Week ①

PHY 637 Decoherence and Open Quantum Systems
Instructor: Sebastian Wüster, IISER Bhopal, 2021

These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

0 Administrative affairs

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(ii) Literature:

- Schlosshauer, *"Decoherence and the quantum-to-classical transition"* [SD]
- May, Kühn, *"Charge and Energy Transfer Dynamics in Molecular Systems"* [MK]
- Weiss, *"Quantum dissipative systems"*, 2nd ed. [WQD]
- Gardiner, Zoller, *"Quantum Noise"* [QN]
- R. Shankar, *"Principles of quantum mechanics"* [SQM]
- Agarwal, *"Quantum Optics "* [AQO]
- Breuer and Petruccione, *"The theory of open quantum systems "* [BP]

The course will mainly follow SD, with MK for non-Markovian dynamics. Where stray topics are taken from elsewhere I will try to indicate this. The following is the course arrangement that I hope we can follow after 17th Jan, but that remains to be confirmed. Until then, we will follow an online-only variant, which will be communicated by email.

(iii) Lectures:

- There will be life lectures in the allotted room for those that are interested in these. If demand exceeds limited space due to virus-spacing rules, we shall adopt a rotation schedule, but from your preliminary google form responses, that will not be the case. I will record those lectures simultaneously and later edit and provide as downloadable video on microsoft teams.
- I am arranging lecture notes into "week" segments, based on similar content. While most of those segments should indeed take a week for us to work through, this will not be true for all and they may take less or more often more time. These will always be available online before the lecture on my webpage and/or teams forum.

(iv) Assessment:

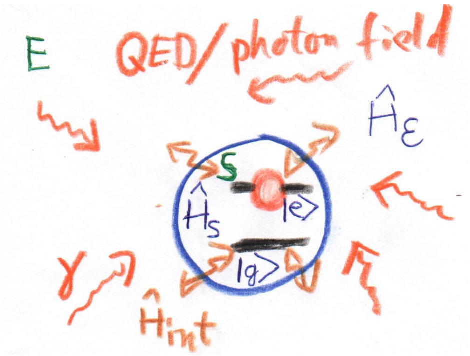
- **3 scheduled Quizzes with examineer 15+15+15=45%** There will be some quizzes lasting 1-1.5 hours, conducted using the examineer webpage . These are ”open notes” quizzes, so make your notes available offline or on a second device beforehand. These will be proctored life and/or via camera. Think of the second quiz as “mid-sem”.
- **Assignments: 35%** There will be about five-six assignments handed out with a two week deadline each. I expect you to form teams of 3-4 students and stick in these teams for the semester. Hand in only one solution per team. The TA is instructed to give full marks for *any serious attempt* at a given question of the assignment, even if the result is wrong. This is to discourage copying and encourage doing it yourself. However, the TA is asked to deduct marks for messy presentation and blatant copying from anywhere. The same teams will be used in tutorials, see below. Submit your final assignment solution via email to the TA. All has to be integrated in a single file, e.g. .pdf. This may be a good opportunity to learn LaTex and nicely typeset your solution, but handwritten and good-quality scanned/photographed is fine too.
- **Numerics component of assignments:** Modern science almost always necessitates the heavy use of computers. Most assignments will contain a numerics component, to be done using XMDS, please see infosheet provided. Please try to install the package on at least one computer in your team, otherwise installations are available in the CC computer pool. Contact the TA if there are installation problems. For each assignment, I will provide a template code package that you have to only minorly edit. See notes on numerics assignments online. No prior experience of either programming or xmds should be required.
- **Flipped classroom and tutorials:** Most weeks, we will convert the Wednesday into a tutorial or TA class by flipping the classroom. That means that that session’s lecture material is provided as recording only and instead we meet in studio-AIR for a tutorial or TA class alternatingly every other week. In the TA class I will expect YOU to present your assignment solutions and in the tutorial you shall discuss within your team and other teams on simple questions designed to get the main concepts across. Since you are supposed to gather in the same teams for assignments and tutorials, I request you to group into online/offline teams depending on whether you are willing to attend the life tutorials in AIR or prefer the online version via e.g. google meet. Both will be combined via projector, so I shall be able to answer questions from both types.
- **Final exam: 20%** The exam will try to test understanding of the essential *physics* concepts taught, not maths. For guidance regarding what are the most important concepts look at the quizzes and assignments. All exams will be designed to give a significant advantage to those students that solved all assignments by *themselves* within their team. Exam will either be conducted online using examineer and shall then make heavy use of examineer’s randomisation features to render teamwork ineffective, or circumstances permitting (preferred) the old fashioned pen and paper way.

Contents

1 Motivation and Review

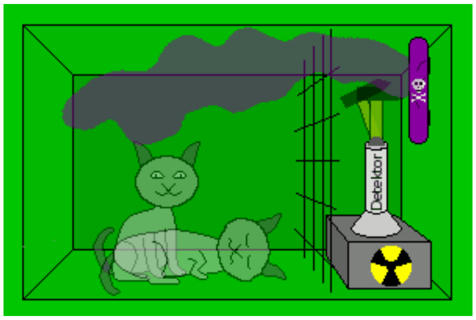
1.1 What is an open quantum system?

- Split the world into a "system" of interest S and an environment E.
- Fundamentally, both ought to be described quantum mechanically.
- Frequently we have a system that is simple/ describable, but an environment that is too large to treat quantum mechanically (see section 2), and that we don't even care about.



left: Essential building blocks of an open quantum system in an example relevant for spontaneous emission: A single atom, for which we consider only two quantum states $|\,g\,\rangle$ and $|\,e\,\rangle$ is our sytem. It interacts via its dipole with electromagnetic radiation (photons γ). This environment is more complex than the atom (many elm. field modes, polarisations, occupations), and is not empty even at $T = 0$. S and E interact via system-environment interactions $\hat{H}_{\text{int}}$. We will later formalize this splitting on the level of the Hamiltonian by writing $\hat{H} = \hat{H}_S + \hat{H}_\mathcal{E} + \hat{H}_{\text{int}}$.

- The *theory of open quantum systems* provides ways to *approximately* determine the evolution of S, despite it being affected by E through interactions $\hat{H}_{\text{int}}$, without having to fully deal with E.
- Besides the practical utility, the theory also provides us with fundamental insight into what is called the "quantum to classical transition": Why does the everyday world around us behave classically, even though all microscopic constituents behave quantum mechanically? This problem is well illustrated by the Schrödinger's cat thought[1] experiment:



left: Schrödinger's cat paradox. Suppose a nucleus is in the grey box that radioactively decays with rate Γ. According to quantum mechanics, after some time it will be in the state $|\,\Psi(t)\,\rangle = \sqrt{\exp\left[-\Gamma t\right]}|\,\text{nucleus original}\,\rangle + \sqrt{1-\exp\left[-\Gamma t\right]}|\,\text{nucleus decayed}\,\rangle$. The detector detects the decay with 100% probability and then triggers the hammer, releasing the poison, killing the cat.

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[1] fortunately, for the cat.

If we treat the entire device fully quantum mechanical, the *total* state after some time is:

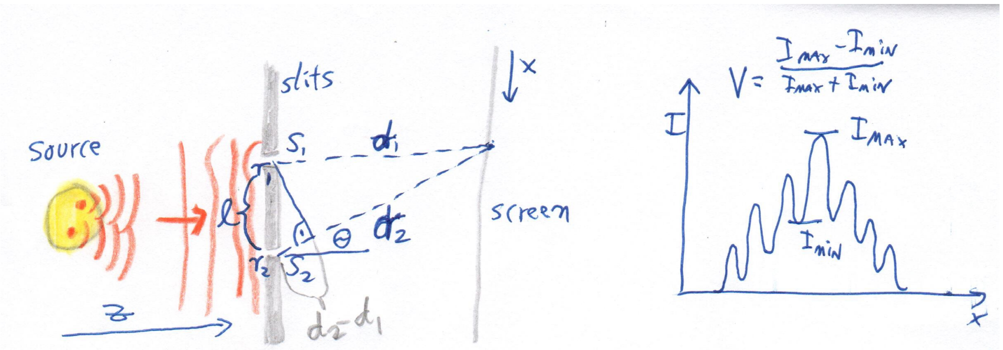
$$| \Psi(t) \rangle = \sqrt{\exp{[-\Gamma t]}} | \text{nucleus original, cat alive} \rangle + \sqrt{1 - \exp{[-\Gamma t]}} | \text{nucleus decayed,cat dead} \rangle. \tag{1.1}$$

However superpositions of alive and dead cats contradict our experience, so where does this go wrong? See also e.g. this video .

1.2 What is (de-)coherence?

It turns out a major effect of environments on open quantum systems is (quantum) decoherence. So let us attempt a brief definition of that.

- An ensemble n of waves $\{\exp{[i(\omega_n t - k_n x + \varphi_n)]}\}$ is termed coherent if it will show spatial or temporal interference patterns after averaging over the ensemble, based on e.g. $\exp{[ix]} + \exp{[ix]} = 2\exp{[ix]}$ but $\exp{[ix]} + \exp{[ix + i\pi]} = 0$.
- Depending on which type of interference or which ensemble we are referring to, we can distinguish spatial-, temporal- or spectral coherence.



top: Sketch of Young's double slit experiment and the resultant interference pattern (for a case of imperfect fringe visibility V). $\mathbf{r}_{1,2}$ are the location of the slits and $d_{1,2}$ the distance from either slit to a chosen location x on the screen.

Consider the paradigmatic experiment on coherence and interference shown above. The field at a position on the screen is given by

$$\begin{aligned} E(\mathbf{x}, t) &= E_1(\mathbf{x}, t) + E_2(\mathbf{x}, t), \text{ with} \\ E_n(\mathbf{x}, t) &= E\left(\mathbf{r}_n, t - \frac{d_n}{c}\right) \frac{1}{d_n} e^{i(k - \frac{\omega}{c}) d_n} \end{aligned} \tag{1.2}$$

as a superposition of light from slit 1 with light from slit 2. Light is assumed mono-chromatic with frequency ω, wavenumber k and speed of light c, and we ignore polarisation thus using a scalar electric field E. We can ignore the complex exponential at the end of the second line since $c = \omega/k$.

The actual intensity observed on the screen is:

$$I(\mathbf{x}, t) \sim \overline{E(\mathbf{x}, t) E(\mathbf{x}, t)^*}, \tag{1.3}$$

where $\overline{\cdots}$ denotes an average over times longer than an optical cycle. The need for this average will be crucial in the following.

We define $t_n = d_n/c$, and can then write

$$I(\mathbf{x},t) \sim \frac{1}{d_1^2}\overline{E(\mathbf{r}_1,t-t_1)E(\mathbf{r}_1,t-t_1)^*} + \frac{1}{d_2^2}\overline{E(\mathbf{r}_2,t-t_2)E(\mathbf{r}_2,t-t_2)^*}$$
$$+ 2\mathrm{Re}\left\{\frac{1}{d_1 d_2}\overline{E(\mathbf{r}_1,t-t_1)E(\mathbf{r}_2,t-t_2)^*}\right\}. \tag{1.4}$$

The first two terms are just the intensities at slit 1 and 2 assumed constant $= I_0$ now. If we had a *perfect plane wave* impinging on the screen ($E = \sqrt{I_0}\exp\left[i(\omega t - kz)\right]$), the second term becomes $2I_0\mathrm{Re}\left\{\overline{\exp\left[i\omega(t-d_1/c)\right]\exp\left[-i\omega(t-d_2/c)\right]}\right\} = 2I_0\cos\left(2\pi\frac{l}{\lambda}\theta\right)$ and creates full contrast interference fringes[2]. However for a *perfect plane wave* we would need a laser source. Some extended incoherent source will have the electric field fluctuating in time and position as shown (orange lines).

These fluctuations affect the electric field correlation function

$$G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) \equiv \overline{E(\mathbf{r}_1,t_1)E(\mathbf{r}_2,t_2)^*}. \tag{1.5}$$

which enters the last line in (1.4) and thus the fringe visibility V. It measures to what extent the electric field at position $\mathbf{r}_1$ and time t_1 will have on average the same phase as that at position $\mathbf{r}_2$ and time t_2

Further reading: This discussion is adapted from Hecht and Ganesan ”Optics” / Walls and Milburn ”Quantum Optics”. See also:
”Bass, Handbook of optics” chapters 2.8 and 4.
”Römer, Theoretical Optics” chapter 12.

1.2.1 Quantum coherence

- Also in quantum mechanics, coherence refers to the degree of visibility of interference effects.
- As we shall see, this visibility can be detrimentally affected by a large environment. Interferences that we might want to measure in a quantum system, depend on how the system has interacted with the environment, which can be thought of as causing the system state to fluctuate. Averaging over the un-observed environment then causes interferences to disappear.

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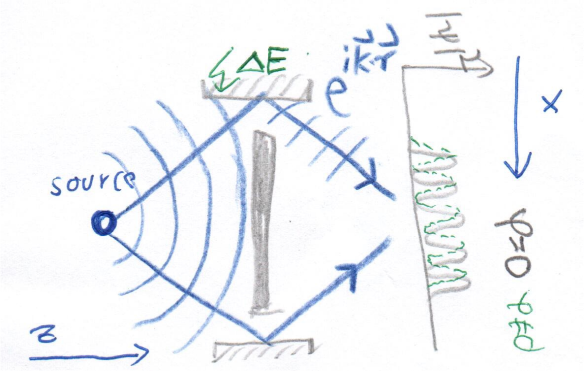
[2] Note the average is over some short interval of time t and drops out.

Example 1, Matter wave interferometry:



left: In a similar setup as Young's double slit, consider a matter-wave interfering with itself after reflection of some boundaries shown. Environmental fluctuations at the boundary scramble relative phases and wash out the interference pattern.

Consider the self-interfering matter wave in the example above. Along the x-direction we have $\Psi(x) = \mathcal{N}\left(e^{ik_x x}e^{-i\Delta E\frac{T}{\hbar}} + e^{-ik_x x}\right)$, where $\mathcal{N}$ is a normalisation factor, k_x the wave number (momentum along x) and $e^{-i\Delta E\frac{T}{\hbar}}$ a phase factor that we assume came from Schrödinger's equation through some interaction with the environment (slits) lasting time T at energy ΔE with the boundary at the upper point of reflection.

The interference pattern is given by

$$|\Psi(x)|^2 = \mathcal{N}^2\cos^2\left(k_x x + \varphi\right). \tag{1.6}$$

with $\varphi = -\Delta ET/(2\hbar)$. Depending on ΔE, fringe positions will shift as indicated in the sketch. To see a matter wave interference pattern we have to do repeated experiments. If now ΔE differs for different states of the environment and we average over the latter, fringes will be lost.

We will consider this example again in much more detail in section 3.2.3.

Thus de-coherence is the loss of some initially present interference visibility, due to loss of fixed phase relations φ of different quantum waves in an average.

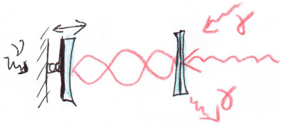
1.3 Most quantum systems are open

quantum technologies

- have: semiconductors, lasers, MRT
- want: quantum sensors, smart materials,...

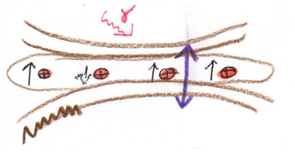
Opto-mechanics

- cavity with oscillating mirror
- Phonon and photon leakage



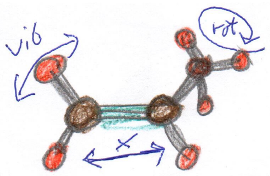
Quantum computers/
Quantum information

- Q-Bits in ion-trap



Molecular physics

- Complex molecule, other DGFs



Broad relevance

- In principle, every quantum system except "the entire universe" is open. However assuming a closed system can be a good approximation for short times (we see later why).
- In general, the larger a "system", the more prominent the environmental influence becomes.
- Environment can be helpful/ exploited.

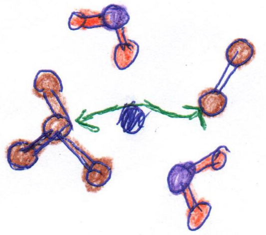
- Conceptually, we can make an open system closed by including the environment. "Openness" depends on the *choice* of S and E. The choice is however usually well motivated and constrainted by practicalities or interest.

