-}P_t(-) - w_{-+}P_t(+)\,, \tag{31}$$

$$\dot{P}_t(-) = w_{-+}P_t(+) - w_{+-}P_t(-)\,. \tag{32}$$

Since $P_t(+) = 1 - P_t(-)$

$$\dot{P}_t(+) = w_{+-} - (w_{+-} + w_{-+})P_t(+)\,, \tag{33}$$

The solution

$$P_t(+) = \frac{w_{+-}}{w_{+-} + w_{-+}}\left[1 - e^{-(w_{+-}+w_{-+})t}\right] + P_0(+)e^{-(w_{+-}+w_{-+})t}\,. \tag{34}$$

relaxes to the stationary state independent of initial condition

$$P_\infty(+) = \frac{w_{+-}}{w_{+-} + w_{-+}}\,, \tag{35}$$

with **relaxation time** $(w_{+-} + w_{-+})^{-1}$. For symmetric $w_{+-} = w_{-+} = w$ $P_\infty = 0.5$ and the relaxation time is $1/(2w)$.

IV.1 Unitarity and Born's principle

Pre-probabilities are complex functions and their space (Hilbert space) is equipped with a scalar product, $\langle\phi|\psi\rangle := \int \mathrm{d}x\, \phi^*(x)\psi(x)$ such that $|\psi(x)|^2$ can serve as a probability distribution. This is Born's principle in quantum theory.

$$P_t(x) = |\,\langle x \mid \psi_t\rangle\,|^2 \ , \tag{36}$$

$$\psi_t = U_t\psi_0 = e^{-iHt}\psi_0 \ , \tag{37}$$

$$\boxed{\partial_t\psi_t = -iH\psi_t} \ . \tag{38}$$

(38) is called **general Schrödinger equation**. It fits in our scheme of generated dynamics with $\sigma = \psi$ and $T_t = U_t$ and $\mathcal{L} = H$. Here, by construction, the probability is conserved and time reversibility is guaranteed by

$$U_t^{-1} = U_{-t} = U_t^\dagger \ . \tag{39}$$

Probability density $P_t(x)$ and **probability flux** $j_t(x)$ are independent quantities following from the **pre-probability** $\psi_t(x)$, which thus serves as the state of quantum processes, which are **reversible stochastic processes**.

IV.2 Quantum: Two Value System

With the help of the eigenstates $C_{xm} := \langle x \mid m \rangle$ the time evolution reads

$$\psi_t(x) = \sum_m C_{xm} e^{-i\omega_m t} \langle m \mid \psi_0 \rangle \ , \tag{40}$$

$$\langle m \mid \psi_0 \rangle = \sum_{x'} C^*_{x'm} \psi_0(x') \ . \tag{41}$$

For two values $x = +, -$ and $m = 1, 2$ the diagonal elements of H are real numbers H_{++} and H_{--}. The off-diagonal elements are complex conjugated $H_{-+} = H^\star_{+-}$. The frequencies are

$$\omega_{1,2} = \frac{H_{++} + H_{--}}{2} \pm \sqrt{\frac{(H_{++} - H_{--})^2}{4} + \mid H_{+-} \mid^2} \, , \tag{42}$$

and the eigenstates are

$$C_{+1} = \frac{-H_{+-}}{\sqrt{(\omega_1 - H_{++})^2 + \mid H_{+-} \mid^2}} , \quad (43)$$

$$C_{+2} = C_{+1} \cdot \frac{\omega_1 - H_{++}}{H_{+-}} , \quad (44)$$

$$C_{-2} = \frac{-H_{-+}}{\sqrt{(\omega_2 - H_{--})^2 + \mid H_{+-} \mid^2}} , \quad (45)$$

$$C_{-1} = C_{-2} \cdot \frac{\omega_2 - H_{--}}{H_{-+}} . \quad (46)$$

Choosing the initial state as $\psi_0 = +$ one finds so-called Rabbi oscillations in the probability of a two value quantum system (frequently called two level system),

$$P_t(+) = 1 - 4 \mid C_{+1} \mid^2 \cdot (1 - \mid C_{+1} \mid^2) \cdot \sin^2 \left(\frac{(\omega_1 - \omega_2)t}{2} \right) . \quad (47)$$

For degenerate states $\omega_1 = \omega_2$, of course, there are no oscillations. Starting with an eigenstate, of course, the probability stays 1. **Oscillations** rather than relaxation is the indicator of reversible stochastic processes.

IV.3 Free Particle vs. Diffusion

Free particle means translation invariance and rotational (in 1D reflection) invariance . Thus $H = H(\partial_x^2)$ and does not explicitly depend on x. Once we require Galilei invariance (velocities add) we find $H = (-1/2m)\partial_x^2$ with positive parameter m characterizing inertia. The corresponding Schrödinger equation reads

$$\boxed{\partial_t \psi_t(x) = \frac{i}{2m}\partial_x^2 \psi_t(x)}\,. \tag{48}$$

It looks like a diffusion equation when we identify D with $i/2m$. The fundamental solution (Green's function) can be found by Fourier analysis as for the diffusion equation:

$$\boxed{G(x, x_0, t) = \sqrt{\frac{m}{2\pi i t}}\exp\left(-\frac{mx^2}{2it}\right)}\,. \tag{49}$$

Free Particle vs. Diffusion: Flux, Spreading, Drift, Interference

- The flux is related to the phase gradient of the pre-probability $\psi = \sqrt{P}e^{i\varphi}$,

$$\boxed{j_t(x) = P_t(x)\frac{\partial_x \varphi}{m}}. \tag{50}$$

- The width of a quantum wave packet grows linearly in time while the peak moves with a velocity. The diffusive wave packet has no drift at all and its width grows only as a square root in time.
- When quantum wave packets meet they interfere (superposition of amplitudes) while diffusive packets just superimpose probabilities.

03. Methods of Solutions and Approximations

Martin Janßen

bcgs intensive week course, july 2020

Content

Overview on Methods

The time-dependent (semi-) group time evolution operator

$$T_t = e^{tG} = T_1^t \tag{1}$$

or its corresponding complex frequency dependent resolvent

$$(z - iG)^{-1} \tag{2}$$

are operator valued functions of G or T_1, not easy to evaluate.

- In discrete time, one can proceed by iteration $T_t = T_{t-1}T_1 = T_1^t$.
- For discrete variables a **spectral decomposition** of T_1 or G essentially solves the dynamics. We sketch this here and come back to it when discussing open systems.
- Symmetries can help to reduce complexity of calculations. We will touch it later.
- If $G = G_0 + G_1$ with solved G_0 problem, one can make expansion in G_1. This time dependent perturbation theory can be found in standard lectures on quantum theory and it will not be treated here.

Overview on Methods

- When the variables can be treated as continuous, the use of the translation operator ∂_x transforms the **generator to a differential operator**. This helps in truncated **Lie series expansions**, useful for deterministic processes.
- The spectral decomposition of ∂_x allows for a **path integral representation of the time evolution operator** for stochastic processes, both of Markov and quantum type. This opens a great flexibility for further approximations which go beyond standard perturbation theory.
- There is also a supersymmetric path integral representation for the resolvent operator which seems - to me - promising to study. However, due to lack of time and expertise it will not be addressed further in this lecture course.

I. Spectral decomposition of Liouville

σ as probabilities or pre-probabilities or facts we represent as elements taken from a Hilbert space $\mathcal{X}$ to have expectation values by weighted superpositions. With fact states the weights are exclusively 0 and 1. The Liouville $\mathcal{L} = iG = i \log T_1$ acts as operator on $\mathcal{X}$. Quite generally we may write

$$\mathcal{L} = \mathcal{H} - i\Gamma \,; \text{with } \mathcal{H}^\dagger = \mathcal{H} \;;\; \Gamma^\dagger = \Gamma \geq 0 \,. \tag{3}$$

$\Gamma \geq 0$ excludes unbounded exponentially large growing of properties. We assume $\mathcal{X}$ to have finite dimension N (from beginning or by discretization) and $\mathcal{L}$ should not have any further symmetries such that its eigenvalues $\lambda_k = \omega_k - i\gamma_k$ (ω, γ real and $\gamma \geq 0$) can be assumed to be non-degenerate. We can then [Dieudonné: On biorthogonal systems, Michigan Math. J. 2 (1953); Brody: Biorthogonal Quantum Mechanics arXiv:1308.2609] find a **bi-orthogonal partition of unity** by normalized left and right eigenstates $\langle L_k \,|$, $|\, R_k \rangle$, which means ...

....

$$\langle L_k|R_{k'}\rangle = \delta_{kk'} \; ; \; \sum_{k=1}^{N} \mid R_k\rangle \langle L_k \mid = 1 \, . \tag{4}$$

Left and right eigenstates have to be distinguished. Left and right eigenstates are generally not orthogonal amongst themselves. Hermitian conjugates of left and right eigenstates are eigenstates of $\mathcal{L}^\dagger$ with complex conjugated eigenvalues λ_k^*. Left and right eigenstates become identical with real eigenvalues when Γ vanishes and $\mathcal{L}$ is Hermitian, as in quantum processes.
Now we can write the **spectral decomposition** of $\mathcal{L}$ as

$$\mathcal{L} = \sum_{k=0}^{N} \lambda_k \mid R_k\rangle \langle L_k \mid \; . \tag{5}$$

An evolving state is a superposition of **oscillations** (λ_k real finite), **relaxations** (λ_k imaginary finite), **damped oscillations** (λ_k complex finite), or a **stationary state** (zero-mode: λ_k=0):

$$\boxed{\mid \sigma_t\rangle = \textstyle\sum_{k=0}^{N} A_k e^{-i\omega_k t - \gamma_k t} \mid R_k\rangle \; ; \; A_k = \langle L_k|\sigma_0\rangle} \, . \tag{6}$$

Remarks on (6):

- In case of accidental degeneracies there will appear additional terms of type $t^n e^{-i\omega_k t-\gamma_k t}$ with $n+1$ limited by the dimensionality of the eigenspace.
- When the discretized system becomes larger and the spectrum becomes denser with increasing N and when it cannot be resolved any longer, the sums should be replaced by appropriate integrals and the time behavior can become much more involved than described by (6). However, it can be traced back to (6) in a controlled way by studying the behavior under increasing discretization number N.

II.1 Generator Coefficients

Kernels like $G(x,x')$ in $\dot{\sigma}_t(x) = \int dx'\, G(x,x')\sigma_t(x')$ can be represented by a series of local differential operators of arbitrary high order, because ∂_x is the generator of translations:

$$\int \mathrm{d}x'\, f(x,x') = \int dh\, f(x,x+h) = \sum_{n=0}^{\infty} (\partial_x)^n \int dh\, \frac{h^n}{n!} f(x-h,x)\,. \tag{7}$$

G operating on functions of variable x can be expressed as

$$G_x \cdot = \sum_{n=0}^{\infty} (\partial_x)^n \left[G_n(x)\cdot\right]\,, \tag{8}$$

with **generator coefficients** uniquely determined by

$$G_n(x) = \frac{(-1)^n}{n!} \int \mathrm{d}x'\, (x'-x)^n G(x',x)\,. \tag{9}$$

$G(x',x)$ can then be expressed as

$$G(x',x) = \sum_{n=0}^{\infty} \left[(\partial_{x'})^n \delta(x'-x)\right] \cdot G_n(x)\,. \tag{10}$$

II.2 Kramers-Moyal coefficients

In the Markov case the generator coefficients are known as **Kramers-Moyal coefficients** which can, due to the transition rate character of $M(x, x') =: w(x' \to x)$ for $x \neq x'$, be written in terms of moments of deviations $\Delta x := x' - x$

$$D_n(x) := \lim_{\Delta t \to 0} \frac{(-1)^n}{n!} \langle (\Delta x)^n \rangle_w / \Delta t \,. \tag{11}$$

In particular, $D_0(x) = 0$ due to probability conservation, $D_1(x)$ is denoted as **drift coefficient** and $D_2(x)$ as **diffusion coefficient**. The Markov equation for systems with only drift and diffusion is called **Fokker-Planck equation** (FPE). For continous Markov processes FPE is very often a reasonable approximation, provided enough randomness happens already on time scales shorter than the resolution time scale (a "large N phenomenon").

Comment on Langevin Equation

The Fokker-Planck equation for the probability distribution can be written as a so-called Langevin equation (a stochastic differential equation) for the time dependent stochastic variable $x(t)$ which simply rests on the role of the two coefficients, drift and diffusion,

$$\lim_{\Delta t \to 0} \langle \Delta x \rangle / \Delta t = -D_1(x) \tag{12}$$

$$\lim_{\Delta t \to 0} \left\langle (\Delta x)^2 \right\rangle / \Delta t = 2D_2(x) \tag{13}$$

The second equation shows the fractal non-differentiable character of paths $x(t)$. Without diffusion there is only drift - back to the deterministic situation $\dot{x} = -D_1(x)$.

II.3 Hamilton coefficients

In the quantum case with Dirac Notation $H(x', x) = \langle x'|H|x\rangle$

$$H_n(x) = \frac{(-1)^n}{n!} \int \mathrm{d}x' \, (x' - x)^n \, \langle x'|H|x\rangle \; . \tag{14}$$

are called **Hamilton coefficients** There is no restriction on these coefficients apart from Hermiticity of H which not only means on average over x, but due to the local character: **even coefficients are rea**l and **odd coefficients are imaginary.**
$H_0(x)$ is called **potential field**, $-iH_1(x)$ is called **gauge field**, since it can be regauged in combination with a regauge of the wave function's phase and constant $H_2 = -1/2m$, with m called mass, ensures real flux. A well known form of a Hamilton operator for up to second order coefficients reads

$$H = (-1/2m) \left(\partial_x + iqA(x)\right)^2 + V(x) \tag{15}$$

III.1 Lie Series

The formal series solution of e^{tG} (**Lie series**)

$$\boxed{f(t) = \sum_{m=0}^{\infty} \frac{t^m}{m!} \left(\sum_{n=0}^{\infty} (\partial_x)^n \left[G_n(x) \right] \right)^m f(0)} \,. \qquad (16)$$

is defined by pure differentiation and thus can be carried out to arbitrary high order by (computer-) algebra. In some special cases the summation can be done completely and in all other cases it can be used as a quite effective tool for approximations; mainly for deterministic dynamics with only $G = g(x)\partial_x$.The idea is: take short time steps and truncate after low powers and control of errors (compare the run with maximum power n and $n+1$).
As an example with a complete analytical solution we consider the Aristotelian model for motion on earth: $G = -kx\partial_x$. The Lie series applied to an initial x yields
$x(1 + (-k)t + (1/2)(-k)^2 t^2 + \cdots)$ and coincides with the series of the exponential relaxation xe^{-kt} to rest.

III.2 Path Integral for Propagator

For the transition(-amplitude) (called **propagator**)

$$\langle x', t|x, t_0\rangle := \langle x'|T_{tt_0}|x\rangle \ . \tag{17}$$

two central ideas are exploited: (1) the (semi-)group property by iterating the short time propagator and (2) by solving the short time propagator with spectral analysis of translations and linear approximations in time steps.
The (semi-)group property in kernel representation is well known from quantum theory ($1 = U_t^\dagger 1 U_t = \int d\tilde{x} \ |\ \tilde{x}, \tilde{t}\rangle \langle \tilde{x}, \tilde{t}\ |$) and in Markov theory as the **Chapman-Kolmogorov equation**.

$$\langle x', t|x, t_0\rangle = \int d\tilde{x} \ \langle x', t|\tilde{x}, \tilde{t}\rangle \langle \tilde{x}, \tilde{t}|x, t_0\rangle \ . \tag{18}$$

This can be iterated N times. The short-time propagator becomes linear in the time step $\Delta t = (t - t_0)/(N + 1)$

$$\langle x', t + \Delta t|x, t\rangle := \langle x'|1 + G\Delta t|x\rangle \ . \tag{19}$$

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Now we use the kernel representation (10) and use the spectral representation (a concept of **duality**) of the delta-function.

$$\langle x', t+\Delta t|x,t\rangle = \int (dk/2\pi)\, e^{ik(x'-x)} \left[1 + \Delta t \sum_{n=0}^{\infty} (ik)^n G_n(x)\right]. \tag{20}$$

The expression

$$\sum_{n=0}^{\infty} (ik)^n G_n(x) =: G(x,k) \tag{21}$$

will be called **generator function**. In the quantum case it will be called (quantum) **Hamilton function**. This function depends on the definition of the coefficients $G_n(x)$ and therefore on the ordering of derivatives and coefficients in G. The variable k is just an integration variable and has, so far, no meaning as a canonical conjugate of x as in classical Hamilton mechanics. Such meaning only emerges under certain conditions to be discussed later.

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The term $1 + \Delta t G(x,k)$ can be re-exponentiated in the order Δt, such that we finally arrive at a complete integral solution

$$\langle x', t | x, t_0 \rangle = \lim_{N\to\infty} \frac{1}{(2\pi)^{N+1}} \int \mathrm{d}x_N \ldots \int \mathrm{d}x_1 \int \mathrm{d}k_{N+1} \ldots \int \mathrm{d}k_1 \cdot \left[\cdot \exp\left\{ \sum_{j=1}^{N+1} G(x_{j-1}, k_j) \Delta t + \frac{i k_j (x_j - x_{j-1})}{\Delta t} \Delta t \right\} \right] . \tag{22}$$

As a short-hand notation of such **path integral** can be written as

$$\boxed{\langle x', t | x, t_0 \rangle = \int\limits_{x \to x'} Dx(\tau) Dk(\tau)\, e^{\int_{t_0}^{t} \mathrm{d}\tau \{ G(x(\tau), k(\tau)) + i k(\tau) \dot{x}(\tau) \}}} . \tag{23}$$

III.3 L-function and S-functional

We can get rid of the dual variable by formally carrying out this integration at each intermediate step as a kind of Fourier-Laplace transform changing the variable $k(\tau)$ to $\dot{x}(\tau)$,

$$\boxed{\int Dk(\tau)\; e^{\int_{t_0}^{t} \mathrm{d}\tau\{\, G(x(\tau),k(\tau))+ik(\tau)\dot{x}(\tau)\}} =: e^{\int_{t_0}^{t} \mathrm{d}\tau L^{[G]}(x(\tau),\dot{x}(\tau))}}\,. \tag{24}$$

The function resulting from this transformation is called the L-function and its integral over time is a functional of a path $x(\tau)$ and is called the S-functional,

$$S^{[G]}[\mathrm{x}(\tau)] := \int_{t_0}^{t} \mathrm{d}\tau\, L^{[G]}(x(\tau),\dot{x}(\tau))\,. \tag{25}$$

Note, L is not necessarily the Legendre-transform of G, but more generally defined by the Fourier-Laplace transform of (24).

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For Markov processes ($G = M$) the negative of the L-function is called **Onsager-Machlup function** and the exponents are written with a minus sign, $L^{[G]} = -L^{[OM]}$ and $S^{[G]} = -S^{[OM]}$. For quantum processes the L-function is (with a factor of i) called (quantum) **Lagrange function** and written as $L^{[G]} = iL$ and the corresponding S-functional as **action functional** $iS[x(\tau)] = i\int_{t_0}^{t} \mathrm{d}\tau L(x(\tau), \dot{x}(\tau))$.
The Onsager-Machlup function for up to second order reads

$$L^{[OM]}(x, \dot{x}) = \frac{\left(\dot{x} + D^{[1]}(x)\right)^2}{4D^{[2]}(x)} \tag{26}$$

The quantum Lagrangian of a Galilei particle with translation symmetry breaking potential field and gauge field with coupling constant q reads

$$L(x, \dot{x}) = \frac{m}{2}\left(\dot{x} - iqA(x)\right)^2 - V(x)\,. \tag{27}$$

Note, no correspondence principle or "quantization" is needed to find this.

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Thus, the propagator of a Markov process can be written as

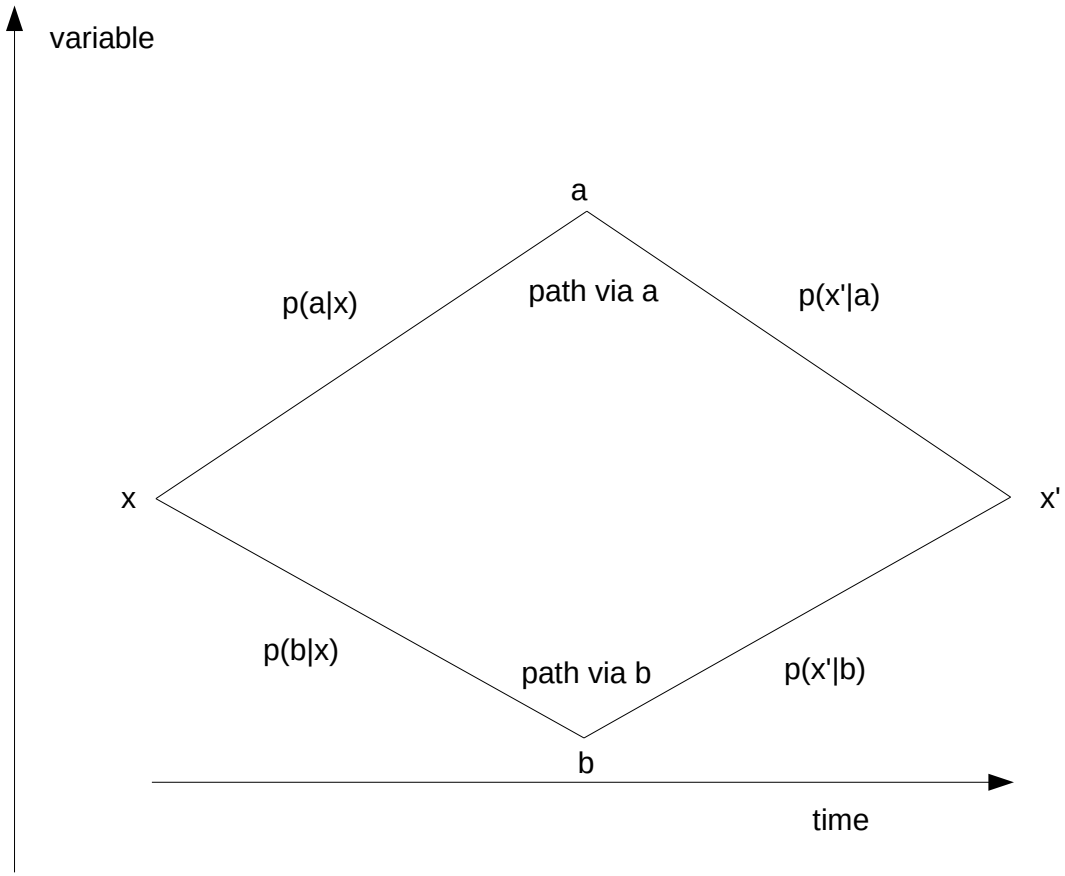
$$\boxed{(x',t|x,t_0) = \int\limits_{x\to x'} Dx(\tau) e^{-\int_{t_0}^{t} \mathrm{d}\tau\, L^{[OM]}(x(\tau),\dot{x}(\tau))}}. \qquad (28)$$

Similarly, the propagator of a quantum process can be written as

$$\boxed{\langle x',t|x,t_0\rangle = \int\limits_{x\to x'} Dx(\tau) e^{i\int_{t_0}^{t} \mathrm{d}\tau\, L(x(\tau),\dot{x}(\tau))}}. \qquad (29)$$

IV.1 Chain Rule for Markov

To illustrate the meaning of a path integral consider just two paths.

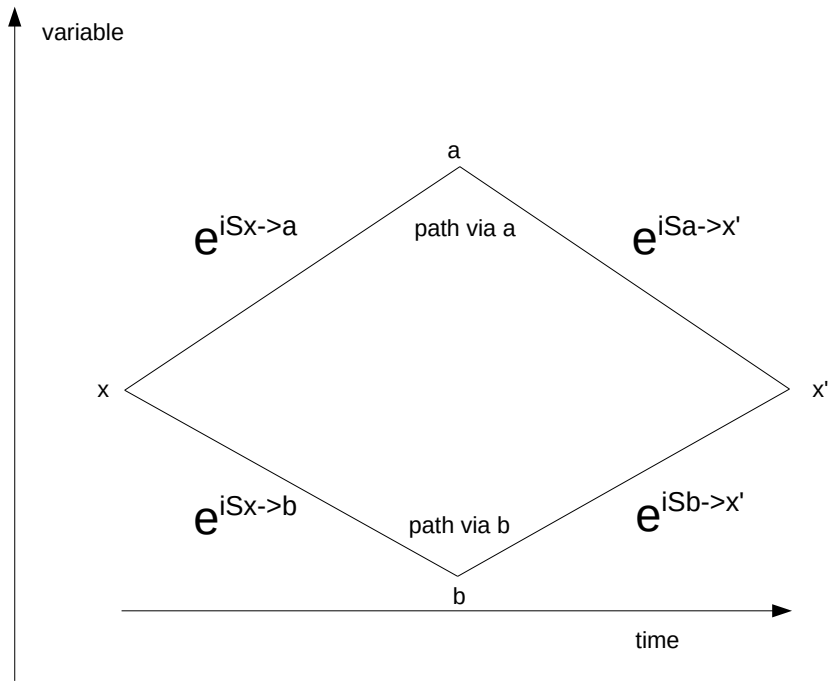


The usual chain rule results as a dynamical law of propagation

$$p(x'|x) = p(x'|a)p(a|x) + p(x'|b)p(b|x) = p_a + p_b \,. \qquad (30)$$

IV.2 Huygens-Born Principle

In the quantum case: Huygen's principle (the amplitude is a superposition of amplitudes with phases accumulated along paths starting at x and ending at x')



$$\begin{aligned}\sqrt{p(x'|x)}e^{i\phi} &= \sqrt{I_a}e^{iS_{x\to a}+iS_{a\to x'}} + \sqrt{I_b}e^{iS_{x\to b}+iS_{b\to x'}} \\ &= \sqrt{I_a}e^{iS_a} + \sqrt{I_b}e^{iS_b}\,. \end{aligned} \tag{31}$$