Really closed systems:

- Few colliding elementary particles
- Nothing much else ???
- Coherence time record: 10 min *Wang et al. Nature Photonics* **11** *(2017) 646.*

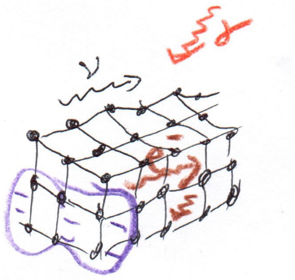
Quantum chemistry

- Chemical reactions
- Solvent influence



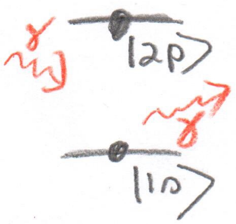
Material science

- Quasi-particle damping
- Dissipation



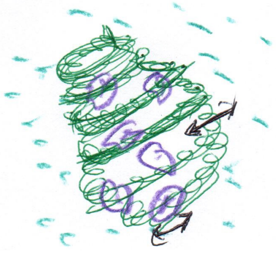
Atomic physics

- Spont. decay
- QED vacuum



(Quantum-?)-biology

- Mag-field sensing
- Sense of smell
- Photosynthesis?



1.4 Course outline

1) Motivation and Review: ∼ 2 weeks
   - What is decoherence? Review of QM elements. Problems with QM. System-environment models (moved into chapter (2) accidentally).

2) Basic Formalism and Interpretation of Decoherence: ∼ 3 weeks
   - Density matrices, purity, ensemble and reduced interpretation. Measurements. Superselection. Relation of decoherence and dissipation, dephasing, noise. Some Tricks and Tools.

3) Markovian open quantum systems: ∼ 3 weeks
   - Master equation, Born and Markov approximations, Lindblad form. Examples with continuum systems, Brownian motion, damped harmonic oscillator. Examples with discrete systems, spins, dephasing, spontaneous decay. Spin-Boson model.

4) Non-Markovian open quantum systems: ∼ 3 weeks
   - Structured baths, memory effects, Redfield and Nakajima Zwanzig equations [scope permitting], examples: molecular vibrations.

5) Quantum-to-Classical Transition and Interpretations of Quantum Mechanics [time permitting]: ∼ 2 weeks
   - Localisation due to environmental scattering, observations, quantum brain, many-worlds.

1.5 Review and Notation

This section aims to remind you of all material from your earlier courses (mainly PHY 303/304: QM-I/II) that is of particular relevance for this lecture. Anything not fully familiar to you should be revised.

1.5.1 The postulates of quantum mechanics

- Quantum mechanics can be built up by starting with a few postulates, and then simply doing math from there (see e.g. R. Shankar "Principles of quantum mechanics", Chapter 4):

(P1) The state of a particle is represented by a vector $|\,\Psi\,\rangle$ in a Hilbert-space.

(P2) All observables are represented by an operator $\hat{O}$, e.g. position operator $\hat{x}$, momentum operator $\hat{p}$. Let the eigenvalues and eigenvectors of the operator be defined by:

$$\hat{O}|\,\phi_n\,\rangle = o_n|\,\phi_n\,\rangle. \tag{1.7}$$

(P3) Then, if the system is in $|\,\Psi\,\rangle$ and the observable corresponding to $\hat{O}$ is measured, the result will be one of its eigenvalues o_k with probability $p_k = |\langle\,\phi_k\,|\,\Psi\,\rangle|^2$. *The state of the system will change to $|\,\phi_k\,\rangle$ as a result of the measurement* (collapse of the wave function). Formally we apply the projection operator $\hat{P}_k = |\,\phi_k\,\rangle\langle\,\phi_k\,|$ onto the wavefunction:

$$|\,\Psi\,\rangle \qquad \underbrace{\to}_{\text{measurement with result } k} \qquad |\,\phi_k\,\rangle\langle\,\phi_k\,|\,\Psi\,\rangle, \tag{1.8}$$

and then normalize the resultant state to one again.

(P4) The quantum state obeys the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\,\Psi(t)\,\rangle = \hat{H}|\,\Psi(t)\,\rangle, \tag{1.9}$$

where $\hat{H}$ is the Hamiltonian.

The claim is that the rest of QM that you know mathematically follows, and enables us to make predictions in agreement with experiment.

In this lecture we will be concerned with the opinion, that the part about wave-function collapse in postulate (P3) and example 3 is fundamentally unsatisfactory (we see later why, in section 3.2.2). This is because the act of "measurement" should also just be time-evolution, described by (1.9).

1.5.2 Single particle quantum mechanics

An open quantum system almost always needs to be a many-body system (so that we can divide it into "system" and "environment"). However each many-body system typically is assembled of some types of single particles, so let's go through the quantum mechanics and notation for those first.

We want to frequently describe a single particle in a basis made of eigenstates of the

Time-independent Schrödinger equation (TISE)

$$\hat{H}_0|\varphi_n\rangle = E_n|\varphi_n\rangle. \tag{1.10}$$

- Where H_0 is the single body Hamiltonian (depends on co-ordinates of one particle)
- $|\,\varphi_n\,\rangle$ is the (typically) infinite single-particle basis. Since it is a basis, we can write any arbitrary single particle quantum state $|\,\phi\,\rangle$ as $|\,\phi\,\rangle = \sum_n c_n|\,\varphi_n\,\rangle$, with coefficients $c_n \in \mathbb{C}$. The space of all normalized ϕ is the single particle Hilbert-space $\mathcal{H}_0$.
- E_n are single particle energies

Example 2, Single particle quantum states:
(i) Free particles in Volume $\mathcal{V}$

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} = -\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}, \qquad E_n = \frac{\hbar^2\mathbf{k}^2}{2m} = \frac{\mathbf{p}^2}{2m}, \tag{1.11}$$

$$|\, \varphi_n \,\rangle \rightsquigarrow \langle\, \mathbf{x} \,|\, \phi_{\mathbf{k}} \,\rangle \;=\; \frac{1}{\sqrt{\mathcal{V}}} e^{i\mathbf{k}\mathbf{x}}. \tag{1.12}$$

where $\mathbf{k}$ is the wavenumber and $\mathcal{V}$ the quantisation volume.
(ii) Spin states: In terms of the spin operator(s) $\hat{\mathbf{S}} = [\hat{S}_x, \hat{S}_y, \hat{S}_z]^T$, we define eigenstates

$$\hat{\mathbf{S}}^2 |\, \chi_{s,m_s} \,\rangle = \hbar^2 s(s+1) |\, \chi_{s,m_s} \,\rangle, \tag{1.13}$$

$$\hat{S}_z |\, \chi_{s,m_s} \,\rangle = \hbar m_s |\, \chi_{s,m_s} \,\rangle, \quad m_s = -s \cdots s. \tag{1.14}$$

$$\tag{1.15}$$

We will mostly need the spin-1/2 case, for which a Matrix representation can be more convenient. We have a basis

$$|\, \varphi_n \,\rangle \rightsquigarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix} \cong |\!\uparrow\rangle = |\, \chi_{\frac{1}{2},+\frac{1}{2}} \,\rangle \text{ or } \begin{bmatrix} 0 \\ 1 \end{bmatrix} \cong |\!\downarrow\rangle = |\, \chi_{\frac{1}{2},-\frac{1}{2}} \,\rangle. \tag{1.16}$$

In terms of this basis, any operator has a 2×2 matrix representation. We particularly need the unit matrix plus Pauli matrices

$$\mathbb{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{1.17}$$

with commutation relations $\left[\sigma_i, \sigma_j\right] = 2i\epsilon_{ijk}\sigma_k$, where ϵ_{ijk} is the completely anti-symmetric tensor. Spin operators are then $\hat{S}_k = \hbar\hat{\sigma}_k/2$, $k \in \{x, y, z\}$, thus $\left[\hat{S}_i, \hat{S}_j\right] = i\hbar\epsilon_{ijk}\hat{S}_k$ A typical Hamiltonian is (e.g. spin in a magnetic field).

$$\hat{H}_0 = \Delta E \;\; \hat{\sigma}_z, \qquad E_{\uparrow\downarrow} = \pm\Delta E, \tag{1.18}$$

We will also refer to eigenstates of $\hat{S}_x$, which are $|\!\leftarrow\rangle = (|\!\uparrow\rangle + |\!\downarrow\rangle)/\sqrt{2}$ and $|\!\rightarrow\rangle = (|\!\uparrow\rangle - |\!\downarrow\rangle)/\sqrt{2}$.

(iii) Simple Harmonic oscillator. Hamiltonian:

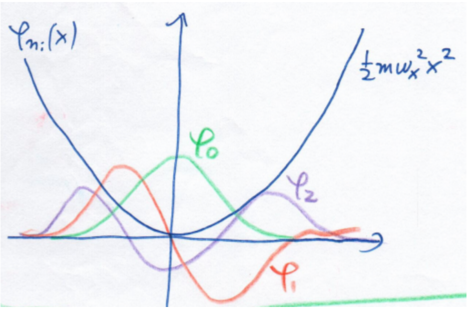
$$H_0 = \frac{\mathbf{p^2}}{2m} + \frac{1}{2}m\omega^2 x^2. \tag{1.19}$$

Example continued:

Spatial wave function /States:

$$\varphi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}\sigma}} e^{-\frac{x^2}{2\sigma^2}} H_n\left(\frac{x}{\sigma}\right), \tag{1.20}$$

where $\sigma = \sqrt{\hbar/(m\omega)}$. Energies: $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$.



left: Sketch of first few oscillator wavefunctions.

Raising and lowering operators We define,

$$\hat{b} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\sqrt{\frac{1}{2m\omega\hbar}}\hat{p}$$

$$\hat{b}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - i\sqrt{\frac{1}{2m\omega\hbar}}\hat{p} \tag{1.21}$$

We can show that $[\hat{b}, \hat{b}^\dagger]$=1 (from $\left[\hat{x}, \hat{p}\right] = i\hbar$) and then re-write the Hamiltonian (1.19) using raising and lowering operators as

$$\hat{H}_0 = \hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right) \tag{1.22}$$

Nextly we deduce (e.g. in Shankar SQM $\cong$ pg.204) the

Function of raising and lowering Operators

$$\hat{b}|\varphi_n\rangle = \sqrt{n}|\varphi_{n-1}\rangle \qquad \hat{b}|\varphi_0\rangle = 0 \tag{1.23}$$

$$\hat{b}^\dagger|\varphi_n\rangle = \sqrt{n+1}|\varphi_{n+1}\rangle \tag{1.24}$$

- These properties follow solely from the commutation relation $\left[\hat{b}, \hat{b}^\dagger\right] = 1$, and hence we would not need to know the position space representation (1.20).

Number Operator $\hat{N} = \hat{b}^\dagger\hat{b}$ and $\hat{N}|\varphi_n\rangle = n|\varphi_n\rangle$. We will also denote oscillator states simply by $|\,n\,\rangle$, hence

$$\hat{N}|\,n\,\rangle = n|\,n\,\rangle \tag{1.25}$$

The states (1.20) are difficult to interpret in the context of our experience with the *classical* harmonic oscillator. This link is easier made with the concept of

Coherent states These are defined by $|\,\alpha\,\rangle \equiv \hat{D}(\alpha)|\,0\,\rangle$ with displacement operator

$$\hat{D}(\alpha) = e^{\alpha\hat{b}^\dagger - \alpha^*\hat{b}}. \tag{1.26}$$

We can then derive the explicit number state representation:

$$|\,\alpha\,\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |\,n\,\rangle. \tag{1.27}$$

- As time goes on, the position space density in a coherent state harmonically oscillates with amplitude $|\alpha|$ and phase $\arg(\alpha)$ around 0, remaining in a Gaussian shape like $|\,\varphi_0\,\rangle$.
- You can verify that coherent states act like eigenstates of the annihilation operator $\hat{b}|\,\alpha\,\rangle = \alpha|\,\alpha\,\rangle$, and $\langle\,\alpha\,|\hat{b} = \alpha^*\langle\,\alpha\,|$.

1.5.3 Measurements

Now that we reviewed a few useful examples for single particle quantum states in section 1.5.2, let us revisit postulate (3) of section 1.5.1 again in one example:

Example 3, Wavefunction collapse: In e.g. a first Stern-Gerlach magnet (preview example 11) with inhomogeneous field along the x-direction, assume you have prepared an atom in the eigenstate with $S_x = +1/2$ namely $|\,\phi\,\rangle = |\leftarrow\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$. You now send it through a second magnet with inhomogeneous field along the z-direction. Q: With which probability do you measure $S_z = +1/2$ and what is the state after that measurement?
A: We find the probability using $p = |\langle\uparrow|\,\phi\,\rangle|^2 = 1/2$. After measuring the result $S_z = +1/2$, we assert the wavefunction has collapsed to $|\,\phi\,\rangle = |\uparrow\rangle = (|\leftarrow\rangle + |\rightarrow\rangle)/\sqrt{2}$ based on postulate P3.

1.5.4 Many-particle quantum mechanics

When including the environment, most of the examples in section 1.3 are many-body systems: We have to describe a “system of interest” and its ”environment”, which clearly necessitates at least two (typically many more) particles, or alternatively degrees of freedom (DGFs) of the same particle (e.g. a complex molecule). Whether we describe N particles with one DGF or one particle with N DGF, the quantum mechanical formalism is the same, reviewed or introduced in the following.

For each particle we have to add one set of co-ordinates and quantum numbers to the wave-function. Lets denote the collection of all such variables with

$$q = \{\mathbf{r}, m_s, \cdots\}. \tag{1.28}$$

For $N = 2$ particles, we then have to write e.g. energy eigenstates $\phi_k(q_1, q_2)$, where the subscripts on q_j now number the particle j. Thus the wavefunction is now a function on a space of twice as many dimensions as the one for a single particle. Formally we need the

Tensor product: (simplified version). Given an arbitrary vector $\mathbf{v} \in \mathcal{V}$ in an N-dimensional vector space $\mathcal{V}$, with components v_n, and another vector $\mathbf{w} \in \mathcal{W}$ in an M-dimensional vector space $\mathcal{W}$, you can think of the tensor product $\otimes$ of these vectors as an $N \times M$ matrix

$$\mathbf{v} \otimes \mathbf{w} = \begin{bmatrix} v_1 w_1 & v_1 w_2 & \cdots & v_1 w_M \\ v_2 w_1 & v_2 w_2 & \cdots & v_2 w_M \\ \vdots & \vdots & \ddots & \vdots \\ v_N w_1 & v_N w_2 & \cdots & v_n w_M \end{bmatrix} \tag{1.29}$$

The space of all these matrices is itself a vector-space again, written $\mathcal{V} \otimes \mathcal{W}$, and called the tensor product of $\mathcal{V}$ and $\mathcal{W}$. We can repeat the operation to add a third "dimension" to the matrix (making it a cube of numbers, rather than a square) etc., thus generating even higher dimensional objects than Matrices (ND arrays).
After forming (1.29) we can turn $\mathbf{v} \otimes \mathbf{w}$ again into a vector (in a $N \times M$ dimensional space), by reshaping:

$$\mathbf{v} \otimes \mathbf{w} = \begin{bmatrix} v_1 w_1 & v_1 w_2 & \cdots & v_1 w_M & v_2 w_1 & v_2 w_2 & \cdots & v_n w_{M-1} & v_n w_M \end{bmatrix}^T . \tag{1.30}$$

- For a more rigorous mathematical definition, see math courses.
- For a simple recipe that suffices in physics typically, see next example below.

Using this we can define the

Many-body Hilbertspace For N particles, each described by a single particle Hilbertspace $\mathcal{H}_0$, the N-body Hilbert space is

$$\mathcal{H}_{MB} = \underbrace{\mathcal{H}_0 \otimes \mathcal{H}_0 \otimes \cdots \otimes \mathcal{H}_0}_{N \text{ times}} \tag{1.31}$$

A basis of this space is given by

$$|\, \psi_{n_1, n_2, \cdots, n_N} \,\rangle = |\, \varphi_{n_1} \,\rangle \otimes |\, \varphi_{n_2} \,\rangle \otimes \cdots |\, \varphi_{n_N} \,\rangle. \tag{1.32}$$

- We ignored aspects arising from the indistinguishability of particles (Bosons, Fermions, see PHY535 on webpage).
- In terms of the basis above we can again write any arbitrary many-body quantum state as

$$|\, \Psi \,\rangle = \sum_{n_1, \cdots, n_N} c_{n_1, \cdots, n_N} |\, \psi_{n_1, n_2, \cdots, n_N} \,\rangle. \tag{1.33}$$

- We see that if the single-particle Hilbert-space is M dimensional, the many-body one is M^N. This gets nasty really quickly. Which is a major motivation for the rest of the present course.
- Orthogonality: Many body states as products of single particle basis are orthogonal, whenever any of the constituents differ, they inherit their orthogonality properties from the single particle states:

$$\begin{aligned}
&\langle\varphi_{n_1}|\langle\varphi_{n_2}||\varphi_{n_1'}\rangle|\varphi_{n_2'}\rangle = \\
&\int d^3\mathbf{x}_1 d^3\mathbf{x}_2\ \varphi^*_{n_1}(\mathbf{x}_1)\varphi^*_{n_2}(\mathbf{x}_2)\varphi_{n_1'}(\mathbf{x}_1)\varphi_{n_2'}(\mathbf{x}_2) \\
&= \left(\int d^3\mathbf{x}_1\ \varphi^*_{n_1}(\mathbf{x}_1)\varphi_{n_1'}(\mathbf{x}_1)\right)\left(\int d^3\mathbf{x}_2\ \varphi^*_{n_2}(\mathbf{x}_2)\varphi_{n_2'}(\mathbf{x}_2)\right) = \delta_{n_1 n_1'}\delta_{n_2 n_2'}. \qquad (1.34)
\end{aligned}$$

Example 4, Many-body states: A state to describe three particles that have spin-1/2 would be e.g. $|\psi\rangle = |\uparrow\rangle|\downarrow\rangle|\uparrow\rangle$, implying the spin of the first particle is up, second down, third up. All $2^3 = 8$ combinations of such states form a basis of the Hilbertspace.
Similarly, if we wanted to describe two harmonic oscillators, calling the position of the first x and the second y, then the state

$$\psi(x, y) = \varphi_0(x)\varphi_1(y) \qquad (1.35)$$

would "say" the first oscillator is in the ground-state, and the second in the first excited state.

After extending states from single body to many-body, we can do the same for operators. We distinguish single body operators, that act on a single object, and $N-$*body* operators, that act on N-particles at once.

The generalisation of Eq. (1.10) to many particles is to add one co-cordinate per particle:

Many-body TISE (general case)

$$\hat{H}(\mathbf{x}_1, ..., \mathbf{x}_n, \hat{\mathbf{p}}_1, ..., \hat{\mathbf{p}}_n)\psi_k(\mathbf{x}_1, ..., \mathbf{x}_n) = E_k\psi_k(\mathbf{x}_1, ..., \mathbf{x}_n) \qquad (1.36)$$

- Typically very high dimensional PDE (e.g. already 9D for 3 particles in 3-dimensions.)
- Often too high dimensional to deal with it directly → We learn techniques to sometimes deal with this problem in this lecture.
- k is an index numbering the eigenstate, as in single particle QM. But now the state is a many-body state. Often it makes sense to de-compose it into a collection of e.g. single particle indices, such as $k \equiv \{n_1, n_2, \cdots n_N\}$, see next dotpoint.

An exemplary Hamiltonian for two equal mass particles that interact (with interaction potential

U) would be written as

$$\hat{H} = -\frac{\hbar^2}{2m}(\nabla^2_{\mathbf{r}_1} + \nabla^2_{\mathbf{r}_2}) + V(\mathbf{r}_1) + V(\mathbf{r}_2) + U(\mathbf{r}_1, \mathbf{r}_2). \tag{1.37}$$

1.5.5 Entanglement

We will see later that decoherence of an open quantum system is crucially linked to the generation of entanglement between the open system and its environment.

Separable and entangled states A many body state is called separable, if it can be written as a product of states for each particle

$$\Psi_{sep}\left(\mathbf{x_1}, \mathbf{x_2}, \cdots, \mathbf{x_n}\right) = \prod_{i=1}^{N} \phi_{n_i}\left(\mathbf{x}_i\right) \tag{1.38}$$

All states that are not separable are called entangled.

Example 5, Entangled versus separable states:
Separable:

$$|\Psi\rangle = |\uparrow\uparrow\rangle = |\uparrow\rangle \otimes |\uparrow\rangle \tag{1.39}$$

$$|\Psi\rangle = \frac{1}{2}\left(|\uparrow\rangle + |\downarrow\rangle\right) \otimes \left(|\uparrow\rangle + |\downarrow\rangle\right) = \frac{1}{2}\left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \tag{1.40}$$

$$\Psi\left(x_1, x_2\right) = \frac{1}{\sqrt{\mathcal{V}}} \exp\left[ik_1 x_1\right] \mathcal{N} \exp\left[-x_2^2/(2\sigma^2)\right]. \tag{1.41}$$

Entangled :

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\right) \tag{1.42}$$

$$\Psi\left(x_1, x_2\right) = \mathcal{N} \exp\left[-\frac{\left(x_1 - x_2\right)^2}{2\sigma_\perp^2} - \frac{\left(x_1 + x_2\right)^2}{2\sigma_\parallel^2}\right] \tag{1.43}$$

- In an entangled state (for two systems A,B) if we measure state A we typically know also about B.
- Entanglement also implies classical correlations, but it is much more than that (keywords: EPR paradox, Bell-theorem).
- The definition gets a bit more complicated for mixed states ($\hat{\rho}$).

1.5.6 Time-evolution, pictures

The word "de-coherence" implies a dynamical process, hence we will have to deal with time-dependent quantum mechanics.

Schrödinger picture: Quantum evolution according to Eq. (1.9), is said to be in the Schrödinger picture. Here the state is time-dependent and operators are typically not. For a time-independent Hamiltonian $\hat{H}$ with $\hat{H}|\,\phi_n\,\rangle = E_n|\,\phi_n\,\rangle$ we can write $|\,\Psi(t)\,\rangle = \sum_n c_n(t)|\,\phi_n\,\rangle$, with $c_n(t) = c_n(0)e^{-iE_nt/\hbar}$. We can also define the time evolution operator

$$\hat{U}(t) = \exp{[-i\hat{H}t/\hbar]}, \tag{1.44}$$

and use it to write $|\,\Psi(t)\,\rangle = \hat{U}(t)|\,\Psi(0)\,\rangle$. The simple expression (1.45) is valid for *time-independent* Hamiltonians only. Otherwise we need to use

$$\hat{U}(t) = \mathcal{T}\left\{\exp{[-i\int_0^t \hat{H}(t')dt'/\hbar]}\right\}, \tag{1.45}$$

where $\mathcal{T}$ denotes time-ordering: In the power series for exp all copies of $\hat{H}$ have to be ordered such that their time arguments *increase* from right to left.

Heisenberg picture: States themselves are not observable. For observables we have to consider operators (matrix elements of these). For simplicity lets consider expectation values, which we can re-write as

$$\bar{O}(t) = \langle\,\Psi(t)\,|\hat{O}|\,\Psi(t)\,\rangle = \langle\,\Psi(0)\,|\hat{U}^\dagger(t)\hat{O}\hat{U}(t)|\,\Psi(0)\,\rangle = \langle\,\Psi(0)\,|\hat{O}(t)|\,\Psi(0)\,\rangle. \tag{1.46}$$

The last expression contains the time-dependent operator $\hat{O}(t) = \hat{U}^\dagger(t)\hat{O}\hat{U}(t)$ and now depends only on the initial state at $t = 0$. The time dependence has moved into the operators. This is called the Heisenberg picture. It is fully equivalent to the Schrödinger picture.

Interaction picture: Let's assume we have a Hamiltonian with a natural splitting into two pieces $\hat{H} = \hat{H}_0 + \hat{V}$. Let's call $\hat{H}_0$ the "free Hamiltonian" and $\hat{V}$ the "interaction". This could be for example a many-body system with the individual energies (non-interacting) in $\hat{H}_0$ and complicated (maybe time dependent) interactions in $\hat{V}$. For us here, we usually have $\hat{V} = \hat{H}_{\text{int}}$, the system-environment interaction (see section 1.1). In some cases, particularly for perturbation theory, it makes then sense to employ a hybrid version of the two pictures above, where we define states $|\,\Psi_I(t)\,\rangle = \hat{U}_I^\dagger(t)|\,\Psi\,\rangle$ with

$$\hat{U}_I(t) = \exp{[-i\hat{H}_0t/\hbar]}. \tag{1.47}$$

The subscript "I" denotes interaction picture quantities, states and operators; without "I" they are in the Schrödinger picture. Operators are defined as

$$\bar{O}_I(t) = \hat{U}_I^\dagger(t)\hat{O}_S\hat{U}_I(t) \tag{1.48}$$

We can then show the evolution equations

$$i\hbar\frac{\partial}{\partial t}|\,\Psi_I(t)\,\rangle = \underbrace{\hat{U}_I^\dagger(t)\hat{V}\hat{U}_I(t)}_{\equiv\hat{V}_I}|\,\Psi_I(t)\,\rangle = \hat{V}_I|\,\Psi_I(t)\,\rangle, \tag{1.49}$$

$$i\hbar\frac{\partial}{\partial t}\hat{O}_I(t) = \left[\hat{O}_I, \hat{H}_0\right], \tag{1.50}$$

that is interaction pictures states evolve according to the interaction Hamiltonian only, and operators according to the free Hamiltonian only.

Further reading: e.g. Sakurai, "Modern quantum mechanics", chapter 5.

1.5.7 Stochastic processes

In some sense decoherence involves the randomizing effect of the environment on the system. To classify this, we need some definitions already at the level of classical stochastic processes.

A stochastic process is based on a time-dependent random variable $X(t)$ (X may be a vector). If we record a sequence of its values x_1, x_2, x_3, $\cdots$ at ordered times $t_1 < t_2 < t_3 < \cdots$, the process is fully defined by the joint probability density

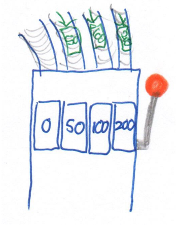
$$p(x_1, t_1; x_2, t_2, x_3, t_3, \cdots) \tag{1.51}$$

i.e. the probability that we recorded value x_1 at time t_1, and after that x_2 at time t_2 etc. We shall also need the conditional probability

$$p(x_1, t_1; x_2, t_2, x_3, t_3, \cdots | y_1, \tau_1; y_2, \tau_2, y_3, \tau_3) \equiv \frac{p(x_1, t_1; x_2, t_2, x_3, t_3, \cdots, y_1, \tau_1; y_2, \tau_2, y_3, \tau_3)}{p(y_1, \tau_1; y_2, \tau_2, y_3, \tau_3)} \tag{1.52}$$

to have recorded that sequence given already earlier having recorded values y_1, y_2, y_3, $\cdots$ at times $\tau_1 < \tau_2 < \tau_3 < \cdots$ (which are all earlier than the t_i).

Example 6, Example I: Money gained from an infinite slot machine:



left: Suppose when pulling the lever on the slot machine, either of the results (0, 50, 100 or 200 Rupies) is spit out with 25% probability each. Let $X(nT)$ bet the amount of cash you earned after n attempts (interval T between attempts). This constitutes a stochastic process (with discrete time steps).

Using Eq. (1.52) we can define a

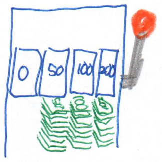
Markov process as a stochastic process for which

$$p(x_1, t_1; x_2, t_2, x_3, t_3, \cdots | y_1, \tau_1; y_2, \tau_2, y_3, \tau_3) = p(x_1, t_1; x_2, t_2, x_3, t_3, \cdots | y_3, \tau_3) \tag{1.53}$$

is valid. This means that the future evolution of the process after t only depends on the state at t, **not** on the entire history.

- The example I above is of a Markovian stochastic process. If you have 500 INR after $n = 10$ attempts, the probabilities for having (500, 550, 600 or 700 Rupies) after attempt $n = 11$ are all 25%, determined only by the status at $n = 10$. What earlier happened during $n = 1, \cdots, 9$ is irrelevant.

Example 7, Example II: Money gained from finite reserves slot machine:



left: The situation changes when we assume a limited reservoir size, say the machine only has 10 notes of each bill to begin with. If it runs out of a certain note, it gives 0 instead of that note. In the same situation as before, we now need know all the results of $n = 1 \cdots 9$: If we collected 10 times 50, we no longer get the 50 bill and the probabilities for step $n = 11$ change to (500 [50%], 550 [0%], 600 [25%] or 700 Rupies [25%]). If we had won the 500 by e.g. 5×100, probabilities are instead as before. In both these cases the state at $t = nT$ with $n = 10$ is identical though. So the future evolution depends on the entire past.

Further reading: Adapted from Gardiner, "Handbook of stochastic methods", chapter 3. See there for (too) much more information.

1.6 Localisation versus quantum diffusion

We end the motivation part with a puzzle why you actually *might* expect quantum effects in our everyday life:

Every non-trivial quantum mechanical position space wave-function represents a coherent superposition of many different position states. One can argue that as long as these are localized enough we would not see the effect of that in everyday experience. Consider however the freely diffusing quantum mechanical wavepacket. For an initial state

$$\Psi(x, t = 0) = \frac{1}{(\sqrt{\pi}\sigma_0)^{1/2}} \exp\left[-\frac{x^2}{2\sigma_0^2}\right], \tag{1.54}$$

with free particle Hamiltonian $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$, the time evolution is given by the broadening wavepacket:

$$|\Psi(x, t)|^2 = \frac{1}{\sqrt{\pi}\sigma(t)} \exp\left[-\frac{x^2}{\sigma(t)^2}\right], \tag{1.55}$$

with width $\sigma(t) = \sigma_0\sqrt{1 + \hbar^2 t^2/(m^2\sigma_0^4)}$, (remember QM1, Griffith section 2.4). If we insert for example $m = 2 \times 14$ amu (Nitrogen molecule in air, N_2) and an initial wave function width (localisation) of $\sigma_0 = 3.5$ nm (roughly the distance to the next molecule in the atmosphere), this spreads significantly on a 1μs time-scale and reaches $\sigma(t) \approx 10$ cm after 10 s. Then all these wave functions massively overlapp, and why would we not see interference features?

For answer you have to be patient until near the end of the lecture!.

Week ②

PHY 637 Decoherence and Open Quantum Systems
Instructor: Sebastian Wüster, IISER Bhopal, 2021

These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

2 System environment models

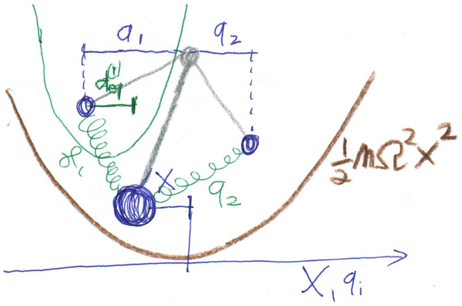
In this section we list mathematical system-environment models that could describe most of the examples in section 1.3. We will follow the classification of SD, chapter 5: An essential distinction that can be made for both, the system *and* environment, is whether it is described by a continuous or a discrete coordinate. A continuous system is then treated like a quantum harmonic oscillator and a discrete one like a spin-system. This provides a total of four possible "canonical models".

The aim of this section is to supply hands on examples for the remainder of the course. You will have to be patient for the full solution of these models in terms of open quantum systems, until much later.

- The classification above is for guidance only, there are more different open quantum systems since their behaviour also strongly depends on the details of the system-environment coupling $\hat{H}_{\text{int}}$.

2.1 Quantum Brownian Motion and damped Harmonic Oscillator

- Classification: System – one oscillator, environment – many oscillators.



left: Consider a central (heavy) harmonic oscillator as the system, that is weakly coupled to a pool of other (light) oscillators, as shown in this figure. We schematically also show the presence of couplings, please refer to equations for the actual details.

We thus write the system and bath part of the Hamiltonian as

$$\hat{H}_S = \frac{\hat{P}^2}{2M} + \frac{1}{2}M\Omega^2\hat{X}^2, \tag{2.1}$$

$$\hat{H}_{\mathcal{E}} = \sum_i^N \left(\frac{\hat{p}_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2\hat{q}_i^2\right), \tag{2.2}$$

in terms of position and momentum operators (capital letters = system oscillator, small letters = environment oscillators).

We also assume quadratic coupling terms $\hat{H}_{\text{int}} = \sum_i \frac{\kappa_i}{2}(\hat{X} - \hat{q}_i - d_{\text{eq,i}})^2$. In the end, the only term from expanding the square that interest us is the linear coupling term, thus we just set:

$$\hat{H}_{\text{int}} = \hat{X} \otimes \sum_i \kappa_i\hat{q}_i \equiv \hat{X} \otimes \hat{E} \tag{2.3}$$

- We write $\otimes$ to highlight the splitting into operators acting on the system versus acting on the environment ($S \otimes \mathcal{E}$).
- All other terms from expanding $(\hat{X} - \hat{q}_i - d_{\text{eq,i}})^2$ simply redefine frequencies, equilibrium positions and the zero of energy for all oscillators involved, hence they are skipped.
- For the case of a general system potential $V(\hat{X})$ instead of the harmonic one $\frac{1}{2}M\Omega^2\hat{X}$, the model of this section is called the Caldeira-Leggett model.