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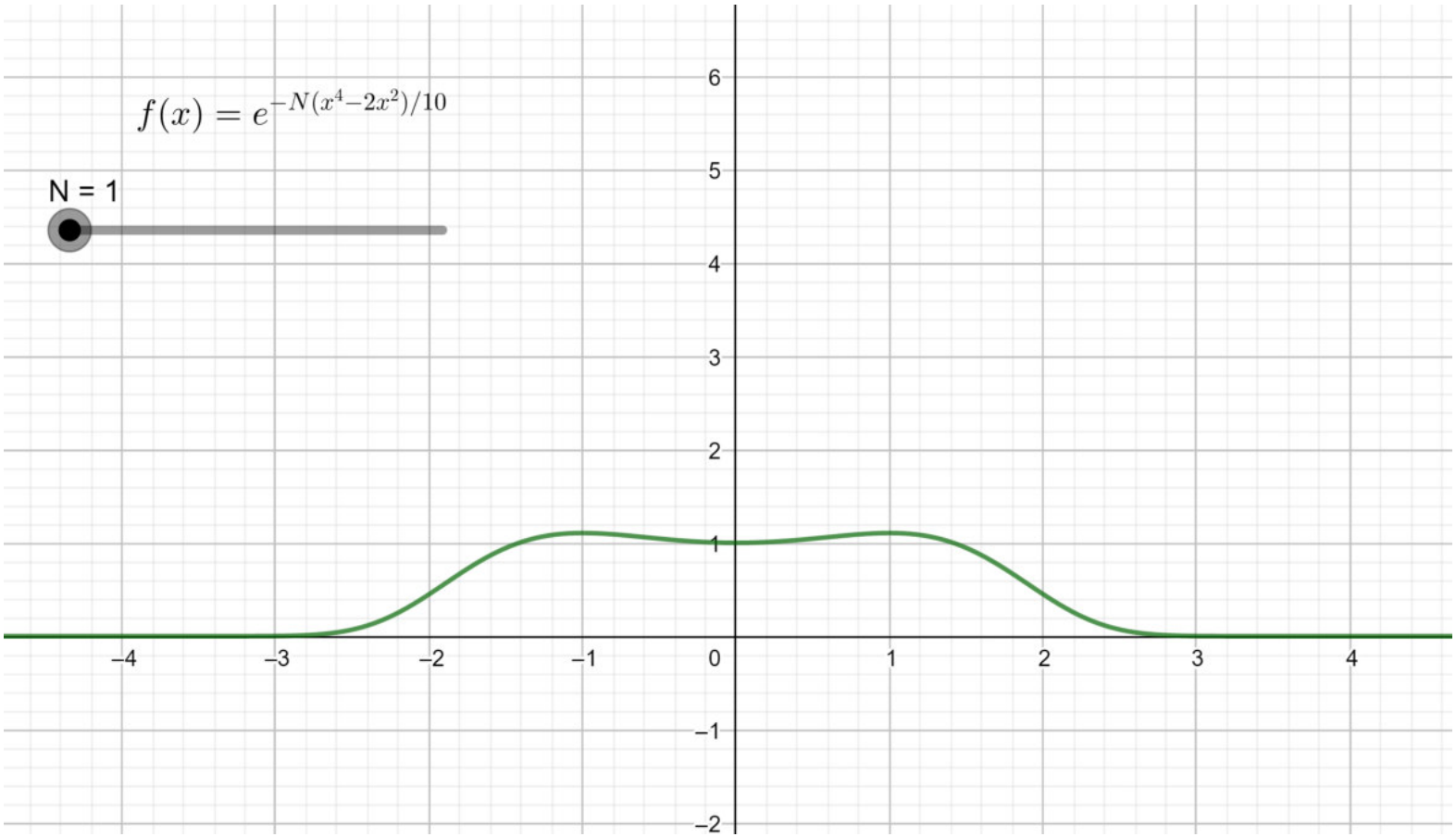
together with Born's rule: wave intensities as probabilities.
For two paths with equal absolute intensities $I_a = I_b = I$ we get for the transition probability a simple interference pattern

$$\boxed{p(x'|x) = 2I(1 + \cos(S_a - S_b))}\,. \tag{32}$$

The total intensity (probability) oscillates between 0 (destructive interference) and $4I$ (constructive interference), while an averaging over phases yields $2I$, as for a Markov process with equal probabilities for each of two paths.

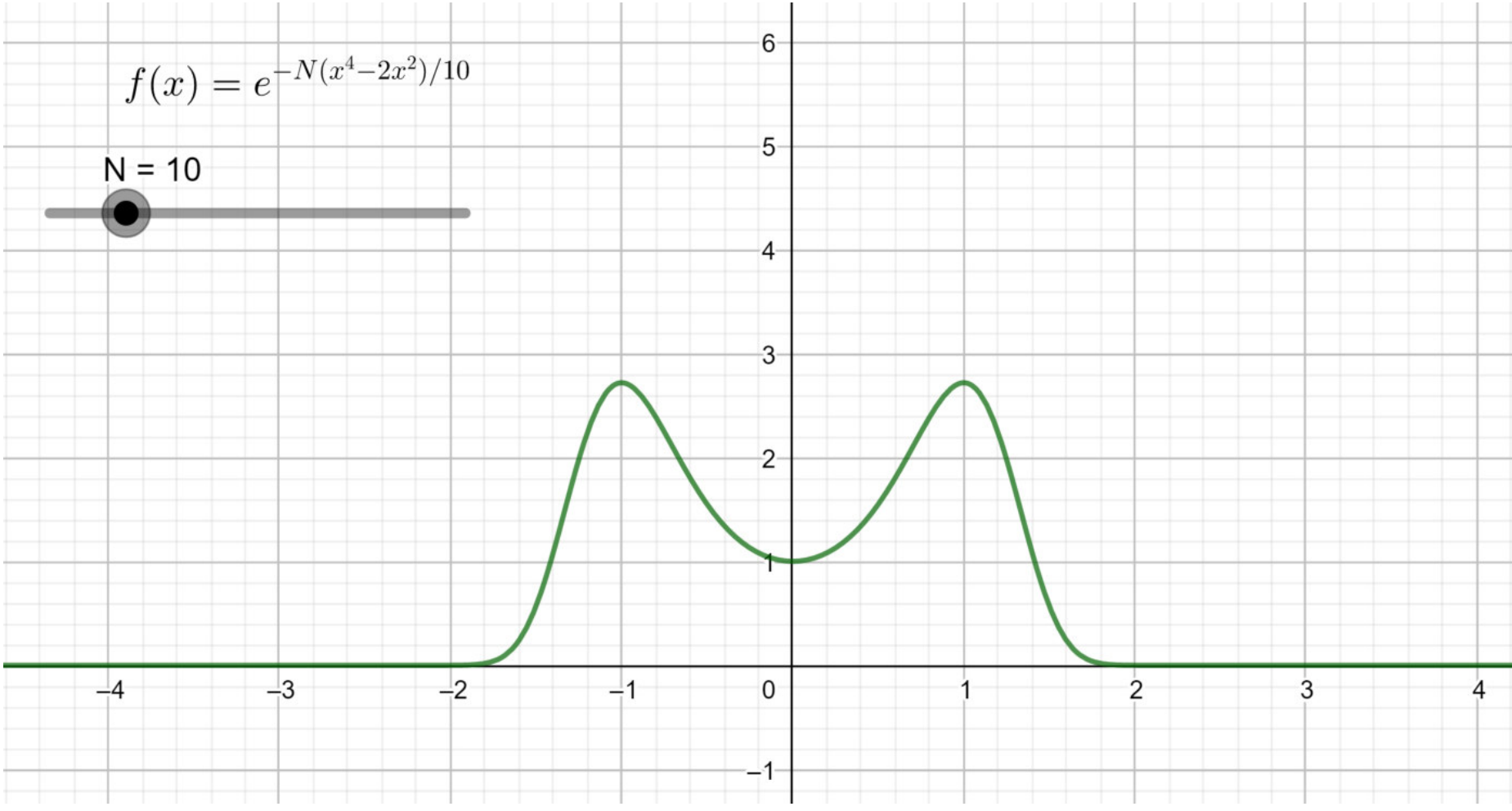
V.1 The large N Effect

The large N-effect is likely the most general reason that we can comprehend the world at all. The large N-effect helps to isolate properties. We show what we mean by this in an example of a graph of a function of the form $\exp\left(-Nf(x)\right)$ with a function $f(x)$ having only little structur:



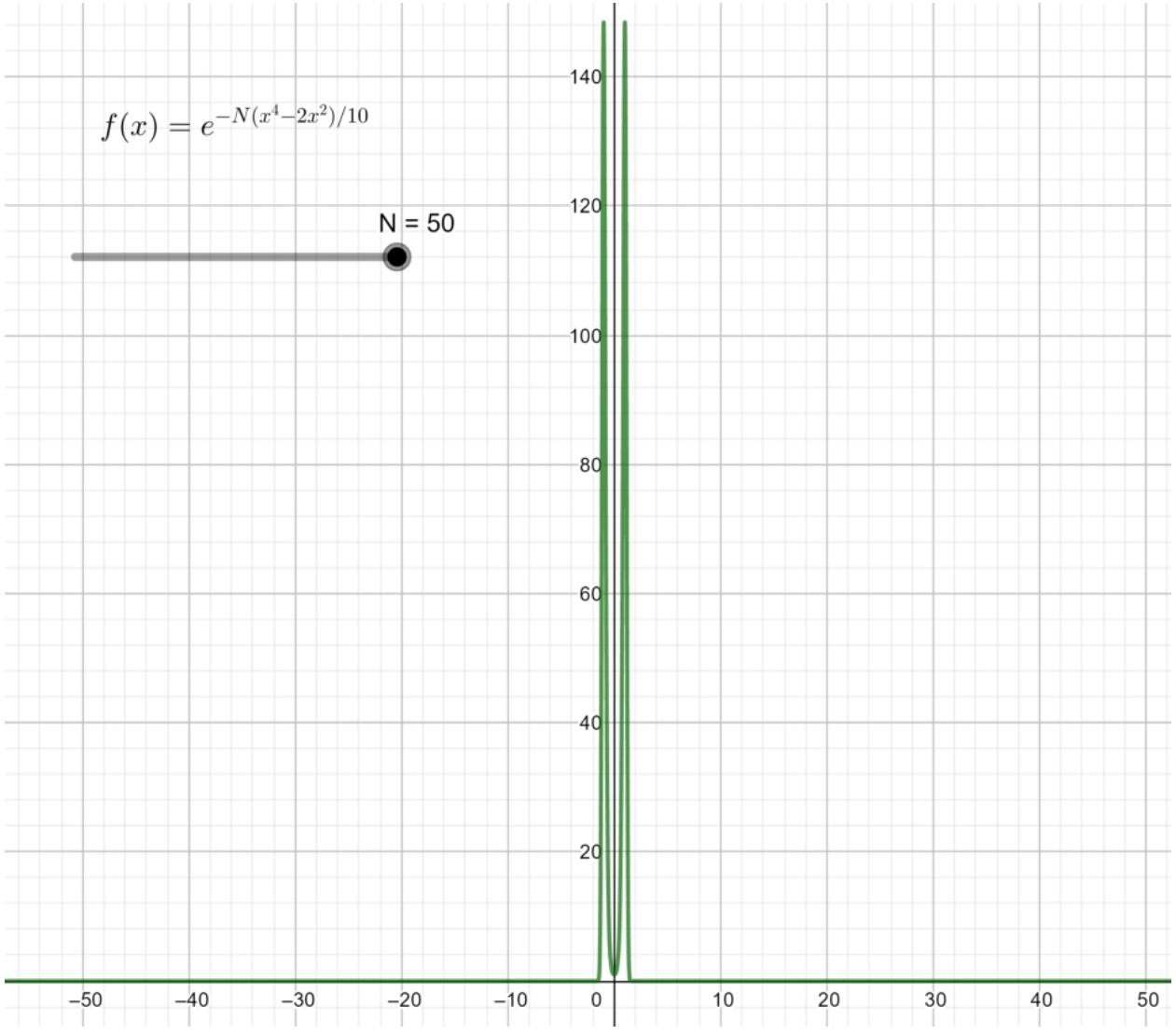
V.1 The large N Effect

Once we increase N to 10, the little structures will be amplified



V.1 The large N Effect

On increasing N to 50 the little structure becomes amplified to separated sharp peaks:



V.1 The large N Effect

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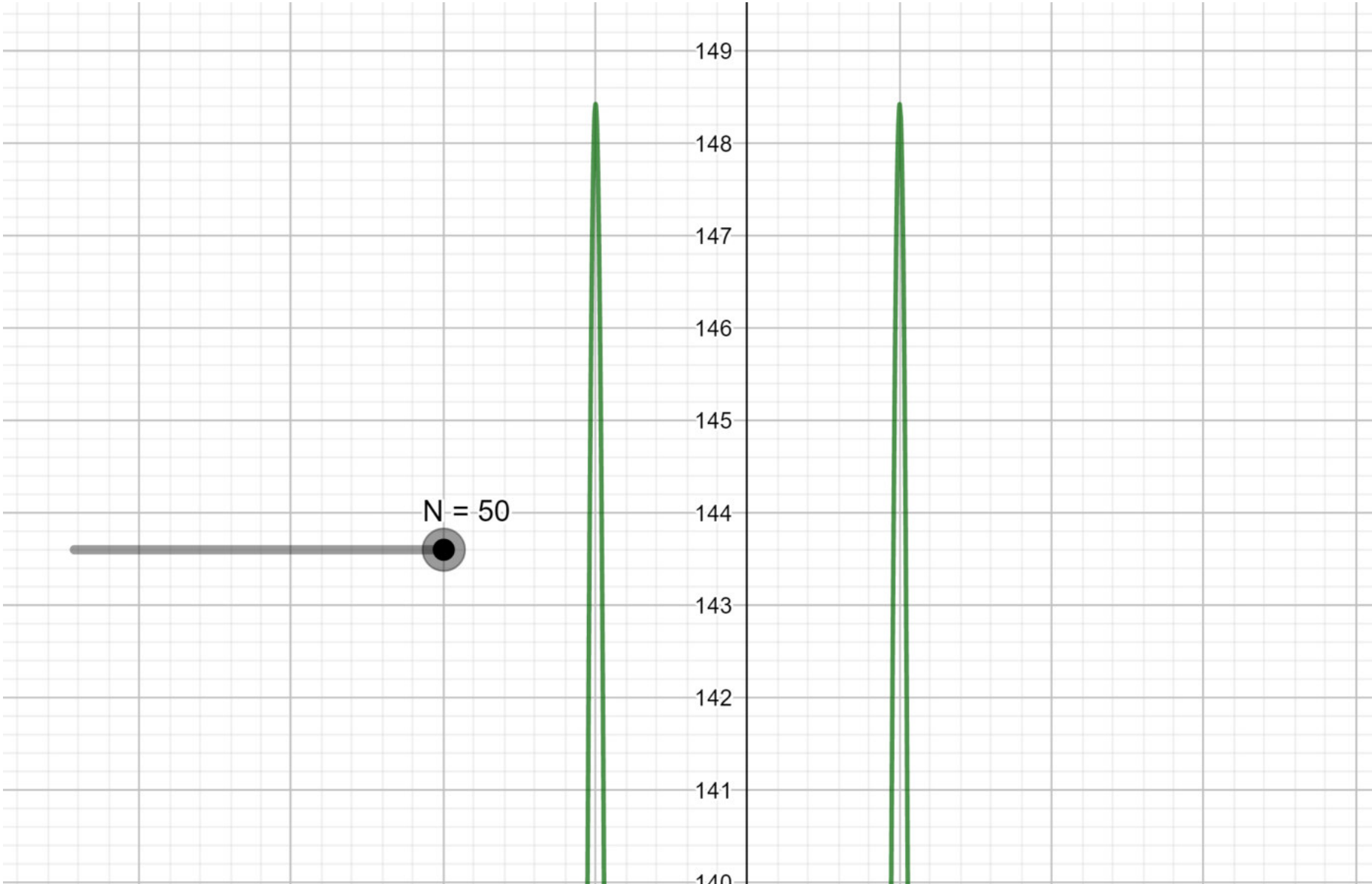

V.1 The large N Effect

The large N-effect in mathematical terms runs under the name of saddle point approximation or method of steepest descend or expansion around stationary action. In a simple form it can be studied from

$$\exp\left(-Nf(x)\right) \tag{33}$$

We expand $f(x)$ around one of its stationary solutions x_0,

$$f(x) = f(x_0) + f^{[2]}(x - x_0)^2 + \mathcal{O}(x - x_0)^3\,, \tag{34}$$

and introduce the rescaled deviation $\eta := (x - x_0)/\sqrt{N}$, resulting in an expansion for the full exponent as

$$Nf(x) = Nf(x_0) + f^{[2]}\eta^2 + \mathcal{O}\left(\eta^3/\sqrt{N}\right)\,. \tag{35}$$

The exponent is dominated by the stationary value and a sub-leading quadratic term. Higher order contributions die out asymptotically with large N. Thus, asymptotically with large N a Gaussian approximation with pronounced peak becomes exact.