We now rewrite all operators in (2.1)-(2.3) by ladder operators as in (1.21), using $\hat{b}$, $\hat{b}^\dagger$ for the system and $\hat{a}_i$, $\hat{a}_i^\dagger$ for the environment, and arrive at our final

Quantum Brownian motion Hamiltonian in the energy basis

$$\hat{H}_S = \hbar\Omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right), \tag{2.4}$$

$$\hat{H}_{\mathcal{E}} = \sum_i \hbar\omega_i\left(\hat{a}_i^\dagger\hat{a}_i + \frac{1}{2}\right), \tag{2.5}$$

$$\hat{H}_{\text{int}} = \left(\hat{b} + \hat{b}^\dagger\right) \otimes \sum_i \bar{\kappa}_i\left(\hat{a}_i + \hat{a}_i^\dagger\right). \tag{2.6}$$

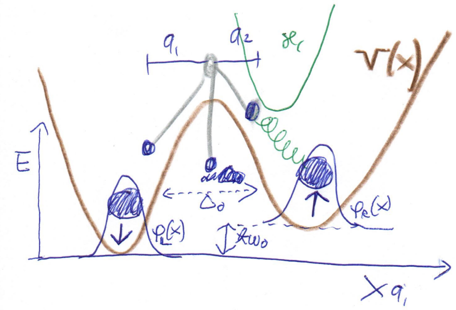
- The new interaction constant is $\bar{\kappa}_i = \kappa_i\sqrt{\frac{\hbar}{2m_i\omega_i}}\sqrt{\frac{\hbar}{2M\Omega}}$, which you see by inverting (1.21) to give e.g. $\hat{X} = \sqrt{\frac{\hbar}{2M\Omega}}\left(\hat{b} + \hat{b}^\dagger\right)$.
- An important feature of (2.3) is the possibility of dissipation: It contains terms such as $\hat{b}\hat{a}_i^\dagger$, which removes an energy quantum from the system oscillator and gives it to the environment.
- Heating on the other hand is also possible, through the cc. term $\hat{b}^\dagger\hat{a}_i$. To find out which will prevail, see later sections.

Example 8, Basis: As in (1.25) we can use oscillator quantum numbers n to define a basis for both, the system (basis $\mathcal{B} = \{|\,n\,\rangle\}$) and the environment (basis $\mathcal{B} = \{|\,m_1, m_2, \ldots, m_N\,\rangle\}$). The compound basis for system+environment is thus $\mathcal{B} = \{|\,n; m_1, m_2, \ldots, m_N\,\rangle\}$. Note {..} means "set of...".

2.2 Spin boson model

- Classification: System – one spin, environment – many oscillators.

We now change the system from the previous section to have a more complex potential $V(x)$ with two local minima, see below. However we then make it simpler again, by assuming the dimension X to be effectively frozen, with only two possible positions inside of the two local minima.



left: Damped double well system realization of the spin-boson model. The system particle (blue ball) couples to the environment oscillators (grey rods) as in section 2.1. However it now feels a different potential $V(x)$. We consider energies where it can only reside in the left well, with wavefunction $\varphi_L(x)$, or right well $\varphi_R(x)$. Identifying $\varphi_L \equiv |\downarrow\rangle$, $\varphi_R \equiv |\uparrow\rangle$, we realize an effective two-level system or spin-1/2 system.

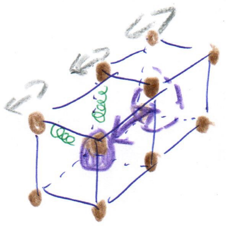
Simplifying the model into its standard form is more involved, but we eventually arrive at the Hamiltonian below with system, bath and coupling Hamiltonians given by

$$\hat{H}_S = \frac{1}{2}\hbar\omega_0\hat{\sigma}_z - \frac{1}{2}\hbar\Delta_0\hat{\sigma}_x, \tag{2.7}$$

$$\hat{H}_{\mathcal{E}} = \sum_i^N \left(\frac{\hat{p}_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2\hat{q}_i^2\right), \tag{2.8}$$

$$\hat{H}_{\text{int}} = \hat{\sigma}_z \otimes \sum_i \kappa_i\hat{q}_i. \tag{2.9}$$

- $\hbar\omega_0$ is the energy difference between the two system states, and $\hbar\Delta_0$ their inter-state transition amplitude (here tunnelling amplitude).
- See (1.17) for spin-operators / Pauli matrices.
- Note: These κ_i have dimension [energy/length] as opposed to the previous section (2.2), where it had [energy/length^2].
- The bath is of the same structure as in section 2.1, but the coupling to it has changed.



left: A physical system that realizes the above is a defect atom (violet) tunnelling in a solid crystal (brown), with crystal-phonons (green) as bath of oscillators.

Further reading: Some derivation of the model can be found in "Leggett *et al.*, Rev. Mod. Phys. **59** 1 (1987)".
See WQD, chapter 3.2, for another concrete example realizing the spin-boson model: Flux in an r.f. SQUID, in contact with a heat bath.

As before we can write this in terms of ladder operators to arrive at a final

Spin-boson model with system, bath and coupling Hamiltonians given by

$$\hat{H}_S = \frac{1}{2}\hbar\omega_0\hat{\sigma}_z - \frac{1}{2}\hbar\Delta_0\hat{\sigma}_x, \tag{2.10}$$

$$\hat{H}_{\mathcal{E}} = \sum_i \hbar\omega_i \left(\hat{a}_i^\dagger\hat{a}_i + \frac{1}{2}\right), \tag{2.11}$$

$$\hat{H}_{\text{int}} = \hat{\sigma}_z \otimes \sum_i \bar{\kappa}_i \left(\hat{a}_i + \hat{a}_i^\dagger\right). \tag{2.12}$$

- Here $\bar{\kappa}_i = \kappa_i\sqrt{\frac{\hbar}{2m_i\omega_i}}$.
- We will also consider the simplified case $\Delta_0 = 0$, for which the Hamiltonian Eq. (2.12) does not induce dissipation. We can see this since in that case $\left[\hat{H}_S, \hat{H}_{\text{int}}\right] = 0$ (always $\left[\hat{H}_S, \hat{H}_{\text{S,E}}\right] = 0$)). Thus the interaction Hamiltonian can not cause a change in system energy.

2.2.1 Simplified Spin-Boson model

Let us look at a simple example of Spin-Boson dynamics in the case $N = 1$ (single oscillator) and $\Delta_0 = 0$. This can be solved analytically (5.3.1 SD) but with some technicalities. Let us describe how a numerical solution would work and use diagrams!

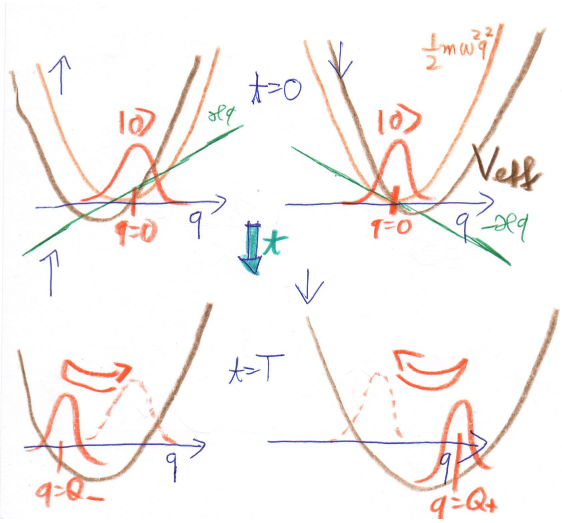
The complete system has a basis $\{|\uparrow, n\rangle = |\uparrow\rangle \otimes |n\rangle, |\downarrow, n\rangle = |\downarrow\rangle \otimes |n\rangle$, combining (1.16) and (1.25). Thus $|\Psi(t)\rangle = \sum_{s,n} c_{sn}(t)|sn\rangle$. Insertion of this into (2.10)-(2.10) gives equations of motion $\dot{c}_{sn}$. Importantly it turns out that none of the $\dot{c}_{\uparrow,n}$ are coupled to the $\dot{c}_{\downarrow,n}$, so we can solve the two "blocks" separately. That means we can ask separately "what happens if the spin is in $|\uparrow\rangle$?", "$\cdots|\downarrow\rangle$?.

One further way to see this, is to realize that the matrix representation of the Hamiltonian and therefore also that of the time-evolution operator decomposes into blocks. If we write our coefficients

$c_{sn}(t)$ all into one large vector, the TISE becomes

$$i\hbar \begin{bmatrix} \dot{c}_{\uparrow 0}(t) \\ \dot{c}_{\uparrow 1}(t) \\ \vdots \\ \dot{c}_{\downarrow 0}(t) \\ \dot{c}_{\downarrow 1}(t) \\ \vdots \end{bmatrix} = \begin{bmatrix} \underline{\underline{H}}_{\uparrow} & 0 \\ 0 & \underline{\underline{H}}_{\downarrow} \end{bmatrix} \cdot \begin{bmatrix} c_{\uparrow 0}(t) \\ c_{\uparrow 1}(t) \\ \vdots \\ c_{\downarrow 0}(t) \\ c_{\downarrow 1}(t) \\ \vdots \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} c_{\uparrow 0}(t) \\ c_{\uparrow 1}(t) \\ \vdots \\ c_{\downarrow 0}(t) \\ c_{\downarrow 1}(t) \\ \vdots \end{bmatrix} = \begin{bmatrix} \underline{\underline{U}}_{\uparrow} & 0 \\ 0 & \underline{\underline{U}}_{\downarrow} \end{bmatrix} \cdot \begin{bmatrix} c_{\uparrow 0}(0) \\ c_{\uparrow 1}(0) \\ \vdots \\ c_{\downarrow 0}(0) \\ c_{\downarrow 1}(0) \\ \vdots \end{bmatrix} \tag{2.13}$$

Example 9, Numerical solution of single-spin, single-boson model: Consider an initial-state $|\,\Psi(0)\,\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right) \otimes |\,0\,\rangle$. We can guess the evolution directly from (2.7)-(2.9):



left: For spin in state $|\uparrow\rangle$ we have $\langle\uparrow|\hat{H}_{\text{int}}|\uparrow\rangle = \kappa\hat{q}$, while $\langle\downarrow|\hat{H}_{\text{int}}|\downarrow\rangle = -\kappa\hat{q}$. In either case the single oscillator feels a shifted harmonic potential $V_{\text{eff}} = \frac{1}{2}m\omega^2 q^2 \pm \kappa q$ as shown in the figure (brown line). However the shift direction depends on the spin. Starting in the ground-state of the un-shifted potential, the oscillator does harmonic motion while its wave-function remains a Gaussian. This represents a coherent state. But the oscillator position during this oscillation depends on the state of the spin.

- If we denote by $|\,\alpha_q\,\rangle$ a coherent oscillator state centered at q (think of it as ground-state shaped Gaussian centered at q), then at the time T when the wavepacket reaches the "turning point" shown in the figure the overall state is

$$|\,\Psi(T)\,\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle \otimes |\,\alpha_{Q-}\,\rangle + |\downarrow\rangle \otimes |\,\alpha_{Q+}\,\rangle\right). \tag{2.14}$$

- This is of the same structure as the cat-state (1.1), except the oscillator may still be microscopic. But we can do the same calculation for $N = 10^{23}$ oscillators with similar results (each oscillator evolves into "their own" coherent state).

- We shall see that the creation of an entangled state (2.14) from a separable state $|\,\Psi(0)\,\rangle$ is at the heart of a quantum measurement and decoherence.

- In subsequent sections we will frequently make reference to the kind of paradigmatic entangling quantum evolution discussed above. We will refer to the evolution by

$$\frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right) \otimes |\,0\,\rangle \rightarrow \frac{1}{\sqrt{2}}\left(|\uparrow\rangle \otimes |\,\alpha_{Q-}\,\rangle + |\downarrow\rangle \otimes |\,\alpha_{Q+}\,\rangle\right), \tag{2.15}$$

where "$A \rightarrow B$" means *Total state A evolves under unitary evolution of the coupled system into total state B.*

- Assignment 1 provides another example based on a spin-spin model, see section 2.3.

2.2.2 Two level atom

We also want to present the example of section 1.1 as an open-system Hamiltonian. To do that we first have to introduce:

QED in a (small) nutshell: In classical electro-dynamics, electric and magnetic field follow from the vector potential $\mathbf{A}(\mathbf{x}, t)$ and scalar potential $\varphi(\mathbf{x}, t)$. In the Coulomb Gauge the latter is zero. In quantum electro-dynamics (QED) the vector potential is given by an operator

$$\hat{\mathbf{A}}(\mathbf{x}, t) = \sum_{n,\nu} \sqrt{\frac{\hbar}{2\epsilon_0 \omega_n \mathcal{V}}} \mathbf{e}_{n\nu} \left(e^{i(\mathbf{k}_n \mathbf{x} - \omega_n t)} \hat{a}_{n\nu} + e^{-i(\mathbf{k}_n \mathbf{x} - \omega_n t)} \hat{a}^\dagger_{n\nu} \right). \tag{2.16}$$

This decomposes the field into modes with index n written as $e^{i(\mathbf{k}_n \mathbf{x} - \omega_n t)}$ with wavenumber $\mathbf{k}_n$, frequency $\omega_n = c|\mathbf{k}_n|$ within a quantization volume $\mathcal{V}$. The index ν is for the polarisation, which is manifest in the polarisation vector $\mathbf{e}_{n\nu}$.
Most importantly each mode is described by operators $\hat{a}_{n\nu}$, $\hat{a}^\dagger_{n\nu}$ that act like ladder operators for the oscillator. The quantum states of the electro-magnetic field that these act on are occupation number states $|\, n_a n_b \cdots \rangle$, where each of the n_i is the number of photons in a mode $n\nu$.

Let us indeed simplify a single atom as in section 1.1 with considering only two electronic states for it, a ground state $|\, g \,\rangle \rightarrow |\downarrow\rangle$ and some excited state $|\, e \,\rangle \rightarrow |\uparrow\rangle$. We indicate here already how we identify these two states with spin-states in this section.

You will learn/ have learnt in PHY402, that transitions between electronic states in an atom because of electro-magnetic radiation are governed by the dipole matrix element

$$\mathbf{d}_{eg} = \langle\, e \,|\hat{\mathbf{A}}(\mathbf{x}, t) \cdot \boldsymbol{\nabla}|\, g \,\rangle. \tag{2.17}$$

It turns out that using a few further approximation (rotating-wave and dipole approximations), we can eventually write the effective

Two-level atom Hamiltonian for interactions with the quantized electromagnetic field following from (2.16) as:

$$\hat{H}_S = \frac{\hbar\omega_{eg}}{2}\hat{\sigma}_z, \tag{2.18}$$

$$\hat{H}_{\mathcal{E}} = \sum_{n\nu} \hbar\omega_n \hat{a}^\dagger_{n\nu}\hat{a}_{n\nu}, \tag{2.19}$$

$$\hat{H}_{\text{int}} = \hbar \sum_{n\nu} \left(g_{n\nu}\hat{a}_{n\nu} + g^*_{n\nu}\hat{a}^\dagger_{n\nu} \right) \left(\hat{\sigma}_+ + \hat{\sigma}_-\right), \tag{2.20}$$

where $\hbar\omega_{eg} = E_e - E_g$ is the energy difference of the two electronic states and $g_{n\nu} = -i\frac{\omega_{eg}\mu_{eg}}{\sqrt{2\hbar\epsilon_0\omega_n\mathcal{V}}}$, $\mu_{eg} = \langle\, e\, | e\mathbf{x} |\, g\,\rangle$. We used $\hat{\sigma}_+ = (\hat{\sigma}_x + i\hat{\sigma}_y)/2 = |\!\uparrow\rangle\langle\downarrow\!|$, $\hat{\sigma}_- = (\hat{\sigma}_x - i\hat{\sigma}_y)/2 = |\!\downarrow\rangle\langle\uparrow\!|$.

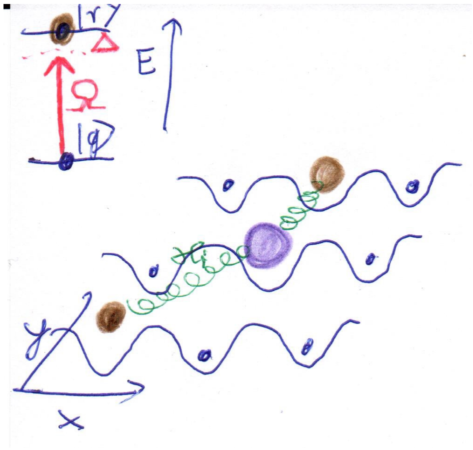
- Since the electro-magnetic field modes $n\nu$ function exactly like harmonic oscillators, this can be classified as a spin system-with oscillator environment, appropriate for this section.
- Comparison of (2.10)-(2.12) with (2.18)-(2.20) shows identical structure, except a changed system-environment interactions $\hat{H}_{\text{int}}$.
- The obvious interpretation of its terms is that a photon gets absorbed and the atom excited ($\hat{a}_{n\nu}\hat{\sigma}_+$) and the reverse.
- We will see later how this coupling of the atom to a quantum-electromagnetic field environment leads to spontaneous decay of the excited state $|\, e\,\rangle$.
- In quantum optics for some cases all elm. field modes $n\nu$ except one can be ignored. In this case the Hamiltonian above realizes the so called Jaynes-Cummings model.

Further reading: This section is based on Walls and Milburn ”Quantum Optics” 10.1.

2.3 Spin-spin model

- Classification: System – one spin, environment – many spins.

Finally we change to a picture where the environment is also given by a collection of spins. See the exemplary system below.



left: Spin-spin environment model realized by an array of optically trapped Rydberg atoms. Each atom is trapped on a single 2D lattice site, so position dynamics is fully suppressed. Atoms can be in a ground state $|\,g\,\rangle$ or Rydberg state $|\,r\,\rangle$. Under certain conditions (see PHY402) a laser can drive transitions between these two states with Hamiltonian $\hat{H} = \frac{\Omega}{2}(|\,r\,\rangle\langle\,g\,| + c.c.) - \Delta|\,r\,\rangle\langle\,r\,|$, with parameters Ω, Δ controlled by laser intensity and frequency. We assume two distinguishable species of atom, system (violet) and environment (brown). Only if two atoms n, m are in a Rydberg state, they interact over large distances of many micrometers with: $\hat{V} = \kappa_{nm}[|\,r\,\rangle\langle\,r\,|]^{(n)} \otimes [|\,r\,\rangle\langle\,r\,|]^{(m)}$ (operator $[\cdots]^{(n)}$ acts on atom n only. Over micrometer distances, if the atoms were in the ground-state there is no interaction (the range of that is nanometers).).

In such a case we can write a

Spin-spin model with system, bath and coupling Hamiltonians given by

$$\hat{H}_S = \frac{1}{2}\omega_0\hat{\Sigma}_z - \frac{1}{2}\Delta_0\hat{\Sigma}_x, \tag{2.21}$$

$$\hat{H}_{\mathcal{E}} = \sum_i^N \frac{1}{2}\omega_i\hat{\sigma}_z^{(i)} - \frac{1}{2}\Delta_i\hat{\sigma}_x^{(i)}, \tag{2.22}$$

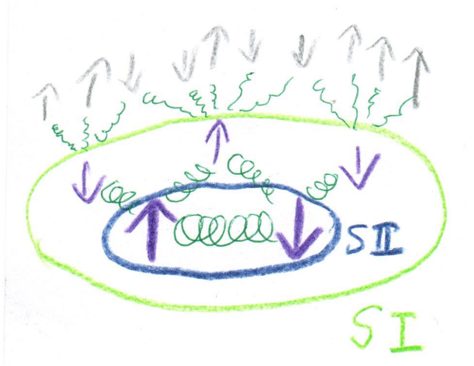
$$\hat{H}_{\text{int}} = \hat{\Sigma}_z \otimes \sum_i \kappa_i\hat{\sigma}_z^{(i)}. \tag{2.23}$$

Here CAPITAL Pauli matrices $\hat{\Sigma}_{x,z}$ act on the system spin, and lower case ones $\hat{\sigma}_{x,z}$ on environmental spins.

- By $\hat{\sigma}_x^{(i)}$ we imply a Pauli matrix that only acts on spin number (i), i.e. $\hat{\sigma}_x^{(2)}|\uparrow\uparrow\uparrow\rangle = |\uparrow\downarrow\uparrow\rangle$.
- Spin-spin models are often good environmental models at low temperature, for example when it is enough to consider the two lowest quantum states for each oscillator in Eq. (2.8).
- Detailed translation of the example above into (2.21)-(2.23): exercise! (Identify: $|\downarrow\rangle \leftrightarrow |\,g\,\rangle$, $|\uparrow\rangle \leftrightarrow |\,r\,\rangle$.
- We have done some preliminary investigations of the spin-spin model in assignment 1.

2.4 Multi-component problems

The paradigmatic examples above are simpler than most real problems, in that the system part has a clear single particle character (i.e. *one* oscillator or *one* spin). In practice of course S may be a many-body system itself.



left: In the left figure of many coupled spins (violet and gray), the size of green twiddles indicates the strengths of mutual couplings. In this case it may be not fully clear if we should choose our system as just the two inner spins (S-II), or maybe all violet spins (S-I). This illustrates a certain ambiguity in our system-environment splitting. We will learn later, that this may even affect the classification of the resultant open-system, i.e. S-II may be Non-Markovian, while S-I is Markovian.

The <u>formalisms</u> you learn in the remainder of the lecture should be able to deal with both cases in the caption above, and give identical answers when all their underlying assumptions are fulfilled. However, the initial <u>classification</u> of the open-system and thus methods to be used for them may differ depending on whether choice I or II is made.

Week ③

PHY 637 Decoherence and Open Quantum Systems
Instructor: Sebastian Wüster, IISER Bhopal, 2021

These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

3 Basic Formalism and Interpretation of Decoherence

In the following we want to proceed with the aim sketched in section 1: to develop a formalism that allows us to deal with the system (S) part of the models introduced in section 2 only, and find a way to effectively take into account the influence of the environment $\mathcal{E}$.

For that we have to revise/ introduce the concept of....

3.1 Density matrices

3.1.1 Pure state density matrices and the trace operation

So far we are mainly used to describe a quantum system in terms of the (pure) state vector $|\,\Psi\,\rangle = \sum_n c_n|\,\phi_n\,\rangle$, where the sum denotes its decomposition in terms of some arbitrary Hilbert-space basis $\mathcal{B} = \{|\,\phi_n\,\rangle\}$. Alternatively we can write the

Pure state density matrix/ density operator defined as the projection

$$\hat{\rho} = |\,\Psi\,\rangle\langle\,\Psi\,| = \sum_{nm} c_n c_m^* |\,\phi_n\,\rangle\langle\,\phi_m\,|. \tag{3.1}$$

- The corresponding matrix ρ has Matrix elements $\rho_{nm} = c_n c_m^*$.
- The elements on the diagonal are $\rho_{nn} = p_n = |c_n|^2$, called populations (see QM-1/2).
- The off-diagonal element $\rho_{nm} = c_n c_m^*$ is called coherence between states n and m.

We can also formulate quantum time-evolution as in section 1.5.6 for the density matrix, it is then governed by the

Von Neumann equation

$$\frac{d}{dt}\hat{\rho}(t) = -\frac{i}{\hbar}\big[\hat{H}(t), \hat{\rho}(t)\big]. \tag{3.2}$$

- Proof: Exercise. Start with $\hat{\rho}(t) = |\,\Psi\,\rangle\langle\,\Psi\,| = \sum_{nm} c_n(t)c_m^*(t)|\,\phi_n\,\rangle\langle\,\phi_m\,|$, differentiate wrt. time, apply product rule and TDSE.

We also introduce the

Trace of an Operator As for matrices this is the sum of all diagonal elements of an operator

$$\mathrm{Tr}[\hat{O}] \equiv \sum_k \langle\,\phi_k\,|\hat{O}|\,\phi_k\,\rangle. \tag{3.3}$$

where $\mathcal{B} = \{|\,\phi_n\,\rangle\}$ is any orthonormal basis of the Hilbertspace.

- This definition is independent of the choice of $\mathcal{B}$.
- We have introduced it in order to write the expectation value of an operator $\hat{O}$ with $\hat{O}|\,\phi_k\,\rangle = o_k|\,\phi_k\,\rangle$ in a quantum state $|\,\Psi\,\rangle = \sum_k c_k|\,\phi_k\,\rangle$ as

  $$\langle\hat{O}\rangle = \mathrm{Tr}[\hat{O}\hat{\rho}] = \sum_k o_k|c_k|^2. \tag{3.4}$$

  This expression is known from using state vectors $|\,\Psi\,\rangle$.
- The trace is linear $\mathrm{Tr}[\hat{A}+\hat{B}] = \mathrm{Tr}[\hat{A}] + \mathrm{Tr}[\hat{B}]$ and cyclic $\mathrm{Tr}[\hat{A}\hat{B}\hat{C}] = \mathrm{Tr}[\hat{B}\hat{C}\hat{A}]$. *Proof of all of this: exercise.*

Example 10, Coherences in a density matrix indicate superpositions: Iff the state $|\,\Psi\,\rangle$ contains a quantum superposition of basis elements $|\,\phi_a\,\rangle$ and $|\,\phi_b\,\rangle$, such as $|\,\Psi\,\rangle = \frac{1}{\sqrt{2}}(|\,\phi_a\,\rangle + |\,\phi_b\,\rangle)$, the coherence ρ_{ab} will be nonzero (in this case $\rho_{ab} = 1/2$). Note, however, that the statement wether or not there is a superposition, and whether or not a coherence is non-zero depends on the choice of basis:
Consider the spin state: $|\,\Psi\,\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$, in terms of the basis $\mathcal{B} = \{|\uparrow\rangle, |\downarrow\rangle\}$

$$\rho = \begin{bmatrix}\frac{1}{2} & \frac{1}{2}\\ \frac{1}{2} & \frac{1}{2}\end{bmatrix} \text{''} = \text{''} \frac{1}{2}\Big(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\Big), \tag{3.5}$$

with non-vanishing coherences. We also illustrate the two notations that we intend to use: the Matrix representation of the density operator (left) and the operator form (right).
To illustrate the basis dependence, we can express $\hat{\rho}$ instead in the basis $\mathcal{B} = \{|\leftarrow\rangle, |\rightarrow\rangle\}$ (eigenstates of σ_x), we have

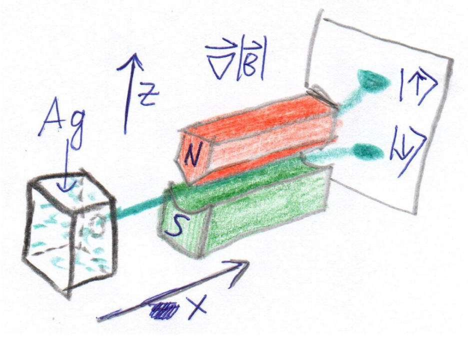
$$\rho = \begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix} \text{''} = \text{''} |\leftarrow\rangle\langle\leftarrow|, \tag{3.6}$$

with no coherences.

3.1.2 Mixed state density matrices

To have an illustrative example for the concepts later in this section, let us first revisit the

Example 11, Stern-Gerlach experiment: undertaken in 1922 to explore the quantization of angular momentum, see figure below. The Ag atom angular momentum is just given by the valence electron spin, hence $s = 1/2$. The magnetic moment of the atom due to the electron is $\hat{\boldsymbol{\mu}} = -g_s\mu_B\hat{\mathbf{S}}/\hbar$, in an inhomogeneous magnetic field this yields a Force $\hat{\mathbf{F}} = -\boldsymbol{\nabla}[-\hat{\boldsymbol{\mu}}\cdot\mathbf{B}]$. With magnetic field and inhomogeneity along z we reach, all up: $F_z = -g_s\mu_B\hat{S}_z\frac{\partial}{\partial z}B_z$.



left: A beam of silver atoms is directed through a region of inhomogeneous magnetic field. The resultant different forces experienced by $|\uparrow\rangle$ and $|\downarrow\rangle$ atoms split the beam up into only two discrete spots. The device has thus demonstrated quantisation of $\hat{\mathbf{S}}$ *and* measured the value of $\hat{S}_z$ for each atom.

- Importantly, the spin-component which is being measured is decided by the direction of the magnetic field strength gradient. If we had oriented the field gradient along x, we would obtain two left-right split dots corresponding to atoms in $|\leftarrow\rangle$, $|\rightarrow\rangle$ (see section 1.5.2).
- Let us try to formally describe the situation in the figure above, where each atom from a

thermal source is randomly in either the $|\uparrow\rangle$ or $|\downarrow\rangle$ state with $50\% - 50\%$ probabilities.[3] Which state would we assign to such an atom? We could try $|\Psi\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$, which would give the correct probabilities for a measurement of $\hat{S}_z$ (50/50).

- However what if we measure $\hat{S}_x$ instead? We recognise the state above as $|\leftarrow\rangle$, eigenstate of $\hat{S}_x$. Thus if we measure $\hat{S}_x$ instead of $\hat{S}_z$, we would get $+1/2$ with 100% probability. However, since we said atoms are with $50\% - 50\%$ chance in $|\uparrow\rangle$ or $|\downarrow\rangle$ and $|\uparrow\rangle = (|\leftarrow\rangle + |\rightarrow\rangle)/\sqrt{2}$, $|\downarrow\rangle = (|\leftarrow\rangle - |\rightarrow\rangle)/\sqrt{2}$, we should in fact get $S_x = +1/2, -1/2$ with $50\% - 50\%$ probability for each atom. How can we write a state that describes both measurements, $\hat{S}_x$ and $\hat{S}_z$ correctly?
- This example points to essential differences in uncertainties in quantum mechanics and classical mechanics.

The tool to describe both types of uncertainties in one unified formalism are density matrices as in section 3.1.1, which is in fact why we introduced them.

We now define the

Mixed state density matrix

$$\hat{\rho} = \sum_n p_n |\phi_n\rangle\langle\phi_n|, \tag{3.7}$$

Here ϕ_n is an orthonormal set of states and p_n the classical probability to be in state n.

- We have $\sum_n p_n = \mathrm{Tr}[\hat{\rho}] = 1$, expressing normalisation of our state.
- We recognize (3.1) as a special case with $p_n = \delta_{nk}$ for some k.
- Consider now the expectation value of an operator

$$\begin{aligned}\langle\hat{O}\rangle = \mathrm{Tr}[\hat{O}\hat{\rho}] &= \sum_n \langle\phi_n|[\hat{O}\sum_m p_m|\phi_m\rangle \underbrace{\langle\phi_m|]|\phi_n\rangle}_{=\delta_{nm}} \\ &= \sum_n p_n \langle\phi_n|\hat{O}|\phi_n\rangle \end{aligned} \tag{3.8}$$

This takes into account both, the classical and quantum mechanical formalism for determining an average. The same can also account for a combination of classical and quantum mechanical uncertainties, see Assignment 3.

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[3] The true situation is that all spins are unpolarized, so they point in any random direction. One can show that this gives equivalent results for our purposes, see e.g. the QM book by Sakurai on how to reach this conclusion.

Example 12, Spin mixture:
Let us apply this to the spin mixture problem discussed on the previous page. We define the state of atoms in the oven via the density matrix $\hat{\rho} = (|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|)/2$, implying we simply have no knowledge of which spin state they are in, but that there is no superposition of $\uparrow + \downarrow$. Then

$$\langle\hat{S}_x\rangle = \mathrm{Tr}[\hat{S}_x\hat{\rho}] \overset{Eq.\ (3.8)}{=} (\underbrace{\langle\uparrow|\hat{S}_x|\uparrow\rangle}_{=0} + \underbrace{\langle\downarrow|\hat{S}_x|\downarrow\rangle}_{=0})/2 = 0, \tag{3.9}$$

as required since we will find $\hat{S}_x = +1/2, -1/2$ with equal probability. Equally we also find $\langle\hat{S}_z\rangle = 0$.

- This sort of mixture is also called proper mixture, and can represent a system that **is** in a pure state, but we don't know in which. The mixture is due to our ignorance. We will learn about improper mixtures shortly.
- For this interpretation we need to know additionally that the system is in a certain set of pure states. For example we can write the density matrix in the example above equally well as $\hat{\rho} = (|\leftarrow\rangle\langle\leftarrow| + |\rightarrow\rangle\langle\rightarrow|)/2$ (exercise), which we would get when saying the system is always either in $|\leftarrow\rangle$ or $|\rightarrow\rangle$. Given only the density matrix as a mathematical object we cannot distinguish the two scenarios. This means measurements cannot distinguish between the two.
- The density matrix just introduced also plays a central role in quantum statistical physics, where we use it with $p_n = \exp[-E_n/(k_B T)]$ to describe a statistical ensemble at temperature T. Alternatively one could describe a quantum ensemble of identical systems also in a pure high-dimensional Hilbertspace (see SD 2.4.5). For ensemble averages both approaches give the same results.

Even though they have the same populations in the basis $\{|\phi_n\rangle\}$, a mixed state $\hat{\rho}$ as in (3.7) is very different from the pure state $|\Psi\rangle = \sum_n \sqrt{p_n}|\phi_n\rangle$. We have seen this in the above discussion of measurements on a state $|\leftarrow\rangle$ and on the density matrix $\hat{\rho} = (|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|)/2$.