V.1 The large N Effect

Let us comment on situations for the large N effect to occur:

- The emergence of the central limit theorem: N is the number of weakly correlated random numbers summed up to an average random number. Fluctuations become more and more Gaussian as N increases. The proof is along the generating function for cumulants, which is additive. N appears in exactly the way discussed here.
- In path integrals for Markov and quantum processes and in equilibrium partition sums: Either due to massive phase cancellations in quantum path integrals (large fluctuating imaginary exponents lead to randomly oscillating contributions in the sum over paths), or due to exponential suppression in weights of path integrals for Markov processes or statistical partition sums.

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- Then, the deterministic solution captures the essential physics behind the path integral with suppressed fluctuations. In quantum processes this corresponds to the "classical limit" (historically described in the WKB approximation). In Markov processes this corresponds to the limit of negligible diffusion, and in thermodynamic equilibrium this corresponds to the zero temperature limit where the energetic ground state characterizes the thermodynamic ground-state.
- The condition for non-fluctuating behavior in real systems is that typical process scales like wavelength, relaxation time and temperature are very small as compared to the systems global scales like effective system size, measurement time and excitation energy.

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- To illustrate the condition of non-fluctuating behavior for quantum processes we compare two systems: (1) A billiard ball of mass 0.15 kg in standard units and typical velocity of 5 m/s on a table of typical dimensions of 1.5 m. The wavelength is $h/(mv) = 8,8 \cdot 10^{-34}$ m and the ratio of the wavelength to the table size is approximately $6 \cdot 10^{-34}$. (2) An electron in a quantum dot of size 10 nm. Its (Fermi-) wavelength is of the same order of magnitude and hence the relation of wavelength to effective system size is of order 1. Obviously in case (1) quantum fluctuations are irrelevant, while they are essential in case (2).

V.2 Deterministic limit of Quantum (and Markov) processes

A path $x_c(t)$ that leaves the action stationary can serve as the starting point for an expansion in deviations from this stationary solution, $\eta(t) := x(t) - x_c(t)$,

$$S[x(t)] = S[x_c(t)] + S_2[\eta(t)] + \delta S[\eta(t)]\,. \tag{36}$$

where $S_2[\eta]$ contains quadratic fluctuations in η and $\delta S[\eta]$ all higher orders. The stationary path fulfills the Lagrange equation of classical mechanics,

$$\frac{\delta S[x(t)]}{\delta x(t)} = \frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} = 0\,. \tag{37}$$

When $\delta S[\eta(t)]$ turns out to be sub-leading, due to a large N-effect, the path integral can be approximated by the so-called stationary action approximation with Gaussian fluctuations as

$$\langle x_b, t_b \mid x_a, t_a\rangle \approx \exp\left\{iS_c(x_b, t_b; x_a, t_a)\right\} F(x_b, t_b; x_a, t_a)\,, \tag{38}$$

where $S_c(x_b, t_b; x_a, t_a)$ is the action for the stationary path under the boundary conditions

...

There are always fluctuations in the propagator.
When fluctuations become negligible or undetectable for practical reasons, the system can **best be described by the classical deterministic Lagrange equation** (in the Markov case by the drift equation alone). This is a consequence of system parameters (e.g. a large parameter N in S pronounces a stationary point) and is an **emergent phenomenon** like the emergence of Gaussian distributions with tiny variance in real statistical ensembles (central limit theorem for large number of additive random variables).

V.3 Emergence of Markov from Quantum

From the time evolution of a wave function

$$\psi_n(t) = \sum_m \langle n,t|m,t_0\rangle\, \psi_m(t_0)\,. \tag{40}$$

the corresponding probability distribution has a non-Markovian non-closed time evolution

$$\boxed{P_n(t) = \sum_{mm'} \langle n,t|m,t_0\rangle \langle m',t_0|n,t\rangle\, \psi_m(t_0)\psi^*_{m'}(t_0)}\,. \tag{41}$$

Diagonal terms ($m = n$) do not contain phase factors, but the off-diagonal terms do. Once, the off-diagonal parts can be neglected, we arrive at a Chapman-Kolmogorov equation characteristic for Markov processes,

$$\boxed{P_n(t) = \sum_m T(n,t;m,t_0) P_m(t_0)}\,, \tag{42}$$

with non-negative transition probabilities,

$$T(n,t;m,t_0) = |\,\langle n,t|m,t_0\rangle\,|^2\,. \tag{43}$$

...

In systems coupled only very tiny to some environment the phases are typically much more sensitive to the coupling than the amplitudes. After a characteristic time scale, called **decoherence time** τ_{dec}, the phases become effectively random and a coarse grained description for P_n cannot resolve the filigree information buried in the rapidly fluctuating off-diagonal contributions. Because of large sums over randomly fluctuating phases with smoothly varying amplitudes, the systems dynamics can effectively be described by a Markov process instead of the original quantum process. Thus, on a time scale larger than the decoherence time τ_{dec}, **the tiny coupling to the environment, not captured explicitly in the dynamics, will finally lead to the typical behavior of Markov processes, which means some relaxation and irreversibility**. We will put this heuristic consideration on a more firm basis when discussing open quantum systems in Chap. 5.

Exercise No. 3

1. Use the Lie series to solve $\dot{x} = -\gamma x$.
2. Show (7) from Eq. (1) of the first lecture and derive (8), (9).
3. Derive (10) from (8).
4. Write down the general form of the Fokker-Planck equation for a multicomponent configuration x^μ
5. Show that $\delta(x(t) - x)$ with drift equation $\dot{x} = -G_1(x)$ solves the Markov equation, if only G_1 is non-zero in the generator expansion.
6. Show the Gauss-Integral $\int \mathrm{d}x\, e^{-ax^2+bx+c} = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}+c}$ in two steps: First $b = c = 0$ and considering the square of the integral as performed in 2d with polar coordinates and then by quadratic extension for b, c finite.
7. Show that the L-function

$$L^{[G]}(x, \dot{x}) = G_0(x) + \frac{-\left(\dot{x} + G_1(x)\right)^2}{4G_2(x)} .$$

is the Legendre transform of a up to second order generator function $G(x, k)$ with respect to $\partial_{-ik} G(x, k) = \dot{x}$

04. Effective Dynamics by Integration and Projection

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bcgs intensive week course, july 2020

Content

I: Discrete vs. Continuous time

Velocities at time t must at least take one time step earlier or later into account. As a **discrete time derivative** we take

$$\overset{\sqcap}{f}_t := f_{t+1} - f_t \,. \tag{1}$$

In case of smooth behavior we can approximate linearly in the step width n as

$$f_{t+n} = f_t + c_t \cdot n + R(t,n) \,; \lim_{n\to 0} R(t,n)/(c_t \cdot n) = 0 \,. \tag{2}$$

and the time derivative equalls the number c_t at time t,

$$\dot{f}_t = \lim_{n\to 0} \frac{f_{t+n} - f_t}{n} = c_t \,. \tag{3}$$

With smoot behavior we can relate the function and its velocity to the same instant of time t and they can be related by a differential equation of the form $\dot{f} = V(f)$ with continuous function V. Then, for a given value of f there is a unique value of $\dot{f}$. This spoils the time reversibility of such differential equations.

I: Discrete vs. Continuous time

- Time reversible differential equations need a second poperty as an initial condition such that a second order differential equation results for each of them:

$$\ddot{f} = A(f) \tag{4}$$

  with continuous function A.
- When the smoothness condition (2) is not fulfilled, a strictly local in time derivative is meaningless and we have to rely on discrete derivatives like (1) which depend on two times, separated by one time step.
- As an important example consider the time evolution of facts ϕ_t. Each component ϕ_{tm} can only have two values, 0 and 1. The components of discrete time derivatives of facts can only take three discrete values:

$$\overset{\sqcap}{\phi}_{tm} \in \{-1, 0, 1\} \ . \tag{5}$$

I: Discrete vs. Continuous time

We conclude:

- It is not possible to associate a smooth local in time velocity to changing facts. **Therefore, we cannot express the discrete velocity of facts as a unique function of the fact at the same instant of time. We need two instants of time. This makes time reversible equations of motion possible with only the facts as initial condition, but at two instants of time.**
- In permutation dynamics, a time reversed process to a process generated by a permutation π will be generated by the inverse permutation π^{-1}. Which of the two is choosen can be fixed when considering the facts at $t = 0$ and $t = 1$.

II: Notions and Notations

For simplicity of the presentation we stick to discrete variables and recall that expectation values of some property A with possible values A_m are given by a probability distribution p with values p_m as

$$\langle A \rangle = \sum_m A_m p_m \, . \tag{6}$$

We refere to this notation as the **set notation of mean**. It is invariant with respect to simultaneous relabeling of A_m and p_m.

$$\langle A \rangle = \sum_m A_m p_m = \sum_m A_{\pi(m)} p_{\pi(m)} \, , \tag{7}$$

with $\pi \in S_N$ a permutation of indices.
We can interpret (6) as an euclidean scalar product between vector $|\, p)$ and co-vector $(A \,|$,

$$\langle A \rangle = (A|p) \, . \tag{8}$$

We refer to this notation as the **vector notation of mean**. It is invariant with respect to orthogonal transformations, including the permutations, of course.

II: Notions and Notations

For any orthogonal transformation O we have

$$(OA|Op) = \left(A|O^T Op\right) = (A|P) = \langle A \rangle \ . \tag{9}$$

The value p_m can be interpreted as the expectation value of fact $\phi^{[m]}$:

$$p_m = \left(\phi^{[m]}|p\right) \ . \tag{10}$$

However, after a non-permutational orthogonal transformation O the transformed fact cannot be interpreted as an original fact state, since

$$\overline{\phi^{[m]}}_l := \left(O\phi^{[m]}\right)_l = \sum_k O_{lk}\phi_k^{[m]} = \sum_k O_{lk}\delta_{km} = O_{lm} \, . \tag{11}$$

Only for permutations O_{lm} has $N-1$ zeroes and one value of 1.

II. Notions and Notations

Facts also have a characteristic property:

$$\phi_l^{[m]} \cdot \phi_l^{[m']} = \phi_l^{[m]} \delta_{mm'} \,. \tag{12}$$

This property gets lost after non-permutational orthogonal transformations,

$$\overline{\phi^{[m]}}_l \cdot \overline{\phi^{[m']}}_l = O_{lm} O_{lm'} \neq O_{lm} \delta_{mm'} \,, \tag{13}$$

such that transformed facts cannot be reinterpreted as different facts. This is **one of four motivations to introduce projection operators** (matrices) representing facts **and density operators** (matrices) representing probabilities. In addition, we enlarge the structure of the vector space by allowing complex numbers and using a unitary scalar product in order to have full power in solving secular equations for spectral decompositions.

II: Notions and Notations

A fact $\phi^{[m]}$ we had already represented by the vector $|m\rangle$ having zero entries for all of N components except for one entry of 1 at the m-th component. Now we represent it by the projection operator (matrix)

$$P^{[m]} := |m\rangle \langle m| \ , \tag{14}$$

where the essential projector properties hold:

$$\sum_m P^{[m]} = 1 \ , \ P^{[m]} P^{[m']} = P^{[m]} \delta_{mm'} \ ; \ {P^{[m]}}^\dagger = P^{[m]} \ . \tag{15}$$

Properties are lifted to Hermitian operators (matrices)

$$A = \sum_m A_m P^{[m]} \tag{16}$$

and probability distributions to so-called density operators

$$\rho = \sum_m p_m P^{[m]} \ . \tag{17}$$

II: Notions and Notations

The linear space of these operators can easily be equipped with its own canonical unitary scalar product the so-called Hilbert-Schmidt metric,

$$(A \mid B) := \mathrm{Tr}\left\{A^\dagger B\right\} = (B \mid A)^* \tag{18}$$

where $\mathrm{Tr}\, A := \sum_m A_{mm}$ is called trace and is the sum over all diagonal elements. It has the nice cyclic invariance property $\mathrm{Tr}\,\{ABC\} = \mathrm{Tr}\,\{BCA\}$. We can now write the expectation value in **matrix notation** as

$$\langle A \rangle = (A \mid \rho) \tag{19}$$

Unitary transformations U on vectors translate to adjoint transformations on operators:

$$\overline{\rho} = U^\dagger \rho U \;;\; \overline{A} = U^\dagger A U \tag{20}$$

II: Notions and Notations

Now, the expectation value is invariant under unitary transformations of both, A and ρ, as can be concluded from the cyclic invariance and $U^\dagger U = 1$,

$$\langle A \rangle = (A \mid \rho) = \left(\overline{A} \mid \overline{\rho}\right) . \tag{21}$$

Furthermore, in matrix notation the unitarily transformed fact projector is again a projector, **our second motivation for matrix notation:**

$$\overline{P^{[m]}}^2 = \overline{P^{[m]}} \tag{22}$$

Its matrix elements are $\overline{P^{[m]}}_{lk} = U_{ml} U_{mk}$ and such projector is usually non-diagonal in the original fact states representation and it will typically not commute with original $P^{[m]}$, such that both cannot be diagonalized simultaneously. Thus the new fact $|\alpha\rangle = U\ |m\rangle$ is typically incompatible with the original fact. However, this is not a drawback but an enrichment, since there are incompatible facts in nature which cannot be decided to be true or false simultaneously (e.g. rotation around two distinct axes or position vs. translation of objects).