To quantify this difference, we introduce two measures[4]:

Purity

$$\zeta(\hat{\rho}) = \mathrm{Tr}[\hat{\rho}^2] \tag{3.10}$$

We can see $\zeta = 1$ if $\hat{\rho}$ is a pure state density matrix (3.1), but $\zeta < 1$ for genuine mixed states (3.7).

- For maximally mixed states $\hat{\rho} = \sum_n^N 1/N|\phi_n\rangle\langle\phi_n|$, we have $\zeta = 1/N$.

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[4] many more exist

- The definition exploits that $\hat{\rho}^2 = \hat{\rho} \Leftrightarrow \hat{\rho}$ is a pure state density matrix.
- Note that the mixed state density matrix (3.7) has no coherences in the basis $|\,\phi_n\,\rangle$, unlike the pure state one (3.1) for the case of a superposition. It is thus sometimes tempting to use the existence of coherences to discriminate between pure and mixed states. With some extra knowledge this sometime works, but in general is not safe, due to the basis dependence of coherences. In contrast, the purity (3.10) is basis in dependent (proof, exercise).

An alternate measure to quantify the degree of "mixedness" of a quantum system is the

Von-Neumann Entropy defined as

$$S(\hat{\rho}) = -\mathrm{Tr}[\hat{\rho}\,\log_2\hat{\rho}] \equiv -\sum_k \lambda_k \log_2(\lambda_k). \tag{3.11}$$

The λ_k are the non-zero eigenvalues of $\hat{\rho}$. We can see $S = 0$ if $\hat{\rho}$ is a pure state density matrix (3.1), but $S > 0$ for genuine mixed states (3.7).

- For pure states only one eigenvalue is non-zero and equal to unity.
- For a maximally mixed state (see above), we have all $\lambda_k = p_k = 1/N$ and thus $S = \log_2(N)$, which is the maximum allowed value.

3.1.3 Reduced density matrices

In the previous section we saw how the density matrix concept helps us to incorporate at the same time uncertainties due to quantum effects and to classical randomness. We shall now see that it also is a useful tool for the objective stated at the outset of this section: To deal with the system $\mathcal{S}$ only, without having to know the entire quantum state of the environment $\mathcal{E}$.

Let $\mathcal{B}_S = \{|\,\phi_k\,\rangle\}$ and $\mathcal{B}_E = \{|\,\varphi_k\,\rangle\}$ be two bases for system and environment, then we use $|\,\phi_k, \varphi_l\,\rangle = |\,\phi_k\,\rangle \otimes |\,\varphi_l\,\rangle$ to write the elements of the complete basis (system+environment).

Further let $\hat{O} = \hat{O}_S \otimes \mathbb{1}$ be operator that acts on the system only. Any information on the system, via measurements on the system only, can be obtained from operators of that form.

Now note:

$$\begin{aligned}
\langle \hat{O} \rangle = \mathrm{Tr}[\hat{\rho}\hat{O}] &\overset{Eq.\ (3.3)}{=} \sum_{kl} \langle\,\phi_k, \varphi_l\,|\hat{\rho}(\hat{O}_S \otimes \mathbb{1})|\,\phi_k, \varphi_l\,\rangle \\
&= \sum_k \langle\,\phi_k\,| \left(\sum_l \langle\,\varphi_l\,|\hat{\rho}|\,\varphi_l\,\rangle \right) \hat{O}_S|\,\phi_k\,\rangle \equiv \sum_k \langle\,\phi_k\,|\mathrm{Tr}_E[\hat{\rho}]\hat{O}_S|\,\phi_k\,\rangle \\
&\equiv \sum_k \langle\,\phi_k\,|\hat{\rho}_S\hat{O}_S|\,\phi_k\,\rangle = \mathrm{Tr}_S[\hat{\rho}_S\hat{O}_S].
\end{aligned} \tag{3.12}$$

In the second equality we used that $\hat{O}$ does not act on states $|\,\varphi_l\,\rangle$. Here we have introduced the

Reduced density matrix of the system

$$\hat{\rho}_S = \mathrm{Tr}_E[\hat{\rho}], \tag{3.13}$$

where $\mathrm{Tr}_E[\hat{O}] = \sum_l \langle\,\varphi_l\,|\hat{\rho}|\,\varphi_l\,\rangle$ is the partial trace over the environment.

- What we can infer from Eq. (3.12), is that the quantity $\hat{\rho}_S$ gives all the information that we can possibly gain from measurements on the system alone. Importantly this excludes measurements that jointly determine the environmental states. We assume those are not possible.
- Let's look at some examples for a spin-spin model (section 2.3), where we chose just two environmental spins for simplicity:

Example 13, Reduced density matrix for separable system and environment: Suppose system and environment are in a separable[a] state: $|\,\Psi\,\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \otimes \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$. States before $\otimes$ refer to the system, after $\otimes$ to the environment. This expands to $|\,\Psi\,\rangle = \frac{1}{2}(|\uparrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\downarrow\rangle)$, somewhat hiding the separability.
We now perform the partial trace over the environment after converting this to a density matrix.

$$\hat{\rho}_S = \mathrm{Tr}_E[\hat{\rho}] = \sum_{s_1,s_2} \langle\,\_s_1 s_2\,|\hat{\rho}|\,\_s_1 s_2\,\rangle, \tag{3.14}$$

where in the first step spin indices s_1, s_2 run over $\uparrow, \downarrow$ each, and we have used the "placeholder" _ to visualize the fact that the scalar products involving environmental spins act on the last two spin indices only.

We arrive at (exercise)

$$\hat{\rho}_S = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \text{"} = \text{"} \frac{1}{2}\Big(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\Big), \tag{3.15}$$

which we recognise as in (3.5) as the density matrix for the pure system state $|\,\Psi_S\,\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$.
We can evaluate the purity (3.10) (exercise) and find $P = 1$ as expected. If system and environment are separable, the reduced density matrix thus contains the same information as if we had ignored the environment altogether and looked at the system only.

---

[a] wrt. the system-environment splitting. The environment part is actually entangled.

Example 14, Reduced density matrix for entangled system and environment: Now consider a state where the system is entangled with the environment: $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |\uparrow\uparrow\rangle + |\downarrow\rangle \otimes |\downarrow\downarrow\rangle)$. Following the same procedure as in example 1 we reach:

$$\hat{\rho}_S = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \text{''}=\text{''} \frac{1}{2}\Big(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\Big), \tag{3.16}$$

the mixed state already given in (3.6). The purity in this case is given by $P = 1/2$, the minimum allowed in a two-dimensional Hilbertspace.
I this example, we would not have known how to write any information fo the "system only" from $|\Psi\rangle$, since an entangled state does not permit that.

- In the examples above we have seen that a reduced density matrix can frequently take the form of a mixed state. Unlike those in section 3.1.2 these are called improper mixtures. The interpretation is not that the system is in a pure state but we don't know which, but rather that the "system+environment" are together in a complicated entangled pure state, which is such that local measurements on the system alone are indistinguishable from the those in a proper mixed case that would be based on ignorance.
- It can be shown that, assuming a pure total state, **iff** the system and environment are separable, the reduced system state will be pure.

Example 15, Reduced density matrix yielding incomplete mixture: Finally let's look at yet one more example: $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes (c_1|\uparrow\uparrow\rangle + c_2|\downarrow\downarrow\rangle) + |\downarrow\rangle \otimes (c_2|\uparrow\uparrow\rangle + c_1|\downarrow\downarrow\rangle))$, with $|c_1|^2 + |c_2|^2 = 1$. Note, that for $c_1 = 1$, $c_2 = 0$ this co-indices with example 14, and for $c_1 = c_2 = 1/\sqrt{2}$, system and environment are separable, as in example 13.
For the general state in the present example 15, we find

$$\hat{\rho}_S = \frac{1}{2}\begin{bmatrix} 1 & c_1 c_2^* + c_1^* c_2 \\ c_1 c_2^* + c_1^* c_2 & 1 \end{bmatrix} \text{''}=\text{''} \frac{1}{2}\Big(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + 2\mathrm{Re}[c_1 c_2^*]\big(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\big)\Big), \tag{3.17}$$

with purity $P = (1 + 4\mathrm{Re}[c_1 c_2^*]^2)/2$. Thus the purity depends on c_1, c_2, and in general represents a not-maximally entangled system-environment, of relevance in the following. We can get all purity values in between the maximum (1) and minimum (1/2) depending on c_1 and c_2.
Note that the resultant density matrix neither quite takes the form (3.1) nor (3.7) but some hybrid of the two.

3.1.4 Local Measurability of Interference and Distinguishability

We now address how the measurability of interference locally in the sytem depends on the structure of its entanglement with some environment. First note that the measurement of $\hat{S}_x$ alluded to in section 3.1.2 "proves" the existence of a coherent superposition $|\,\Psi\,\rangle = c_1|\!\uparrow\rangle + c_2|\!\downarrow\rangle$ though an interference type measurement: the fraction measured in $m_{sx} = -1/2$ is $|\langle \rightarrow |\,\Psi\,\rangle|^2 = |c_1 - c_2|^2/\sqrt{2}$, vanishing only due to the coherence. For this interference to be measured, the <u>coherences</u> in the density matrix must be non-zero in the z-basis.

Consider the generic bi-partite state

$$|\,\Psi\,\rangle = \frac{1}{\sqrt{2}}\Big(|\,\phi_1\,\rangle \otimes |\,\chi_1\,\rangle + |\,\phi_2\,\rangle \otimes |\,\chi_2\,\rangle\Big), \tag{3.18}$$

with states $|\,\phi\,\rangle$ for the system and $|\,\chi\,\rangle$ for the environment. We do <u>not</u> assume the $|\,\chi_k\,\rangle$ to be mutually orthogonal. The density matrix can be written as $\hat{\rho} = \frac{1}{2}\sum_{ij}^{2} |\,\phi_i\,\rangle\langle\,\phi_j\,| \otimes |\,\chi_i\,\rangle\langle\,\chi_j\,|$.

To find the reduced density matrix of the system, we do require an orthonormal basis of the environment, let that be $\{|\,\varphi\,\rangle_n\}$. We can thus expand $|\,\chi_{1,2}\,\rangle = \sum_l c_l^{(1,2)}|\,\varphi_l\,\rangle$. Using Eq. (3.3) we obtain:

$$\begin{aligned}
\hat{\rho}_S &= \mathrm{Tr}_{\mathcal{E}}\left(\frac{1}{2}\sum_{ij}|\,\phi_i\,\rangle\langle\,\phi_j\,| \otimes |\,\chi_i\,\rangle\langle\,\chi_j\,|\right)\\
&= \frac{1}{2}\sum_{ij}|\,\phi_i\,\rangle\langle\,\phi_j\,|\sum_k\langle\,\varphi_k\,|\left(\sum_{ll'}c_l^{(i)}c_{l'}^{(j)*}|\,\varphi_l\,\rangle\langle\,\varphi_{l'}\,|\right)|\,\varphi_k\,\rangle\\
&= \frac{1}{2}\sum_{ij}|\,\phi_i\,\rangle\langle\,\phi_j\,|\sum_k c_k^{(i)}c_k^{(j)*} = \frac{1}{2}\sum_{ij}|\,\phi_i\,\rangle\langle\,\phi_j\,|\langle\,\chi_j\,|\,\chi_i\,\rangle\\
&= \frac{1}{2}\Big(|\,\phi_1\,\rangle\langle\,\phi_1\,| + |\,\phi_2\,\rangle\langle\,\phi_2\,| + |\,\phi_1\,\rangle\langle\,\phi_2\,|\langle\,\chi_2\,|\,\chi_1\,\rangle + |\,\phi_2\,\rangle\langle\,\phi_1\,|\langle\,\chi_1\,|\,\chi_2\,\rangle\Big).
\end{aligned} \tag{3.19}$$

This is a very important result. We see several generic consequences of the bi-partite (in general entangled) state (3.18):

- If the environmental states $|\,\chi_{1,2}\,\rangle$ were <u>fully distinguishable</u> (that is the case if they are orthogonal, $\langle\,\chi_2\,|\,\chi_1\,\rangle = 0$), then there is <u>no coherence</u> between $|\,\phi_{1,2}\,\rangle$ in the reduced system (see example 2).
- If they were identical ($\langle\,\chi_2\,|\,\chi_1\,\rangle = 1$) we had in fact a separable state and there is full coherence.
- In more general cases, the amount of coherence left in the system depends on the <u>overlapp</u>, which characterises in-distinguishability of the states $|\,\chi_{1,2}\,\rangle$ (example 3). If there is no overlapp, states are fully distinguishable.
- We can interpret $\langle\,\chi_2\,|\,\chi_1\,\rangle$ as quantifying the amount of knowledge or information present in the environment regarding the state of the system, due to both together being in the entangled state (3.18). We will discuss this more later.

Week ④

PHY 435 / 635 Decoherence and Open Quantum Systems
Instructor: Sebastian Wüster, IISER Bhopal, 2021

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3.2 Decoherence and measurements

With the tools provided so far, we can now begin our first discussion of how decoherence arises. There will be a strong conceptual link with "measurements", so let's discuss those first.

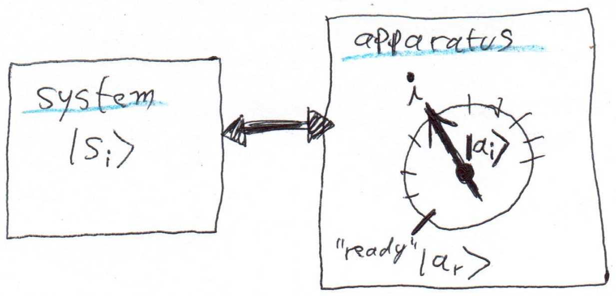
3.2.1 Ideal von Neumann measurements

The postulates in section 1.5.1 attribute a special status to the act of a measurement, that does not seem justified from fundamental principles. We now develop a line of thought due to von Neumann, that attempts to treat the measurement apparatus used to observe a quantum system in a quantum mechanical fashion as well.

Suppose the quantum system $\mathcal{S}$ to be observed has a basis $\{|\, s_n\,\rangle\}$. For the apparatus $\mathcal{A}$ we assume a basis $\{|\, a_n\,\rangle\}$. Let one of those basis states represent the initial state of the apparatus before it has done any measurement, called "ready state" $|\, a_r\,\rangle$. Now suppose the system is in a specific one of the basis states, say $|\, s_i\,\rangle$ initially. The act of measurement then must correspond to the unitary evolution

$$|\, s_i\,\rangle \otimes |\, a_r\,\rangle \to |\, s_i\,\rangle \otimes |\, a_i\,\rangle, \tag{3.20}$$

where the apparatus has made a transition to a state $|\, a_i\,\rangle$ indicating that it has measured $|\, s_i\,\rangle$ for the system. This is sketched in the figure below, adapted from SD. See (2.15) for the "definition" of "$\to$".



left: von Neumann scheme for an ideal quantum measurement.

- We assume here that each state of the system $|\, s_i\,\rangle$ results in the apparatus to take a distinguishable state $|\, a_i\,\rangle$ with 100% probability. In this sense the measurement is assumed perfect.

- Note that in (3.20), after the measurement, the system is still in $|\, s_i \,\rangle$. Such a scheme is called quantum non-demolition (QND) measurement. For the Stern-Gerlach apparatus reviewed in section 3.1.2 to make a QND measurement *before* atoms hit the screen, we need to have a non-destructive way to infer which beam the atoms are in, for example by weakly scattering light off them. *Once atoms hit the screen*, the scheme is no longer QND, since the screen may have changed the spin-state.

Before the measurement, the quantum system will in the general case be in a superposition of its basis states $|\, \psi \,\rangle = \sum_n c_n |\, s_n \,\rangle$. Since the TDSE (1.9) is linear, we can then infer the complete

Von Neumann Measurement Evolution

$$|\, \psi \,\rangle \otimes |\, a_r \,\rangle = \left(\sum_n c_n |\, s_n \,\rangle \right) \otimes |\, a_r \,\rangle \to \sum_n c_n \big(|\, s_n \,\rangle \otimes |\, a_n \,\rangle \big), \tag{3.21}$$

- Note the initial state in (3.21) is separable, the final one entangled (see section 1.5.5). Entanglement has thus been created dynamically.
- For a specific example of unitary dynamics implied by ”→” in (3.21), see the spin-boson evolution in section 2.2.1 and assignment 2. There, the harmonic oscillator can be thought of as having ”measured” the spin, with the left-hand-side (right-hand-side) coherent states corresponding to the $|\, a_i \,\rangle$, that are taken up depending on whether the sytem was in $|\, s_i \,\rangle \in \{|\uparrow\rangle, |\downarrow\rangle\}$.
- Depending on how ”macroscopic” we have assumed our measurement device to be, we would develop the same conceptual worries with the state (3.21) as in the Schrödingers cat example, section 1.1 (it is in fact the same type of state). We might still be OK with the idea, when the apparatus $\mathcal{A}$ is say a single quantum oscillator, maybe a nano-mechanical spring, whereas if $\mathcal{A}$ was an oscilloscope, our intuition would reject it.