II: Notions and Notations

The differential equation of motion in continuous time Markov processes can be written in vector notation as

$$(m|\dot{p}_t) = (m|Mp_t) \tag{23}$$

which clearly shows that $\dot{p}$ at instant of time t is a functional of p at this instant of time. Thus, such processes cannot be reversed in time since the probability flux is uniquely given by the probability distribution and cannot be reversed to start with the same distribution in reversed order. Indeed, the stochastic matrices generated by M usually do not have inverse elements within the group of stochastic matrices. Typically inverse elements become negative and cannot be interpreted as transition probabilities any more. Finally, the vector notation allows for the introduction of vectors representing time derivatives of properties in the following sense:

$$(A|\dot{p}_t) = (A|Mp_t) = \left(M^T A|p_t\right) \; ; \; \dot{A} = M^T A \tag{24}$$

There are fluctuation relations between A and $\dot{A}$.

II: Notions and Notations

The differential equation of motion in continuous time quantum processes, $\rho_t = e^{-i\mathcal{L}t}\rho_0 = e^{-iHt}\rho_0 e^{iHt}$, can be written in matrix notation as

$$\left(P^{[m]} \mid \dot{\rho}_t\right) = \left(P^{[m]} \mid -i\mathcal{L}\rho_t\right) = \left(P^{[m]} \mid -i\left[H, \rho_t\right]\right) \tag{25}$$

The equation of motion is called von-Neuman equation

$$\dot{\rho} = -i\left[H, \rho\right] . \tag{26}$$

Now, due to the commutator, the probability flux is not a functional of the probability distribution, but rather of the **off-diagonal components** of the density matrix. This allows for a time reversible process, **our third motivation for matrix notation**. These off-diagonal components are usually called coherences. I prefer the notion of **flux capacities**. In explicit matrix notation ones has

$$\dot{\rho}_{mm} = \sum_{n \neq m} I_{mn} \; ; \; I_{mn} = 2\,\mathrm{Im}\left(H_{mn}\rho_{nm}\right) . \tag{27}$$

II: Notions and Notations

For a quantum state $\psi_m = \sqrt{p_m} e^{i\varphi_m}$ one has

$$\boxed{\rho_{mn} = \sqrt{p_m p_n} e^{i\varphi_m - \varphi_n}}. \tag{28}$$

The meaning of pre-probabilities is: diagonal elements of ρ capture probabilities and off-diagonal elements capture flux capacities. The fact that only the imaginary part of $H_{mn}\rho_{nm}$ $(n \neq m)$ counts dynamically allows for so-called gauge freedom between ρ and H.

Finally, the matrix notation allows for the introduction of operators representing time derivatives of properties in the following sense:

$$\partial_t \langle A \rangle_t = (A \mid \dot{\rho}_t) = (A \mid -i\mathcal{L}\rho_t) = (i\mathcal{L}A \mid \rho_t) \tag{29}$$

Thus, the so called Heisenberg-equation

$$\boxed{\dot{A} = i\,[H, A]} \tag{30}$$

represents an operator for the time derivative of A. Typically A and $\dot{A}$ do not commute which results in unavoidable fluctuation-relations between them.

III. Integrating out Irrelevant Variables

- When only a reduced set of **relevant variables** are characteristic for our investigation we would like to have closed equations for only them.
- In terms of a probability distribution for the reduced variable $A(\vec{x})$ (typically the number of degrees of freedom of A is much lower than that of $\vec{x}$) the construction of the distribution for A in terms of the distribution for $\vec{x}$ is straightforward

$$\boxed{P_t(A) := \langle \delta(A - A(x) \rangle_{P_t(x)}} \,. \tag{31}$$

  We will show how this integration works a little later.
- If $P_t(x)$ follows a Master equation, so does $P_t(A)$ and the Kramers-Moyal coefficients can easily be derived by simply studying the **moments of deviations** δA **in short time**. This is already the beautifully simple recipe for Markov processes and nothing spectacular happens to the formalism as such.

III. Integrating out Irrelevant Variables

- In terms of pre-probabilities or corresponding projectors something very interesting happens: **a reduced projector is no longer described by a projector but by a more general density matrix** ρ which fulfills three conditions: (a) it is Hermitian, (b) non-negative (for all m $\mathrm{Tr}\left\{P^{[m]}\rho\right\} \geq 0$)and (c) normalized to unity ($\mathrm{Tr}\,\rho = 1$). This is **our fourth motivation for matrix notation**. **However, reduced facts remain facts.**

This can be understood by the following discussion of a vector-state in a product Hilbert space $\mathcal{H}_A \times \mathcal{H}_B$

$$\mid \psi\rangle = \sum_{A_i,B_j} \psi(A_i,B_j) \mid A_i\rangle \mid B_j\rangle \ . \tag{32}$$

The corresponding projector reads

$$P_\psi = \sum_{A_i,B_j,A_k,B_l} \psi^*(A_k,B_l)\psi(A_i,B_j) \mid A_i\rangle \mid B_j\rangle \langle B_l \mid \langle A_k \mid \ . \tag{33}$$

...

. . . Once we consider observables belonging to A and not to B we can calculate their expectation values with the help of a state ρ_A defined by the following constraint:

$$\langle f(A)\rangle = \operatorname*{Tr}_{AB}\{P_\psi f(A)\} = \operatorname*{Tr}_{A}\{\rho_A f(A)\}\ , \tag{34}$$

and ρ_A results from a partial trace along B over P_ψ,

$$\varrho_A \cdot := \operatorname*{Tr}_{B}\{P_\psi \cdot\}\ . \tag{35}$$

The matrix representation of ρ_A is then (our third motivation for a matrix notation)

$$\boxed{(\rho_A)_{ki} = \textstyle\sum_{B_l} \psi^*(A_k, B_l)\psi(A_i, B_l)}\,. \tag{36}$$

We leave it as an exercise to show that this a density matrix. Density matrices which reduce to projectors $\rho = \rho^2$ are called pure states. We leave it also as an exercise to show that reduced fact states are again fact states.

III. Integrating out Irrelevant Variables

In the context of path integral representations we deal with integrals of the type of a partition (sum) integral over an high-dimensional space,

$$Z = \int d^N x \, e^{-S(x_1,\ldots,x_N)} \, . \tag{37}$$

As we will not elaborate further on path integrals in this course I will only sketch some ideas how to get an effective dynamics by integrating out irrelevant variables.

- **Symmetries** of S[x] call for **adjusted coordinates** y some of which will not show up in $S[x[y]]$ and will be integrated out.

We demonstrate this on the simplest possible scenario with just two coordinates a and a^* and $S = S(aa^*)$. Since S has a rotational symmetry in the complex a-plane we introduce radial coordinates r and angle ϕ to write $a = re^{i\phi}$ and the measure transforms like $da \wedge da^* = (dre^{i\phi} + ire^{i\phi}d\phi) \wedge (dre^{-i\phi} - ire^{-i\phi}d\phi) = 2id\phi \wedge dr$

$$Z = \int da \wedge da^* e^{-S(aa^*)} = 2\pi i \int dr^2 \, e^{-S(r^2)} \, . \tag{38}$$

III. Integrating out Irrelevant Variables

- We have a relevant variable X which accumulates many of the variables x_i. We introduce the **constraint** $\delta(X - X[x])$ into the integral, rewrite it by the **Fourier representation** of the δ-function on introducing a dual to X coordinate K, rewrite terms in S by the constraint and try to **integrate out all of the original (now irrelevant) variables**.

We demonstrate this on a very simple scenario of additive X and S to keep it simple: $X = \sum_i x_i$ and $S[x] = \sum_i V(x_i)$. Then, a probability density for X can be written (with normalization constant Z) as

$$P(X) = Z^{-1} \int d^N x \, e^{-\sum_i V(x_i)} \delta(X - \sum_i x_i) =$$

$$= 2\pi Z^{-1} \int dK \int d^N x \, e^{-\sum_i V(x_i) + iK(X - \sum_i x_i)} \, . \qquad (39)$$

On sorting the exponent we can write ...

...

$$P(X) = 2\pi Z^{-1} \int dK e^{iKX} \int d^N x \, e^{-\sum_i (V(x_i) - iKx_i)} = \\ = 2\pi Z^{-1} \int dK e^{iKX} e^{N \cdot \ln\left(\int dx \, e^{-V(x) - iKx}\right)} . \quad (40)$$

Since N is large, we make a Gaussian approximation around assumed minimum at $x = 0$: $V(x) \approx ax^2$ with positive a and calculate the Gaussian integral in x and then in K and find:

$$P(X) = \tilde{Z}^{-1} \int dK e^{iKX} e^{-NK^2/4a} = \\ = \tilde{Z}^{-1} e^{-aX^2/N} , \quad (41)$$

with $\tilde{Z} = \sqrt{\frac{\pi}{a/N}}$ by normalization. In this simple scenario we finally arrived at the full distribution of relevant variable X.

IV. Projecting to Subspace of Relevance

Reducing variables by projection techniques yields a main conclusion: **The resolvent form of quantum processes**

$$\rho(z) = i\,[z - \mathcal{L}]^{-1}\,\rho_0\ ;\ z = \omega + i\epsilon\ ;\ \epsilon \to 0+\,, \tag{42}$$

can be kept with three modifications that capture the essence of effective dynamics of relevant variables in an environment of irrelevant variables. The (semi-) group property, however, can only be restored when neglecting memory effects.

1. When sums over the environmental frequency spectrum should be replaced by integration due to the impossibility to resolve its discrete character, then **a dynamical phase transition to irreversible dynamics occurs**. It shows up in the breaking of Hermiticity of $\mathcal{L}$.
2. The **effective non-Hermitian Liouville becomes frequency dependent** reflecting memory effects due to the environment,

$$\mathcal{L}(\omega) = \mathcal{H}(\omega) - i\Gamma(\omega)\ ;\ \mathcal{H}^{\dagger}(\omega) = \mathcal{H}(\omega)\ ;\ \Gamma(\omega) \geq 0\,. \tag{43}$$

...

IV. Projecting to Subspace of Relevance

...

3. Initial correlations show up in the **frequency dependent** modification of the **initial state** $\rho_0(z)$.

When the frequency dependence of $\mathcal{L}$ and ρ_0 is inessential in the dynamic range to be considered (e.g. for long-time asymptotic behavior corresponding to $z \to 0$) memory effects die out and a semi-group dynamic can be a god approximation.

In the following we give a detailed derivation of the above statements relying on the quite general projector formalism initiated by Nakajima and Zwanzig ≈ 60 years ago. Furthermore, we entirely work in the complex frequency setup instead of a time dependent setup because we know from electrical engineering that this is appropriate to handle memory effects. Mathematically, memory is local in complex frequency while it involves convolution time integrals in a time dependent picture.

Equation of Motion in Open Systems

- Consider a system coupled to an environment. The environment has not to be spatially outside of the system, but it has to contain a huge number of variables which cannot be followed in detail but are coupled to our relevant variables. This characterizes our system as being **"open"**. We do not use any weak coupling assumption but assumptions about the spectral properties instead.
- The reduced density operator is defined by a projector $\mathcal{P}$ on the Hilbert-Schmidt space

$$\rho := \mathcal{P}\rho_{\mathrm{tot}} \,. \tag{44}$$

Here ρ_{tot} is the total density operator of the total closed system. As an example one may take

$$\mathcal{P}\cdot = \operatorname*{Tr}_{E}(\cdot) \otimes \rho_E \,, \tag{45}$$

where ρ_E is the would-be stationary density operator of the environment - if the environment was not coupled to the system.

Equation of Motion in Open Systems

- The reduced density operator ρ is an element of the $\mathcal{P}$-space and can be represented by a $d \times d$ dimensional density matrix when the closed system's Hilbert space is d-dimensional.
- The projector on the complement to the $\mathcal{P}$-space is denoted as $\mathcal{Q} := 1 - \mathcal{P}$. Both projectors fulfill the projector property ($\mathcal{P}^2 = \mathcal{P}$, $\mathcal{Q}^2 = \mathcal{Q}$) and the complement property ($\mathcal{P}\mathcal{Q} = \mathcal{Q}\mathcal{P} = 0$.) The complement space is simply denoted as $\mathcal{Q}$-space.
- We like to construct the dynamic equation for the reduced density operator $\rho(t)$ by using the decomposition,

$$\rho_{\rm tot} = \rho + \Delta\rho^{\rm corr}\,,\ \Delta\rho^{\rm corr} := \mathcal{Q}\rho_{\rm tot}\,, \tag{46}$$

where $\Delta\rho^{\rm corr}$ captures correlations between system and environment. The group-property of the total system transforms to the resolvent equation of the total system

$$\rho_{\rm tot}(z) = i\left[z - \mathcal{L}_{\rm tot}\right]^{-1}\rho_{\rm tot0}\,. \tag{47}$$

Equation of Motion in Open Systems

We start by decomposing ρ's,

$$\begin{aligned}\rho(z) &= i\mathcal{P}\left[z-\mathcal{L}_{\rm tot}\right]^{-1}(\mathcal{P}+\mathcal{Q})\rho_{\rm tot\,0} \\ &= i\mathcal{P}\left[z-\mathcal{L}_{\rm tot}\right]^{-1}\mathcal{P}\rho_0 + i\mathcal{P}\left[z-\mathcal{L}_{\rm tot}\right]^{-1}\mathcal{Q}\Delta\rho_0^{\rm corr}\,, \end{aligned} \quad (48)$$

and $\mathcal{L}$,

$$\mathcal{L}_{\rm tot} = \mathcal{L}_{\mathcal{P}} + \mathcal{L}_{\mathcal{P}\mathcal{Q}} + \mathcal{L}_{\mathcal{Q}\mathcal{P}} + \mathcal{L}_{\mathcal{Q}}\,, \quad (49)$$

and use the algebraic identities

$$[A-B]^{-1} = A^{-1} + A^{-1}B[A-B]^{-1}\,, \quad (50)$$

$$[A-B]^{-1} = A^{-1} + [A-B]^{-1}BA^{-1}\,, \quad (51)$$

which can be verified by multiplication with $A-B$ from the right or from the left, respectively.