The conceptually very simple line Eq. (3.21) now allows us to clearly state three major problems with the concept of a quantum measurement. Two of these can be resolved by decoherence, but one of them cannot.

3.2.2 Measurement Problems

I: The preferred basis problem

Suppose we have done our ideal van-Neumann measurement and wish to conclude from the entanglement structure in the final state of Eq. (3.21), that the apparatus has indeed ”measured” which state of the specific system basis $|\, s_n \,\rangle$ the system ”was in”. I.e. after some still not quantum mechanically described collapse, the system is in state $|\, s_n \,\rangle$ with probability $|c_n|^2$.

However we can pick an arbitrary other basis for the apparatus, say $|\, a'_n \,\rangle$, express our former basis as $|\, a_n \,\rangle = \sum_k \langle\, a'_k \,|\, a_n \,\rangle |\, a'_k \,\rangle$, and then rewrite the final state in (3.21) as (exercise)

$$\sum_n c_n \big(|\, s_n \,\rangle \otimes |\, a_n \,\rangle \big) = \sum_k d_k \big(|\, s'_k \,\rangle \otimes |\, a'_k \,\rangle \big), \tag{3.22}$$

with new system states $d_k |\, s'_k \,\rangle = \sum_n c_n |\, s_n \,\rangle \langle\, a'_k \,|\, a_n \,\rangle$, where d_k normalises the state $|\, s'_k \,\rangle$.

- Since those two bases discussed above are mathematically equivalent, after the "quantum-measurement", the question arises: What picks the preferred basis in terms of which we obtain results after wave-function collapse?

Example 16, Stern-Gerlach measurement problem: The problem is particularly severe, if the coefficients c_n are such that also the $|\, s'_n \,\rangle$ form an orthogonal basis of the system. Let's consider the Stern-Gerlach example (section 3.1.2) again, supposedly measuring a system (gold atom) in the state $|\, \psi \,\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$. According to (3.21), the system+apparatus will evolve into $|\, \Psi \,\rangle = (|\uparrow\rangle |\, a_\uparrow \,\rangle + |\downarrow\rangle |\, a_\downarrow \,\rangle)/\sqrt{2}$, where the apparatus state $|\, a_\uparrow \rangle$ can be thought of as the position wave-function for the atom having moved into the upper beam due to the spin-dependent force felt in the magnetic field.
However following (3.22) we could also write $|\, \Psi \,\rangle = (|\leftarrow\rangle |\, a_\leftarrow \,\rangle + |\rightarrow\rangle |\, a_\rightarrow \,\rangle)/\sqrt{2}$, where $|\, a_\leftarrow \,\rangle = (|\, a_\uparrow \,\rangle + |\, a_\downarrow \,\rangle)/\sqrt{2}$ and $|\, a_\rightarrow \,\rangle = (|\, a_\uparrow \,\rangle - |\, a_\downarrow \,\rangle)/\sqrt{2}$ (exercise). Thus simply from the entanglement-structure of the system+apparatus state, we could argue that the machine has measured both non-commuting observables $\hat{S}_x$, $\hat{S}_z$, which cannot be possible.
In fact we know that the apparatus would have to be designed differently if we wanted to measure $\hat{S}_x$, namely with magnetic field oriented along the x-axis instead of the z-axis.

II: The problem of Nonobservability of Interference

- The entangling dynamics of the kind (3.21) generically arises whenever a quantum system evolves while interacting with an environment. This suggests that entangled and superposition many-body states should be omnipresent also in the macroscopic world, since everything more or less interacts with something else. However, quantum mechanics is clearly not apparent in the large majority of macroscopic phenomena around us. In other words, we typically do not observe interference effects with macroscopic objects. Explaining this is the "problem of Nonobservability of Interference".

III: The problem of Outcomes

- The final question is, after having arrived at the superposition state (3.21) due to the unitary dynamics describing the measurement apparatus, why do we not actually "experience" that superposition? Why do we instead find a specific outcome and what selects which of the possible outcomes we find?
- This is actually an unresolved problem (yours), decoherence cannnot provide any answer for that.
- A possible approach that was proposed, is to extend quantum mechanics by a "physical collapse model", i.e. a mechanism that creates the otherwise only postulated wave function collapse. Other ideas embrace macroscopic superpositions in more philosophical ways. We will try to survey some of these ideas in the last week(s) of the lecture, time permitting.

3.2.3 Environmental monitoring and Decoherence

After having pointed out three major problems with the concept of a quantum-measurement, let us proceed to their partial resolution by the concept of decoherence through "environmental monitoring". The latter term is coined, since it turns out that the evolution in a von Neumann measurement (3.21) actually has the same structure as the evolution of a quantum system in contact with an environment, see e.g. (2.15). Thus if we consider (3.21) to be the evolution of a measurement apparatus "monitoring" our quantum system in state $|\,\psi\,\rangle = \sum_n c_n |\,s_n\,\rangle$, we have to consider the generalisation of (3.21) into

Entangling System-Environment Evolution

$$|\,\Psi(0)\,\rangle = |\,\psi\,\rangle \otimes |\,E(0)\,\rangle = \left(\sum_n c_n |\,s_n\,\rangle\right) \otimes |\,E(0)\,\rangle \to |\,\Psi(t)\,\rangle = \sum_n c_n \big(|\,s_n\,\rangle \otimes |\,E_n(t)\,\rangle\big), \tag{3.23}$$

as representing monitoring of the system by the environment.[a] We have adapted (3.23) to the example preceding (2.15): $|\,E(0)\,\rangle$ is the initial state of the environment (there oscillator), with a total state not entangled with the system. As time t goes on, the state evolves into one that is more and more entangled with the system, with the environment evolving into state $|\,E_n(t)\,\rangle$ if the system was in $|\,s_n\,\rangle$, (in the example the $|\,E_n(t)\,\rangle$ were the two *different* coherent states of the oscillator).

---

[a] We distinguish the total state $|\,\Psi\,\rangle$ from the system state $|\,\psi\,\rangle$.

- Note that (3.23) does not contain any non-trivial evolution within system and environment separately, only that due to interactions. However a component (3.23) will always be part of any coupled evolution.

The just discovered formal equivalence of system-environment and system-"measurement apparatus" evolution, motivates the definition of the

Measurement limit of interactions /quantum measurement limit, as the case where for system-environment models as discussed in section 2, we can neglect all Hamiltonians except $\hat{H}_{\mathrm{int}}$. Thus the evolution is entirely dominated by the system-environment interactions.

We can now use the simple mapping (3.23) to *qualitatively* resolve 2 of the 3 problems outlined earlier. For a *quantitative* resolution, await chapter 4.

The reason for Non-observability of Interference (resolving measurement problem II)

The entangling evolution (3.23) ought to be unavoidable and generic for any insufficiently isolated quantum system, suggesting many-body entangled states are everywhere. However assuming we can only observe the system itself, precisely this can be the reason why we do not observe macroscopic quantum effects, as seen already in section 3.1.4:

Since we can only observe the system, all observables follow from its reduced density matrix, which for the final state in (3.23) is (see calculation in (3.19))

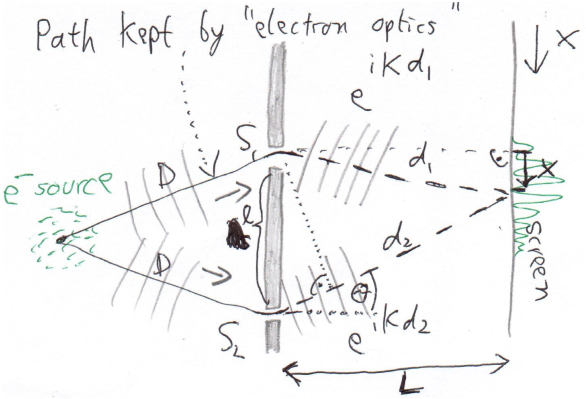
$$\hat{\rho}_S = \frac{1}{2}\bigg(|\, s_1 \,\rangle\langle\, s_1 \,| + |\, s_2 \,\rangle\langle\, s_2 \,| + |\, s_1 \,\rangle\langle\, s_2 \,|\langle\, E_2(t) \,|\, E_1(t) \,\rangle + |\, s_2 \,\rangle\langle\, s_1 \,|\langle\, E_1(t) \,|\, E_2(t) \,\rangle \bigg). \tag{3.24}$$

- We have reduced the number of system states to two again and used $c_1 = c_2 = 1/\sqrt{2}$ in (3.23) for simplicity.

Once $\langle\, E_1(t) \,|\, E_2(t) \,\rangle \approx 0$, we will see no interference in the system anymore. The time by which this happens typically is very short for a macroscopic environment, as we see in examples later. Let us first consider an explicit example discussing "interference fringes" :

Example 17, Decoherence in the matter-wave double slit experiment: Let us consider the matter-wave version of the double slit experiment in section 1.2, sketched below. After the region of the slits, we can write the total electron matter wave roughly as $\psi(\mathbf{r}) = \frac{1}{\sqrt{2}}\mathcal{N}\left(\exp\left[ikd_1\right] + \exp\left[ikd_2\right]\right)$, with coordinates indicated in the sketch. The electron probability on the screen is then $|\psi(\mathbf{r})|^2 \approx \mathcal{N}^2\big(1 + \cos\left(k(d_1 - d_2)\right)\big)$. Rewriting in terms of angle on the screen we obtain $|\psi(\theta)|^2 \approx \mathcal{N}^2\big(1 + \cos\left(kl\theta\right)\big)$, as following from the result for (1.4) in optics as well.

Example continued:



left: Sketch of the matter-wave double slit experiment, all essential features are as with the optical setup, even though practical challenges are vastly different.

Now assume the electron might have interacted with the slit material at the moment of its crossing. This interaction will be microscopically different in the left and right slit. After passing the slit, we then assume a total state $|\,\Psi(\mathbf{r})\,\rangle = \frac{1}{\sqrt{2}}\mathcal{N}\left(\exp\left[ikd_1\right]|\,L\,\rangle + \exp\left[ikd_2\right]|\,R\,\rangle\right)$, where we write the electron state in the position representation and the (abstract) state of the slit material as $|\,L/R\,\rangle$, depending on whether the electron has gone through the **L**eft or **R**ight slit.

Since our screen does not measure the slit state, we have to now utilize the reduced density matrix for the electron, obtained like in (3.19), (3.24). Let us first express the state above in terms of position x on the screen, using $d_1 \approx L + x^2/(2L)$, $d_2 \approx L + (l-x)^2/(2L)$ (sorry for the double use of L. In a state, it means "left", in the expression for d_1 it is the distance between slits and screen, see figure), to find $|\,\Psi(x)\,\rangle = \frac{\mathcal{N}e^{ikL}}{\sqrt{2}}\left(\exp\left[ikx^2/(2L)\right]|\,L\,\rangle + \exp\left[ik(l-x)^2/(2L)\right]|\,R\,\rangle\right)$, and hence

$$\hat{\rho}(x,x') = |\,\Psi(x)\,\rangle\langle\,\Psi(x')\,| = \frac{\mathcal{N}^2}{2}\bigg(e^{ik\frac{(x^2-x'^2)}{2L}}|\,L\,\rangle\langle\,L\,| + e^{ik\frac{((l-x)^2-(l-x')^2)}{2L}}|\,R\,\rangle\langle\,R\,| + e^{ik\frac{(x^2-(l-x')^2)}{2L}}|\,L\,\rangle\langle\,R\,| + e^{ik\frac{((l-x)^2-x'^2)}{2L}}|\,R\,\rangle\langle\,L\,|\bigg) \tag{3.25}$$

resulting in

$$\hat{\rho}_S(x,x') = \frac{\mathcal{N}^2}{2}\bigg(e^{ik\frac{(x^2-x'^2)}{2L}} + e^{ik\frac{((l-x)^2-(l-x')^2)}{2L}} + e^{ik\frac{(x^2-(l-x')^2)}{2L}}\langle\,R\,|\,L\,\rangle + e^{ik\frac{((l-x)^2-x'^2)}{2L}}\langle\,L\,|\,R\,\rangle\bigg). \tag{3.26}$$

For the electron probability on the screen, $\hat{\rho}_S(x,x)$, we obtain

$$\hat{\rho}_S(x,x) = \frac{\mathcal{N}^2}{2}\bigg(2 + \exp\left[-ikl(x-l/2)/L\right]\langle\,R\,|\,L\,\rangle + \exp\left[ikl(x-l/2)/L\right]\langle\,L\,|\,R\,\rangle\bigg). \tag{3.27}$$

indicating an unperturbed interference pattern only if $|\,L\,\rangle = |\,R\,\rangle$ (for example if the electron actually has not affected the screen and $|\,L\,\rangle = |\,R\,\rangle = |\,\phi_{\text{screen}}(t=0)\,\rangle$). If $\langle\,L\,|\,R\,\rangle = 0$, no interference is seen at all.

- We can identify $|\, L/R \,\rangle$ also with the states of some measurement device that allows us to infer which slit the electron has taken, leading to the result that whenever we or the environment obtain some "which-path-information", the interference pattern is gone.

- There are significant technical challenges in the matter-wave experiment compared to optics. For electron-optics we require relatively fast electrons, $E = 50$ keV in the first experiment [C. Jönsson Z. Phys. **161** 454 (1961), Am. J.Phys. **42** 4 (1974)], with a de-Broglie wavelength $\lambda = 0.05\mathring{A}$. Since this is much less than the size of an atom, we cannot actually make slits that are small against the wavelength, as we would in optics.

- See this movie of the above experiment based on single electrons [A. Tonomura *et al.* Am. J. Phys. **57** 117 (1989)]. This version of the experiment is one of the most paradigmatic demonstrations of particle-wave duality.

- One can nowadays perform such experiments with complex particles such as bio-molecules [Gerlich *et al.* Nat. Comm. **2** 263 (2011)]. While for electrons decoherence as described above can be made small, for these systems it cannot. The next plans, are to do it with a virus.

Another element that is included in (3.24) through the time-dependence of $E_n(t)$, is the slow loss of coherence over some characteristic decoherence time. For this we can make use of our earlier spin-boson model example, see section 2.2.1 and assignment 2:

Example 18, Dynamical decoherence in the spin-boson model: Let us go back to the example in section 2.2.1 of a spin interacting with an oscillator in the simplified spin-boson model. We determine the reduced density matrix for the spin only, applying (3.24) to (2.14) and obtain

$$\hat{\rho}_S = \frac{1}{2}\bigg(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\downarrow|\langle\,\alpha_{Q+}\,|\,\alpha_{Q-}\,\rangle + |\downarrow\rangle\langle\uparrow|\langle\,\alpha_{Q-}\,|\,\alpha_{Q+}\,\rangle\bigg). \tag{3.28}$$

Using Eq. (1.27), we can calculate the overlap of two coherent states as $\langle\,\alpha\,|\,\beta\,\rangle = e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2-2\beta^*\alpha)}$. In assignment 2 you found $\alpha_{Q+} = -\alpha_{Q-} = \bar{\kappa}/\omega(1-e^{i\omega t})$, We find $\langle\,\alpha_{Q+}\,|\,\alpha_{Q-}\,\rangle = e^{4\frac{\kappa^2}{\omega^2}(\cos[\omega t]-1)}$, which for short times becomes

$$\langle\,\alpha_{Q+}\,|\,\alpha_{Q-}\,\rangle = e^{-2\kappa^2 t^2}. \tag{3.29}$$

The spin thus has "decohered" (precluding the visibility of interferences), after a time scale $\Gamma_{\text{decoh}} \sim \kappa^{-1}$.

- We can make the decoherence dynamics even more explicit by calculating the time dependent Purity $P(t)$, using Eq. (3.10), from (3.28).

- In the preceding example, coherence / purity would periodically be restored after intervals $T = 2\pi/\omega$. This is because the single oscillator that we coupled the spin to is not really a large environment. Repeating the calculation with a large and larger number of oscillators, we see that the time of "revival" where $P(t) = 1$ again becomes later and later, until it becomes irrelevant.

- In the preceding example we are fortunate to be able to just calculate the dynamics of the entire setup (system+environment), and then form the reduced DM for the system. In general this will not be possible. In chapter 4 we learn how to avoid the detour of calculating the entire setup if we anyway care only about the system, and still quantitatively model the de-coherence dynamics, including the decoherence time.