Equation of Motion in Open Systems

Therefore we can write for the projected total resolvent

$$\begin{aligned}
\mathcal{P}[z-\mathcal{L}_{\rm tot}]^{-1}\mathcal{P} &= [z-\mathcal{L}_{\mathcal{P}}]^{-1} + \\
&+ [z-\mathcal{L}_{\mathcal{P}}]^{-1}\left(\mathcal{L}_{\mathcal{Q}}+\mathcal{L}_{\mathcal{PQ}}+\mathcal{L}_{\mathcal{QP}}\right)[z-\mathcal{L}_{\rm tot}]^{-1}\mathcal{P}\,, \\
\mathcal{Q}[z-\mathcal{L}_{\rm tot}]^{-1}\mathcal{P} &= \mathcal{Q}\,[z-\mathcal{L}_{\mathcal{Q}}]^{-1}\mathcal{P} + \\
&+ [z-\mathcal{L}_{\mathcal{Q}}]^{-1}\left(\mathcal{L}_{\mathcal{P}}+\mathcal{L}_{\mathcal{PQ}}+\mathcal{L}_{\mathcal{QP}}\right)[z-\mathcal{L}_{\rm tot}]^{-1}\mathcal{P}\,, \\
\mathcal{P}[z-\mathcal{L}_{\rm tot}]^{-1}\mathcal{Q} &= \mathcal{P}\,[z-\mathcal{L}_{\mathcal{Q}}]^{-1}\mathcal{Q} + \\
&+ \mathcal{P}\,[z-\mathcal{L}_{\rm tot}]^{-1}\left(\mathcal{L}_{\mathcal{P}}+\mathcal{L}_{\mathcal{PQ}}+\mathcal{L}_{\mathcal{QP}}\right)[z-\mathcal{L}_{\mathcal{Q}}]^{-1}\,.
\end{aligned}$$

Due to the complementary character of projectors we conclude

$$\mathcal{P}[z-\mathcal{L}_{\rm tot}]^{-1}\mathcal{P} = [z-\mathcal{L}_{\mathcal{P}}]^{-1} +$$

$$+ [z-\mathcal{L}_{\mathcal{P}}]^{-1}\left(\mathcal{L}_{\mathcal{PQ}}\,[z-\mathcal{L}_{\mathcal{Q}}]^{-1}\,\mathcal{L}_{\mathcal{QP}}\right)[z-\mathcal{L}_{\rm tot}]^{-1}\mathcal{P}\,, \qquad (52)$$

$$\mathcal{P}[z-\mathcal{L}_{\rm tot}]^{-1}\mathcal{Q} = \mathcal{P}\,[z-\mathcal{L}_{\rm tot}]^{-1}\,\mathcal{L}_{\mathcal{PQ}}\,[z-\mathcal{L}_{\mathcal{Q}}]^{-1}\,. \qquad (53)$$

(52) tells that the total resolvent projected to $\mathcal{P}$-space can be written as the resolvent of an effective Liouville operating solely on $\mathcal{P}$-space, ...

$$\mathcal{P}[z-\mathcal{L}_{\rm tot}]^{-1}\mathcal{P}=[z-\mathcal{L}(z)]^{-1}\,, \tag{54}$$

. . . where the effective Liouville reads

$$\boxed{\mathcal{L}(z)=\mathcal{L}_{\mathcal{P}}+\mathcal{L}_{\mathcal{PQ}}\,[z-\mathcal{L}_{\mathcal{Q}}]^{-1}\,\mathcal{L}_{\mathcal{QP}}}\,. \tag{55}$$

The **first term $\mathcal{L}_{\mathcal{P}}$ is the closed system's Liouville** in the absence of an environment and **the second term describes virtual processes in the system triggered by the environment**, $\mathcal{L}_{\mathcal{PQ}}\,[z-\mathcal{L}_{\mathcal{Q}}]^{-1}\,\mathcal{L}_{\mathcal{QP}}$, hopping to $\mathcal{Q}$-space, there taking a lift with isolated $\mathcal{Q}$-propagator and finally hopping back to $\mathcal{P}$-space. The effective Liouville can be used as well in (53) and we find

$$\mathcal{P}[z-\mathcal{L}_{\rm tot}]^{-1}\mathcal{Q}=[z-\mathcal{L}(z)]^{-1}\,\mathcal{L}_{\mathcal{PQ}}\,[z-\mathcal{L}_{\mathcal{Q}}]^{-1}\,. \tag{56}$$

With (55) and (56) we can rewrite (48)

$$\boxed{\rho(z)=i\,[z-\mathcal{L}(z)]^{-1}\,(\rho_0+\Delta\rho_0^{\rm corr}(z))}\,, \tag{57}$$

with

$$\Delta\rho_0^{\rm corr}(z)=\mathcal{L}_{\mathcal{PQ}}\,[z-\mathcal{L}_{\mathcal{Q}}]^{-1}\,\Delta\rho_0^{\rm corr} \tag{58}$$

Equation of Motion in Open Systems

$\Delta\rho_0^{\mathrm{corr}}(z)$ appears as a **virtual change of initial state within the system**, caused by the initial correlation $(\mathcal{Q}\rho_{\mathrm{tot}0})$ that gets a lift by the isolated $\mathcal{Q}$-propagator and hops to $\mathcal{P}$-space.

- Equation (57) is the announced result. It is an equation of motion defined solely for states of the system.
- The environment enters in an operative way through the couplings, $\mathcal{L}_{\mathcal{PQ}}, \mathcal{L}_{\mathcal{QP}}$, and the isolated $\mathcal{Q}$-propagator, $[z - \mathcal{L}_{\mathcal{Q}}]^{-1}$.
- By decomposing the $\mathcal{Q}$ propagator in its Hermitian and Anti-Hermitian part for $\epsilon \to 0+$ by

$$\boxed{[z - \mathcal{L}_{\mathcal{Q}}]^{-1} = \mathrm{P}\,[\omega - \mathcal{L}_{\mathcal{Q}}]^{-1} - i\pi\delta(\omega - \mathcal{L}_{\mathcal{Q}})}, \qquad (59)$$

where P stands for the Cauchy principal value on integration and $\delta(x)$ for the delta-function on integration. From this decomposition all of the remaining statements of this section can be concluded.

04. Exercises

1. For a trajectory $x(t)$ a time reversed path with time reversal at $t = 0$ is defined by: $\tilde{x}(t) = x(-t)$. Show that $\dot{\tilde{x}}(t) = -\dot{x}(-t)$ and $\ddot{\tilde{x}}(t) = \ddot{x}(-t)$. A dynamic is said to be time reversal symmetric if $\tilde{x}(t)$ is also a solution of the dynamics, if $x(t)$ is a solution. Show that a dynamic equation $\dot{x} = v(x)$ cannot be time reversal symmetric by considering $t = 0$ and that a dynamic equation of type $\ddot{x} = a(x)$ is not in conflict with time reversal symmetry at $t = 0$.
2. We have seen that fact states don't have local in time derivatives, but only discrete derivatives with values$\in \{-1, 0, 1\}$. Argue, that on averaging with a probability distribution p with components p_m a local in time derivative of averaged facts can make sense and why one could think of this as a large N effect.
3. Show the cyclic invariance and the unitary invariance of the trace and verify (21) and (22).
4. Show by the von-Neumann equation that current flux in quantum processes is given by (27).
5. Show that (31) is the appropriate distribution for all functions of reduced variable $A(x)$. ...

. . .

6. Show that (36) is a density matrix, not a projector, in general, but in case of facts it reduces to facts. Construct it for two two-value systems with originally pure states for
(a) product state

$$\mid \psi\rangle = \mid A+\rangle \mid B-\rangle \ ,$$

(b) entangled states

$$\mid \psi\rangle = \sqrt{\frac{1}{2}} \left(\mid A+\rangle \mid B-\rangle \pm \mid A-\rangle \mid B+\rangle \right) \ .$$

7. Show by using (59) that the effective Liouville can be written in the form of (43).

05. Open systems: approach to equilibrium and decoherence

Martin Janßen

bcgs intensive week course, july 2020

Content

I.1: The Problem of Equilibrium

The thermodynamic laws formulate universal experiences:

0. Systems of many constituents under stationary boundary conditions reach a stationary state after some characteristic relaxation time.
1. Energy is always preserved, but can change into many forms.
2. Processes run by themselves only in a certain time order.

- However, irreversibility described in 0. and 2. is in direct contradiction to the reversibility of the known basic equations of motion by Newton, Maxwell, Einstein and von-Neumann.
- A most general formulation of thermodynamic laws - without resorting to an explicit dynamic theory - is achieved in the axiomatic thermodynamics (Clausius, Caratheodory, Lieb and Yngvason) where the entropy as a state quantity serves to identify processes that run the correct time ordering. In addition, entropy serves as a state variable that corresponds to the everyday concept of heat.

I.1: The Problem of Equilibrium

- With the statistical interpretation (Boltzmann, Einstein, Gibbs) of **entropy as measure for the degree of dispersion of energy over possible states**, a new interpretation and calculational options arose for the equations of state of matter.
- The interpretation is: The natural time ordering is such that in the overwhelming majority of cases the dispersion of energy over possible states increases with increasing time.
- However, a justification of this statistical thermodynamics in the context of actual dynamic laws still appears contradictory. In the literature there is no common agreement on how to solve this fundamental puzzle.
- Here is my view, heavily influenced by my teacher J. Hajdu and by J. Polonyi, on solving the puzzle:
- **The irreversibility arises in open systems as a dynamic phase transition with breaking of the time reversal symmetry.**

I.1: The Problem of Equilibrium

My solution in short:

- A system is connected to an environment (possibly within the system's volume) with a large number of variables, the dynamics of which cannot be resolved in detail and can only be captured by an energy density in an effective dynamics of the open system.
- This creates a relaxator in the effective Liouville by a dynamic phase transition that captures irreversibility.
- The open system reaches a typically unique stationary state after a characteristic relaxation time.
- If the energy is conserved in the stationary state the micro-canonical distribution of statistical thermodynamics is favored as stationary state.

I.2: The Problem of Decoherence

Decoherence is a popular notion with lots of vague interpretations.
I like to fix it for this lecture by exclusion and by a definition.
It is often written or said that in a superposition of two states (which are assumed to be orthonormal),

$$|\psi\rangle = \alpha\,|1\rangle + \beta\,|2\rangle\ ,\ |\alpha|^2 + |\beta|^2 = 1 \tag{1}$$

the systems is in a sense in both states simultaneously. This does not make sense! Orthogonal states correspond to mutually exclusive properties which can never be true simultaneously.
To clarify the meaning of a superposition let us have a look at the projector $P_\psi = |\psi\rangle\langle\psi|$ as a matrix in the $1, 2$ basis:

$$P_\psi = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \beta\alpha^* & |\beta|^2 \end{pmatrix} \tag{2}$$

Therefore, the probabilities for finding one of the two states to be true are $|\alpha|^2$ and $|\beta|^2$, respectively. ...

I.2: The Problem of Decoherence

However the off-diagonal elements (coherences) show that there will likely appear Rabi oscillations of these probabilities in a quantum process when starting with such state ψ, because the coherences serve as flux capacities

What can be said also is: If state ψ corresponds to a property which can be true or false, for finite α, β, it is incompatible with the properties 1 and 2, because its overlap is neither 1 nor 0. In the first case it would be the same property as 1 and in case 0, ψ would be 2, a mutually exclusive property to 1.

So neither mutual exclusion nor incompatibility of states should be misinterpreted as simultaneous existence.

Now we can say what is ment by quantum coherence: Since coherences of a superposition are current capacities, their presence will likely lead - in a reversible quantum process - to oscillatory behavior in the probabilities to find one of several mutually exclusive properties. Very often in every day experience such oscillatory behavior is not observed. This leads us to our definition of decoherence. ...

I.2: The Problem of Decoherence

...

We say that a system shows **decoherence**, when the **coherences in a certain basis begin to decrease and become exponentially small** after some characteristic time scale, called decoherence time τ_{dec}.

The shrinking of decoherences **goes along with the shrinking of flux capacities** and finally **must lead to a stationary state**.

Therefore **decoherence can only show up within an irreversible process and the basis to be used is related to the stationary state** the system evolves to.

It is thus substantiated to look for **decoherence in an open quantum system** context.

II.1: Relaxation to a Stationary State in Open Systems

The Laplace transformed density of states $\rho(z)$ allows for an easy analysis of the long time limit in the usual sense as a long time average, defined by

$$f_\infty := \lim_{\epsilon \to 0+} \epsilon \int_0^\infty f(t) e^{-\epsilon t} dt \tag{3}$$

for a quite arbitrary time dependent function $f(t)$. Any oscillations that could still be present at large times in $f(t)$ will be averaged out. In the same sense it holds true that the long time limit is given by

$$f_\infty = \lim_{z \to 0} -iz f(z) \tag{4}$$

where $f(z)$ is the Laplace transformed of $f(t)$.
We take this limit on the equation of motion for open systems of Chap. 4,

$$\rho_\infty = \lim_{z \to 0} z \left[z - \mathcal{L}(z) \right]^{-1} \left(\rho_0 + \Delta\rho_0^{\mathrm{corr}}(z) \right) \tag{5}$$

and exclude that $\Delta\rho_0^{\mathrm{corr}}(z)$ may accidentally have a singular behavior for $z \to 0+$. ...

II.1: Relaxation to a Stationary State in Open Systems

. . . The long time limit is then determined by the zero limit of $z/(z - \mathcal{L}(z)$. This limit is non-vanishing due to the existence of zero modes of $\mathcal{L}(0+)$.

Let us denote the projector on the space of zero modes of $\mathcal{L}(0+)$ by $\Pi^0_{\mathcal{L}(0+)}$, then the long time limit of the density operator reads

$$\rho_\infty = \Pi^0_{\mathcal{L}(0+)} \left(\rho_0 + \Delta\rho_0^{\mathrm{corr}}(0+)\right) . \tag{6}$$

That the effective Liouville must have a zero mode is a consequence of probability conservation which means $\mathrm{Tr}\,\rho(z) = i/z$ and $\mathrm{Tr}\,\mathcal{L}(z)\rho_0 = 0$ for every z and ρ_0. Thus, the effective Liouville has the unit matrix 1 as a left eigenmatrix with eigenvalue 0 and, consequently, there must exist a right eigenmatrix with eigenvalue 0, too. In generic systems the zero mode will be non-degenerate and by normalizing the right zero mode to unit trace we can write the projector on the zero mode as

$$\Pi^0_{\mathcal{L}(0+)} = |\rho_\infty)\,(1| . \tag{7}$$

The notation refers to the Hilbert-Schmidt scalar product. . . .

II.1: Relaxation to a Stationary State in Open Systems

. . .

In generic open systems a stationary state is reached in the long time limit being independent of initial conditions, even if strong initial correlations with the environment had been present.

The heuristic estimate for the relaxation time τ after which the long time limit emerges is given by the virtual processes (hopping rate $1/\tau_{hopp}$ and characteristic time T_Q of oscillations for low frequencies ω within Q-space present in the effective Liouville) and reads $\tau = \tau_{\rm hopp} \cdot (\tau_{\rm hopp}/T_Q)$.

Equation (7) will change to a sum of projectors on different eigenstate combinations of zero modes in the case of degenerate zero modes. It is obvious that in such case the scalar product of left eigenmatrices with the initial state is not simply unity and these scalar products store information about the initial state. This opens a way to design non-generic open systems such that initial conditions can influence the final stationary states as discussed by V. Albert in 2018 for systems with semi-group dynamics.

II.2: Relaxation to a Stationary State in Open Systems with Energy conservation

Since $\mathcal{L}(0+) = \mathcal{H}(0+) - i\Gamma(0+)$ is no longer frequency dependent we can use it to construct a semi-group dynamics. It is known since 1976 (Lindblad) that in such case the Liouville can be written as $[H, \rho_\infty] - i\Gamma\rho_\infty = 0$, where H is the effective Hermitian Hamiltonian of the open system and Γ a relaxator, which is not necessarily Hermitian.

Now, we make an assumption. **We assume that the stationary state is an energy conserved state** within the system,

$$[H, \rho_\infty] = 0\,, \tag{8}$$

For such equilibrium situation we then also have

$$\Gamma\rho_\infty = 0\,. \tag{9}$$

Thus, the stationary state commutes with the Hamiltonian and will be diagonal in the energy representation $H\,|n\rangle = E_n\,|n\rangle$ and now its time to look at representations of the relaxator.

Technicalities

A density matrix in any orthonormal basis $\{|n\rangle\}_{n=1\ldots d}$ with $\langle n|m\rangle = \delta_{mn}$ can be written as $\rho = \sum_{nm} \rho_{nm} |n\rangle \langle m|$ with $\rho_{nm} = \langle n| \rho |m\rangle$.
Any super-operator $\mathcal{A}$ can with such ONB be written as

$$\mathcal{A}\cdot = \sum_{mn,rs} \mathcal{A}_{rs,mn} |r\rangle \langle s| \langle m| \cdot |n\rangle \ , \tag{10}$$

with

$$\mathcal{A}_{rs,mn} = \langle r| \mathcal{A}(|m\rangle \langle n|) |s\rangle \ . \tag{11}$$

For $\mathcal{L}$ and thus for Γ the probability conservation leads to $\mathrm{Tr}\,\Gamma\cdot = 0$ which leads to

$$\sum_m \Gamma_{mm,rs} = 0 \ \text{ for } \ \text{all } r,s \ . \tag{12}$$

II.2: Stationary State with Energy Conservation

The stationary state is diagonal in energy representation $\rho_\infty = \sum_n p_n \, |n\rangle \langle n|$ with non-negative probabilities p_n and (9) reads

$$0 = \sum_n \Gamma_{rs,nn} p_n \quad \text{for} \quad \text{all } r, s \; . \tag{13}$$

We specify to $r = s$ and decompose to bring in probability conservation (12)

$$0 = \sum_{n \neq r} \Gamma_{rr,nn} p_n + \Gamma_{rr,rr} p_r = \sum_{n \neq r} \left(\Gamma_{rr,nn} p_n - \Gamma_{nn,rr} p_r \right) \; . \tag{14}$$

Decomposing $W_{nr} := -\mathrm{Re}\ \Gamma_{nn,rr}$, $Y_{nr} := \mathrm{Im}\ \Gamma_{nn,rr}$ we find

$$\sum_{n \neq r} W_{rn} p_n - W_{nr} p_r = 0 \, , \tag{15}$$

$$\sum_{n \neq r} Y_{rn} p_n - Y_{nr} p_r = 0 \, , \tag{16}$$

II.2: Stationary State with Energy Conservation

Equation (15) looks like a stationary version of a Pauli Master equation commonly known to describe the irreversible evolution into equilibrium states with transition rates W_{rn}, fulfilling the equipartition law,

$$W_{rn}p_n - W_{nr}p_r = 0 \;\text{ for }\; r \neq n\,. \tag{17}$$

W_{rn} can indeed for $n \neq r$ be expected as non-negative transition rates since $\sum_{n\neq r} W_{nr} = -W_{rr} \geq 0$. The equipartition law expresses a so called micro reversibility of the dynamics saying that for the joint probability to find states r and n, separated by one time step, together, it does not matter which of both is taken at the earlier time or at the later time. From (17) the stationary distribution follows by recursion

$$p_n = \frac{W_{n0}}{W_{0n}} p_0\,. \tag{18}$$

...

II.2: Stationary State with Energy Conservation

. . . In a system with strict energy conservation, the transition rates within the energy shell are all equal (both according to Fermi's Golden Rule as well as according to the principle of ignorance) and one gets the micro canonical uniform distribution,

$$p_n \equiv 1/d\,. \tag{19}$$

In a system in a heat bath, the transition rate to the energetically higher state is by the Boltzmann factor $\frac{W_{nm}}{W_{mn}} = ce^{-(E_n - E_m)/T}$ of the energy difference over bath temperature T smaller than the reverse process, and for the stationary distribution one finds the canonical distribution,

$$p_n = \frac{e^{-E_n/T}}{\sum_{k=1}^{d} e^{-E_k/T}}\,. \tag{20}$$

III.1: Effective Eigenvalues of Effective Liouville

We like to find the time dependent density of states of an open quantum system from the spectrum of eigenvalues of the effective Liouville. We take the equation of motion and use the spectral decomposition of the resolvent

$$\rho(z) = i\left[z - \mathcal{L}(z)\right]^{-1}\rho_0(z) = \tag{21}$$

$$= -i\sum_{k=0}^{N}\frac{a_k(z)}{\left[z-\lambda_k(z)\right]}R_k(z)\,. \tag{22}$$

Here $R_k(z)$ is the right eigenmatrix of the effective Liouville corresponding to eigenvalue $\lambda_k(z)$ and

$$a_k(z) = \left(L_k(z) \mid \rho_0(z)\right) \tag{23}$$

is the scalar product between the corresponding left-eigenmatrix $L_k(z)$ and the effective initial state $\rho(z)$. Left- and Right-eigenmatrizes are chosen orthogonal and normalized as described in Chap. 2.

III.1: Effective Eigenvalues of Effective Liouville

Now we assume that $a_k(z)$ and $R_k(z)$ are non-singular in z and that isolated poles appear for $\rho(z)$ at so-called effective eigenvalues $z_k = \omega_k - i\gamma_k$ with $\gamma_k \geq 0$, defined by

$$z_k - \lambda_k(z_k) = 0\,. \tag{24}$$

Then the inverse Laplace transform can be performed, defined by,

$$\rho(t) = \frac{i}{2\pi} \int_{-\infty+i0+}^{\infty+i0+} dz\, e^{-izt} \left[z - \mathcal{L}(z)\right]^{-1} \rho_0(z)\,, \tag{25}$$

with the method of residue resulting in

$$\boxed{\rho(t) = \rho_\infty + \sum_{k=1}^{N} \frac{1}{2} \left(A_k e^{-i\omega_k t} + A_k^\dagger e^{i\omega_k t}\right) e^{-\gamma_k t}}\,. \tag{26}$$

Here the stationary state ρ_∞ has been separated and right eigenvectors at z_k with factors $a_k(z_k)$ and factors $1/(1 - d\lambda/dz(z_k))$ have been put together to matrices A_k and it was written in a way to make Hermiticity obvious.

III.2: Decoherence with Respect to the Stationary State

From (26) we can take the matrix elements in a basis where ρ_∞ is diagonal, as before, and write

$$\boxed{\rho_{nm}(t) = p_n \delta_{nm} + \sum_{k=1}^{N} \frac{1}{2} \left((A_k)_{nm} \, e^{-i\omega_k t} + (A_k)^*_{mn} \, e^{i\omega_k t} \right) e^{-\gamma_k t}} \, . \tag{27}$$

It can be seen that coherences die out exponentially fast and that the smallest non vanishing value of γ_k sets the time scale of decoherence and for the re-population of energy states, usually associated with dissipation.

$$\tau = \tau_{dec} = \frac{1}{\gamma_{\min}} \, . \tag{28}$$

In non-generic cases, the diagonal elements are totally unaffected, e.g., when the interaction with the environment preserves the systems energy throughout the process. Such cases are called pure dephasing cases, since no re-population occurs but only decay of coherences. However, this is an unusual situation.

05. Exercises

1. Verify Eqs. (3) and (4) of this chapter.
2. It is said in the lecture that degenerate zero modes may storage information about an initial state but non-degenerate zero modes do not. Why ist that? Think about the role of probability conservation and use Eqs. (6) and (7).
3. Heuristic estmates of time scales are very instructive for understanding what is going on. We simplify by associating typical time scales with parts of the Liouville as follows: $\mathcal{L}_{\mathcal{P}} \sim T_P^{-1}$, with T_P a typical period of oscillations within the isolated system $(z - \mathcal{L}_{\mathcal{Q}})^{-1} \sim T_Q^{[\omega]}$, with $T_Q^{[\omega]}$ a typical period of oscillations in the isolated environment for frequency range around ω. For low frequency range the characteristic time of period is simply denoted as T_Q. Finally $\mathcal{L}_{\mathcal{PQ}}, \mathcal{L}_{\mathcal{PQ}} \sim \tau_{\mathrm{hopp}}^{-1}$, where $\tau_{\mathrm{hopp}}^{-1}$ is the hopping rate between system and environment and the corresponding hopping time is τ_{hopp}.

...

05. Exercises

...

3. Now, find out the conditions for
   - 0.1 When is the effect of the environment small on the system?
   - 0.2 When can initial correlations be neglected?
   - 0.3 When is the relaxation time much larger than the hopping time?
   - 0.4 What is the effect of the hopping time being much larger than the geometric mean of system time and environment time?
4. Verify the technicalities from Eq. (10) to Eq. (14) or find bugs.
5. Take as an equation $\sum_{n \neq r} W_{rn}(p_n - p_r) = 0$. Keep in mind that probability conservation must be respected and find a criterion in terms of a determinant for a 3-level system, when the solution of such equation is not uniquely given by $p_n \equiv 1/3$.
6. Check the integration by residue from Eq. (25) to Eq. (26). Expand $\lambda_k(z)$ around each pole z_k into a series of powers $(z - z_k)$. ...

05. Exercises

...

7 What does probability conservation, $\mathrm{Tr}\,\rho = 1$, mean for the matrices $(A_k)_{mn}$ and $(A_k)^*_{mn}$ in Eq. (27)?

8 Very often one reads that decoherence is typically much faster than dissipation (re-population of energy states). What do you think now?

06. Deterministic representations of stochastic processes: averaging over what?

Martin Janßen

bcgs intensive week course, july 2020

Content

I.1: Why looking for?

Stochastic processes are described by probabilities for properties evolving in time by equations of motion based on (semi-)group dynamics. They are not necessarily in conflict with determined time evolution of the properties themselves. It is just easier to predict a relative frequency for large numbers N than to predict it for $N = 1$ due to the large N effect. In several interpretations of quantum theory it is fashionable to think that a prediction of individual facts is impossible and not that it is just harder than to predict relative frequencies.

When we observe determined behavior of properties on average as scientists we usually ask what is the behavior on an individual level. To assume that on an individual level a present state does not determine the state in the next time step, but has a huge number of equally possible outcomes, amounts to stop asking for sufficient reasons of events, which is exactly opposite to a scientific approach to reality.

I.1: Why looking for?

A conception that in each moment the world separates into infinitely many **undetermined** worlds one of which is actually chosen with instantaneous influences over arbitrary distances as a supernatural miracle usually would be declared as superstition.

Therefore, let us ask for a deterministic representation of stochastic processes including quantum processes to keep the scientific principle of searching for a sufficient reason intact.

I.2: What is a deterministic representation?

The stochastic process is characterized by an initial distribution $P_{t_0}(x)$ and corresponding time dependent distribution $P_t(x)$ for each time $t > t_0$. If one manages to find **for each initial value** $x(t_0)$ **a unique path** $x(t)$, such that **for each distribution** $P_{t_0}(x)$ **of initial values** $x(t_0)$ the resulting paths $x_k(t)$ (k labeling such corresponding paths) **lead to the time dependent distribution on averaging** over quasi-continuously many paths

$$\boxed{P_t(x) = \lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} \delta(x - x_k(t))}, \qquad (1)$$

we call this **ensemble of paths a deterministic representation** of the stochastic process. It is obvious that a deterministic representation is **by no means unique** for a given stochastic process. Think of changes in paths that have no effect on the averaging. For discrete variables x the δ-function has to be replaced by a Kronecker δ,

$$\boxed{P_t(x) = \lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} \delta_{x,x_k(t))}}, \qquad (2)$$

II.1 Integral Curves of Flux - Hydrodynamic Deterministic Representation

For every stochastic process with **continuous variable in continuous time a deterministic representation can be explicitly constructed in hindsight**, i.e. when the evolution of the distribution is known already. The corresponding paths $x(t)$ are simply the **integral curves of the probability flux** $v_t(x) := j_t(x)/P_t(x)$,

$$\dot{x}(t) = v_t(x(t))\,. \tag{3}$$

By construction the paths are smooth. I denote it as the **hydrodynamic deterministic representation** of the stochastic process. In case of external randomness e.g. by random scatterers acting on a particle we know that realistic paths should not smoothly follow the flux field, but are irregular motions, better described as fractal curves rather than smooth paths. Thus, when it is possible to observe individual **paths in Markov processes**, they **usually do not coincide with the hydrodynamic deterministic representation**....

II.2 Bohmian Mechanics

. . . In the case of quantum systems the hydrodynamic deterministic representation is known as **de Broglie-Bohm theory** or Bohmian mechanics. Its appealing feature is that no other variables besides the original configuration variables have to be taken into account. **Randomness just stems from the unknown initial conditions** of configuration variables. Two predictions: (1) In stationary states the deterministic realization stays at rest, distributed like the initial distribution. It is then plausible that stationary states of charged particles do not radiate. (2) Paths do not intersect each other (unique velocity field). For example, paths in a double slit experiment:

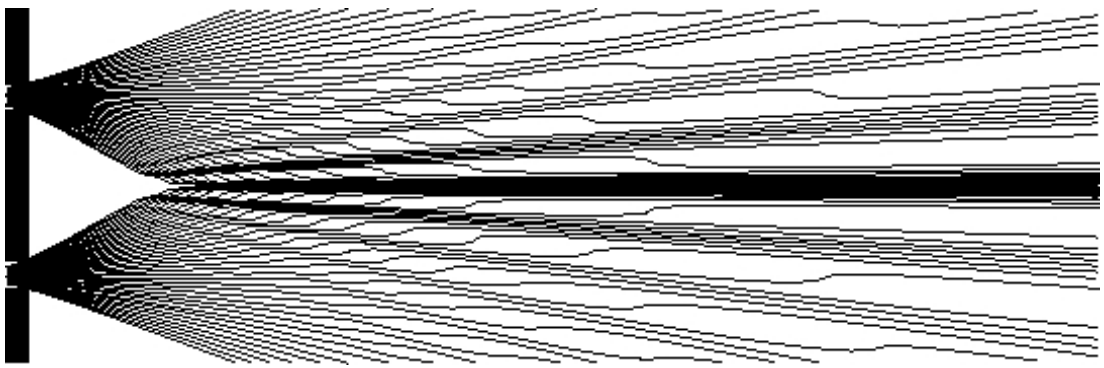

Figure: Paths for the two-slit experiment. (adapted by Gernot Bauer from Philippidis, Dewdney, Hiley 1979: 23, fig. 3) taken from Stanford Encyclopedia of Philosophy

II2. Bohmian Mechanics

. . . However, it does not mean that we can actually pin down this motion in a probabilistic prognostic sense. For example, the conditional probabilities for finding an interference pattern at detectors with particles entering through known initial slit positions vanishes and the corresponding wave function and its flux do not show any interference patterns. Thus, it is speculative that this hydrodynamic deterministic representation describes the true particle motion, because it is not unique and **we do not know how to experimentally check the priority of this hydrodynamic representation** as long as the accuracy to resolve individual paths is limited by the phase sensitivity of **observational influence destroying just that interference pattern for which we like to see the paths**.

II2. Bohmian Mechanics for Discrete Variables

When extending Bohmian dynamics to discrete variables (MJ unpublished) (e.g. for occupation numbers in quantum field theory) we have to define the probability flux in a convenient way. We do it the most general way in continuous time by Kirchhoff's law with Hamiltonian H. With projector $P_n = |n\rangle\langle n|$ we have as **flux gain and flux loss** at n, respectively,

$$I^{\text{gain}}_{nm}(n) := -iP_nHP_m \; ; \; I^{\text{loss}}_{nm}(n) := -iP_mHP_n \, . \tag{4}$$

The **total flux** at n by gain and loss with m is given as

$$\boxed{I_{nm}(n) = -i\left(P_nHP_m - P_mHP_n\right)} \, . \tag{5}$$

On average with density matrix ρ we have

$$\mathrm{I}_{nm}(n) := \langle I_{nm}(n)\rangle = -i\left(H_{nm}\rho_{mn} - \rho_{nm}H_{mn}\right) \tag{6}$$

and reproduce von Neumann for total flux at n on average

$$\partial_t \langle P_n\rangle = \dot{\rho}_{nn} = \sum_{m\neq n} \mathrm{I}_{nm}(n) = -i\sum_{m\neq n}\left(H_{nm}\rho_{mn} - \rho_{nm}H_{mn}\right) \, . \tag{7}$$

II2. Bohmian Mechanics for Discrete Variables

Now, a deterministic hydrodynamic representation could be reconstructed as follows

1. Solve for ρ_t and calculate $\mathrm{I}_{nm}(t)$.
2. Solve the initial value problem **for relative frequency** $h_n(t)$

$$h_n(t) = h_n(t_0) + \int_{t_0}^{t} dt' \sum_{m \neq n} \mathrm{I}_{nm}(t') \,, \tag{8}$$

and distribute initial values according to

$$\langle h_n(t_0) \rangle = p_n(t_0) = \rho_{nn}(t_0) \,. \tag{9}$$

3. The determined relative frequencies $h_n(t)$ will be identical on average with the time dependent probability of the quantum process and form a deterministic representation of that process. This is also true for relativistic quantum field theories.

However, as you may have noticed, $h_n(t)$ **is a smooth real valued function**, even if you start with $h_n(t_0) \in \{0, 1\}$ and therefore cannot reproduce rational values like $0, 1$ at later times t.

II.3 Critics on Hydrodynamic Deterministic Representations

The hydrodynamic deterministic representation is **a representation in hindsight**, where you first have to solve for the time dependent quantum state under realistic boundary conditions, taking all relevant influences into account. In a second step you can calculate the integral curves of the resulting flux. One would rather like to find a deterministic representation that is prior to an averaging process and finally, after averaging, yields the quantum mechanical time dependent probabilities.
Furthermore, **in the discrete variable case**, the **hydrodynamic deterministic representation does not work at all.** The velocity/flux field can take any real value but the discrete numbers must change by discrete differences in a given time step. Thus, the velocity/flux field does not lead in a unique deterministic way to the discrete quantities in the next time step. The general problem with a hydrodynamical deterministic representation is that **probability flux is smooth and no individual discrete process can fit that.**

III.1 From Permutation Dynamics To Markov Processes

The easiest way to go from dynamics of facts to dynamics of prognosticating relative frequencies, which just is dynamics of probabilities, is by averaging facts over probability distributions p. For Markov processes we take the vector notation of permutation dynamics on facts (see Chaps. 2,4),

$$\boxed{\phi_{t+1}^{[\pi(k)]} = T_1^{[\pi]} \phi_t^{[k]} \;\; ; \; p_m = \left(\phi^{[m]} \mid p \right)} \,. \tag{10}$$

Thus, averaging fact dynamics over distribution p can, by transposing the action of T on facts to an action of T^T on the distribution, written like a Markov chain equation:

$$p_{t+1} = T^{[\pi^{-1}]} p_t \,, \tag{11}$$

where $T^{[\pi^{-1}]} \in S_N$. Such permutation matrices are very special stochastic matrices and so (11) only reproduces a very limited and seemingly unrealistic stochastic Markov dynamics. In particular it is reversible and amounts to just relabeling the indices of p_n.

III.2 Averaging over Dynamics

Now comes a crucial point. Stochastic irreversible motions come from a loss of resolution of dynamics of many, thus irrelevant, variables. It amounts to averaging over different dynamics and reduction to relevant variables. So, let us first average permutation matrices over some distribution. Each matrix element of a permutation matrix is in $\{0, 1\}$ and on averaging over a probability distribution each matrix element will become a non-negative real number in the interval $[0; 1]$ and the averaged matrix fulfills

$$\sum_n T_{nm} = \sum_m T_{nm} = 1 \; ; \; T_{mn} \in [0; 1] \, , \tag{12}$$

which means - as is known in the literature as the Birkhoff-von-Neumann-theorem - that on averaging permutation matrices **a general double stochastic matrix** T results. It is also known that the corresponding Markov process has the **unique uniform stationary state** $p_n = 1/N$.

III.3 Reduction to relevant variables

Now, reducing to relevant variables $n = 1, \ldots M$, $M \ll N$, leaving the transition rates between relevant states untouched leads to a reduced matrix

$$\tilde{T}_{nm} = \frac{T_{nm}}{\sum_{n=1}^{M} T_{nm}} \tag{13}$$

in order to keep the probability conserved on the relevant variables. Now it is easy to check, that the matrix $\tilde{T}$ is still stochastic but typically not also double stochastic. Thus we conclude:
Averaging over some distribution of permutation dynamics and reducing to a number of relevant variables leads to a dynamics with some generic stochastic matrix.
Thus, Markov processes in general can be viewed as an average over a distribution of permutation dynamics with reduction to a reduced set of relevant variables.

IV.1 From Permutation Dynamics To Quantum Processes: Averaging over initial State

For quantum processes we take the matrix notation of permutation dynamics on facts (see Chaps. 2,4),

$$\boxed{P_{t+1}^{[\pi(m)]} = T_1^{[\pi]} P_t^{[k]} \left(T_1^{[\pi]}\right)^\dagger \;;\; p_m = \left(P^{[m]} \mid \rho\right) \;;\; \rho = \sum_m p_m P_m} \,. \tag{14}$$

Averaging the facts over some distribution ρ_0 at a fixed initial time t_0 and on taking the adjoint time evolution in the scalar product of expectation values one can then rewrite the dynamic as a unitary time evolution for the density operator

$$\rho_t = \left(T_1^{[\pi^{-1}]}\right)^t \rho_0 \left(\left(T_1^{[\pi^{-1}]}\right)^\dagger\right)^t \,. \tag{15}$$

which is the **quantum process time evolution, however restricting the unitary matrices to only permutation matrices**.

IV.2 From Permutation Dynamics To Quantum Processes: Unknown Basis

Now comes a crucial point. We know from non-abelian symmetry groups and Fourier analysis that **incompatible, but complementary** properties of real life can be mathematically described by projection operators, P^I, P^{II}, that do not commute and have scalar products, $\left(P^I|P^{II}\right)$ neither 1 nor 0.

$$\left[P^I, P^{II}\right] \neq 0 \tag{16}$$

but are related by some unitary matrix U_0 such that

$$\left[P^I, U_0 P^{II} U_0^\dagger\right] = 0\,. \tag{17}$$

Such $U_0^\dagger$ can be viewed as a transformation to the appropriate basis of facts corresponding to the actual properties which are either true or false. Unfortunately, **often we do not know this appropriate basis**. Therefore, for the time evolution of the density operator we may have to change to such initial basis and find...

IV.2 From Permutation Dynamics To Quantum Processes: Unknown Basis

$$U_0\rho_t U_0^\dagger = \left(T_1^{[\pi^{-1}]}\right)^t U_0\rho_0 U_0^\dagger \left(\left(T_1^{[\pi^{-1}]}\right)^\dagger\right)^t . \tag{18}$$

Since t is a discrete natural number we can plug left of each T_1 a factor of $1 = U_0U_0^\dagger$ and corresponding factors $1 = U_0^\dagger U_0$ to the right of each factor $T_1^\dagger$ and find

$$U_0\rho_t U_0^\dagger = U_0U_1^t\rho_0 \left(U_1^\dagger\right)^t U_0^\dagger , \tag{19}$$

with a unitary matrix

$$U_1 = U_0^\dagger T_1^{[\pi^{-1}]} U_0 . \tag{20}$$

Thus, we can conclude. A deterministic permutation dynamics for some unknown properties with initial facts distributed according to an initial density matrix ρ_0 is described by a quantum dynamics with one step time evolution operator U_1.

IV. From Permutation Dynamics To Quantum Processes

We summarize our findings of this chapter:

- Hydrodynamic deterministic representations of stochastic processes
  - are often unrealistically smooth in Markov processes,
  - hard to verify in continuous quantum processes due to sensitivity of interference patterns,
  - do not work at all for discrete variables, because of smooth probability flux.
- Permutation dynamics are deterministic reversible dynamics.
- On averaging over a distribution of permutations the reversibility is dynamically broken and by further reduction to relevant variables a typical Markov process emerges for these relevant variables. **Every stochastic Markov process can be represented by a deterministic permutation process. The averaging is over different permutations and incorporates reduction of variables.**....

IV. From Permutation Dynamics To Quantum Processes

On averaging the initial facts within some unknown basis the permutation dynamics turns into a typical quantum process which stays reversible for closed systems. Every quantum process can be represented by a deterministic permutation process. The averaging is over initial facts in some unknown basis.

$$\boxed{U_1 = U_0 T_1^{\pi^{-1}} U_0^\dagger} \tag{21}$$

$T_1^{[\pi]}$ is the one-step generator of permutations with π.
U_0 rotates from a chosen basis to the appropriate fact basis which usually is unknown.
U_1 is the resulting one-step unitary quantum process generator.

06. Exercises

1. Show that integral curves of flux with initial values distributed according to $P_{t_0}(x)$ (3) are a deterministic representation of the stochastic process.
2. Verify (6) and (7).
3. Construct a simple example for a process of discrete variables where the deterministic representation of (8) is in conflict with the discrete nature of variables. A two value system suffices.
4. Check that matrices $\tilde{T}$ of (13) are stochastic but usually no more double stochastic.
5. Show (19) from (18) with the definition of (20).