- Importantly, the superposition character is not lost in the many-body state (3.23). It has in some sense "moved" from within the system only to the combination system+environment. We thus can no longer observe it, if we are confined to measuring the system only, which is fully described by (3.24). If we can make a sophisticated measurement on system+environment, we could still hope to demonstrate the quantum superposition character of (3.23). In all relevant cases, this is not possible.

Example 19, Decoherence in a spin-spin model: Finally consider a genuine many-component spin-spin model as in section 2.3, where we assume all dynamics is dominated by the system environment interaction (2.23) and neglect the other two Hamiltonians. This allows us to determine the full time evolution for an arbitrary number of spins.
We start from an initial state $|\,\Psi(0)\,\rangle = (a|\uparrow\rangle + b|\downarrow\rangle) \otimes \sum_{s_1,s_2,\dots} c_{s_1,s_2,\dots}|\,s_1,s_2,\dots\rangle$, where $s_i \in \{+1/2,-1/2\}$ and the part before $\otimes$ is the initial state of the system, the rest that of the spin-environment. You find (exercise/ SD 2.10.)

$$|\,\Psi(0)\,\rangle = a|\uparrow\rangle \otimes |\,\mathcal{E}_0(t)\,\rangle + b|\downarrow\rangle \otimes |\,\mathcal{E}_1(t)\,\rangle, \tag{3.30}$$

with $|\,\mathcal{E}_0(t)\,\rangle = |\,\mathcal{E}_1(-t)\,\rangle = \sum_{s_1,s_2,\dots} c_{s_1,s_2,\dots} e^{-i\left(\sum_n^N \kappa_n (-1)^{[1/2-s_n]}\right)t/\hbar}|\,s_1,s_2,\dots\rangle$. We have seen this entanglement structure multiple times before.
For the system spin we will find $\hat{\rho}_S = \Big(|a|^2|\uparrow\rangle\langle\uparrow| + |b|^2|\downarrow\rangle\langle\downarrow| + ab^* r(t)|\uparrow\rangle\langle\downarrow| + a^* b r^*(t)|\downarrow\rangle\langle\uparrow|\Big)$, with decoherence factor $r(t) = \sum_{s_1,s_2,\dots} |c_{s_1,s_2,\dots}|^2 e^{-2i\left(\sum_n^N \kappa_n (-1)^{[1/2-s_n]}\right)t/\hbar}$.
You have derived this in assignment 1.
It is possible to make some statistical arguments for randomly oriented environmental spins, to show that $r(t)$ scales as $r(t) \sim 2^{-N}$ with the number of spins, and as $r(t) \sim 2^{-\Gamma^2 t^2}$ with time.

- The main purpose of this example, is to show the generic feature, that coherence is suppressed exponentially with increasing size N of the environment.

3.2.4 Pointer states and Environmental Superselection

Earlier we had argued that entangling system-environment evolution such as (3.21) is the *generic case*[5]. However it does not happen for all initial states, as shown in the following example.

---

[5] That means, take a random initial state, almost always this will be part of the dynamics.

Example 20, No decoherence in the spin-boson model: Now consider the spin-boson model with a different initial state than considered in the example of section 2.2.1 or assignment 2. However we still begin in a superposition state $|\,\Psi(0)\,\rangle = \frac{1}{\sqrt{2}}\left(|\leftarrow\rangle + |\rightarrow\rangle\right) \otimes |\,0\,\rangle$. Since we can express this as $|\,\Psi(0)\,\rangle = |\uparrow\rangle \otimes |\,0\,\rangle$ and Schrödinger evolution is linear, we can read off the final state from our earlier results as $|\,\Psi(0)\,\rangle = |\uparrow\rangle \otimes |\,\alpha_{Q-}\,\rangle$. Here the system *has not* entangled itself with the environment. Consequently upon forming the reduced density matrix of the system $\hat{\rho}_S = |\uparrow\rangle\langle\uparrow| = \frac{1}{2}\Big(|\leftarrow\rangle\langle\leftarrow| + |\rightarrow\rangle\langle\rightarrow| + |\leftarrow\rangle\langle\rightarrow| + |\rightarrow\rangle\langle\leftarrow|\Big)$, which has fully preserved the initial coherence/ superposition despite the interaction with the environment.

This tells us that in the presence of an environment, not all bases of the system Hilbertspace are equivalent, in the sense that superpositions expressed in certain bases will decohere, while in other bases they may not. We define

Pointer states as the preferred states of the system in contact with a certain environment. This means those states which during evolution give rise to least entanglement with the environment.

We can find the pointer states in the quantum measurement limit (see end of section 3.2.3). In this case only $\hat{H}_{\text{int}}$ is relevant. We demand that an initial product of some system and some environment state $|\,\Psi(0)\,\rangle = |\,s_i\,\rangle|\,E_0\,\rangle$ remains in product form under the action of the Hamiltonian

$$|\,\Psi(t)\,\rangle = e^{-i\hat{H}_{\text{int}}t/\hbar}|\,s_i\,\rangle|\,E_0\,\rangle \overset{!}{=} \lambda_i|\,s_i\,\rangle e^{-i\hat{H}_{\text{int}}t/\hbar}|\,E_0\,\rangle = |\,s_i\,\rangle|\,E_i(t)\,\rangle. \tag{3.31}$$

We can see that (3.31) is fulfilled if $|\,s_i\,\rangle$ is an

Eigenstate of the system-part of the interaction Hamiltonian: By this we mean that

$$\hat{H}_{\text{int}}|\,s_i\,\rangle|\,E\,\rangle = \alpha_i|\,s_i\,\rangle|\,E'\,\rangle. \tag{3.32}$$

for arbitrary environment state $|\,E\,\rangle$. Then $|\,E'\,\rangle$ is *some*, typically different environment state.

While it does not always have to be the case, in all the examples of section 2 we have the form

$$\hat{H}_{\text{int}} = \hat{O}_S \otimes \hat{O}_{\mathcal{E}}, \tag{3.33}$$

with $\hat{O}_S$ acting only on the system and $\hat{O}_{\mathcal{E}}$ only on the environment. In that case, the pointer states are simply the eigenstates of $\hat{O}_S$.

Example 21, Pointer states of spin-boson model: Using the discussion above, we see that the pointer states of the spin-boson model, with interaction term $\hat{H}_{\text{int}} = \hat{\sigma}_z \otimes \sum_i \bar{\kappa}_i \left(\hat{a}_i + \hat{a}_i^\dagger\right)$ are eigenstates of $\hat{O}_S = \hat{\sigma}_z$, hence $|\uparrow\rangle$ and $|\downarrow\rangle$.

This matches our experience in earlier examples, where we saw that $\hat{H}_{\text{int}}$ evolves an initial state $|\leftarrow\rangle \otimes |0\rangle$ into an entangled state, while it leaves $|\uparrow\rangle \otimes |0\rangle$ as a separable product.

- In general superpositions of pointer states will not be pointer states.
- However in some cases this can happen, then we talk about a "pointer subspace" or "decoherence free subspace".
- The singling out of a preferred basis by the system-environment interaction also has been given the name environment induced superselection or "ein-selection".

Example 22, Pointer states of Stern-Gerlach apparatus: If we return to the example given after (3.22), of a Stern-Gerlach apparatus measuring a spin, we found the competing bases of the apparatus $\{|a_\uparrow\rangle, |a_\downarrow\rangle\}$ versus $\{|a_\leftarrow\rangle, |a_\rightarrow\rangle\}$, where we had said $|a_\uparrow\rangle$" = " atom went to upper beam ($|a_\downarrow\rangle$" = " atom went to lower beam). The distinction between upper and lower beam is in terms of the position operator $\hat{x}$.

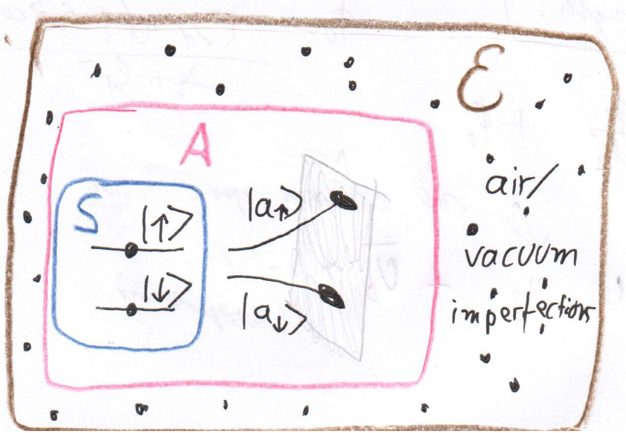
Now consider that the atom is always in contact with some surrounding environment (let it be black-body radiation or vacuum imperfections, i.e. other atoms floating around). This environment may be too complicated to fully tackle, but what we can tell, is that the system-environment interaction will be mainly a function of the position of the atom $H_{\text{int}} = \hat{f}[\hat{x}]$. Thus pointer states are position eigenstates[a]. This now singles out our measurement basis $\{|a_\uparrow\rangle, |a_\downarrow\rangle\}$ (which are position eigenstates) from $\{|a_\leftarrow\rangle, |a_\rightarrow\rangle\}$, which both are superpositions of the atom being in the upper and lower beam simultaneously. The latter would immediately decohere in contact with the environment so that the superposition (3.39) ceases to exist.

---

[a] If you find these pathological, consider a very strongly localized Gaussian wavepacket.

Preferred basis of a measurement apparatus (resolving measurement problem I)

Let's see more explicitly how we can use example 22 to resolve the preferred basis problem. For this we apply the concept of pointer states to a measurement apparatus, which is measuring a quantum system, while the apparatus in turn is in contact with an environment.



left: The layout is sketched in the left. We assume for simplicity that the system $\mathcal{S}$ only interacts directly with the apparatus $\mathcal{A}$, and also the environment $\mathcal{E}$ only interacts directly with the apparatus.

While the discussion here is generally applicable to a macroscopic measurement apparatus, we shall refer to the Stern-Gerlach experiment to be specific. While we will not need it in the following, you may feel good to see a possible model Hamiltonian for this scenario:

$$\mathcal{H}_{\mathcal{S}} = \Delta E \hat{\sigma}_z, \qquad \mathcal{H}_{\mathcal{A}} = \frac{\hat{\mathbf{P}}}{2m}, \qquad \mathcal{H}_{\mathcal{E}} = \sum_n \frac{\hat{\mathbf{p}}_n}{2m},$$

$$\mathcal{H}_{\mathcal{SA}} = \kappa_{\mathcal{SA}} \mathbf{B}(z) \cdot \hat{\sigma}_z, \qquad \mathcal{H}_{\mathcal{AE}} = \sum_n U(\hat{\mathbf{X}} - \hat{\mathbf{x}}_n). \tag{3.34}$$

Capital $\hat{\mathbf{X}}$ and $\hat{\mathbf{P}}$ are position and momentum of the atom of which we want to measure the spin. Small $\hat{\mathbf{x}}_n$ and $\hat{\mathbf{p}}_n$ label decohering environment atoms. These can collide with the to-be-measured atom via interaction potentials U. Finally the system interacts with the apparatus through the Zeeman energy of the spin in a magnetic field.

For simplicity we will consider sequential events, where the system first interacts with the apparatus, and subsequently the apparatus with the environment. Prior to the measurement let

$$|\,\Psi\,\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle) \otimes |\,a_r\,\rangle \otimes |\,E_0\,\rangle. \tag{3.35}$$

After passing through the magnet ($\mathcal{H}_{\mathcal{SA}}$), the state will be

$$|\,\Psi\,\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle|\,a_\uparrow\,\rangle + |\downarrow\rangle|\,a_\downarrow\,\rangle)\,|\,E_0\,\rangle, \tag{3.36}$$

where e.g. $|\,a_\uparrow\,\rangle$ indicates an atom in the upper beam as shown in the figure above. Finally the environment kicks in, and produces

$$|\,\Psi\,\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle|\,a_\uparrow\,\rangle|\,E_\uparrow\,\rangle + |\downarrow\rangle|\,a_\downarrow\,\rangle|\,E_\downarrow\,\rangle), \tag{3.37}$$

where $|\,E_\uparrow\,\rangle$ denotes an environment that was <u>locally</u> modified near the upper beam due to the measured atom. This locality is crucial and arises because $\mathcal{H}_{\mathcal{AE}}$ (or U) depend on the position $\hat{\mathbf{X}}$ only. Assuming that $\langle\,E_\downarrow\,|\,E_\uparrow\,\rangle \approx 0$ since they are many-body states, we can now find the reduced density matrix for system and apparatus from (3.19) as

$$\hat{\rho}_{\mathcal{SA}} = \frac{1}{2} (|\uparrow\rangle|\,a_\uparrow\,\rangle\langle\uparrow|\langle\,a_\uparrow\,| + |\downarrow\rangle|\,a_\downarrow\,\rangle\langle\downarrow|\langle\,a_\downarrow\,|), \tag{3.38}$$

which is now a classical mixture, but correctly correlates spin-states and measurement results.

Let us now recall the measurement problem: We found in (3.22) that subsequent to a von Neumann measurement, there are multiple ways expressing the entangled state that would seem to indicate that our apparatus has measured lots of non-commuting observables at once:

$$\sum_n c_n\big(|\, s_n \,\rangle \otimes |\, a_n \,\rangle\big) = \sum_k d_k\big(|\, s'_k \,\rangle \otimes |\, a'_k \,\rangle\big). \tag{3.39}$$

In our present setting, this means that we can rewrite (3.36) mathematically equivalently as

$$|\, \Psi \,\rangle = \frac{1}{\sqrt{2}}\,(|\leftarrow\rangle|\, a_{\leftarrow} \,\rangle + |\rightarrow\rangle|\, a_{\rightarrow} \,\rangle))\,|\, E_0 \,\rangle. \tag{3.40}$$

However, if we now consider interaction with the environment, it becomes important that $\mathcal{H}_{\mathcal{AE}}$ contains only the position operator $\hat{\mathbf{X}}$ and thus $|\, a_{\uparrow} \,\rangle$, $|\, a_{\downarrow} \,\rangle$ are the pointer states of the apparatus, see example 22. We thus have to rewrite (3.40) again in terms of $|\uparrow\rangle$ and $|\downarrow\rangle$ and thus reach (3.38) again. A similar construction containing $|\, a_{\leftarrow} \,\rangle$ and $|\, a_{\rightarrow} \,\rangle$ would not make sense, since these are highly non-classical quickly decohering states of the apparatus.

We thus find the

Resolution of the preferred basis problem A measurement apparatus measures that basis $\{|\, s_n \,\rangle\}$ of the system, which after the measurement has evolved into an entangled state of the kind (3.39) involving the pointer states $\{|\, a_n \,\rangle\}$ of the apparatus.

We still have a problem with outcomes (not resolving measurement problem III)

After all the $|\, E_n(t) \,\rangle$ in Eq. (3.23) have become orthogonal, the reduced density matrix for the system will be

$$\hat{\rho}_S = \sum_n |c_n|^2 |\, s_n \,\rangle\langle\, s_n \,|. \tag{3.41}$$

This correctly describes the *measurement statistics* of a large number of repeat measurements on an identical system, giving a chance $|c_n|^2$ to find the eigenvalue for $|\, s_n \,\rangle$, the system being in $|\, s_n \,\rangle$ subsequently.

It still does not describe in any more satisfactory way than (non-open) quantum mechanics, why we do not measure some effect of all the components n in a single measurement, but instead only one of the n is selected as the outcome and the state subsequently changed to $|\, s_n \,\rangle$.

Week ⑤

PHY 435 / 635 Decoherence and Open Quantum Systems
Instructor: Sebastian Wüster, IISER Bhopal, 2021

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We had seen in the previous week, that whether or not a given system+environment will exhibit quantum interferences in the system will (i) depend on the joint system-environment state and (ii) then can be determined via the reduced density matrix of the system $\hat{\rho}_{\mathcal{S}}$. Before we move in week 6 to powerful methods that allow directly working with $\hat{\rho}_{\mathcal{S}}$, we provide here some techniques that facilitate handling entangled system+environment states, and interpreting reduced density matrices.

3.2.5 What decoherence is not

There are several concepts that can mimick decoherence or are related to it, but different, that we briefly discuss now.

I: Decoherence versus Dissipation
Dissipation is the loss of energy from the system into the environment. This happens already on a classical level, and then of course also in quantum-mechanics. We have already seen a model in section 2.2, that clearly <u>does not</u> exhibit dissipation. As stated there, this happens when $\left[\hat{H}_S, \hat{H}_{\text{int}}\right] = 0$, since then $\hat{H}_S$ is a conserved observable. We have later seen, in section 3.2.3, that the model <u>does</u> exhibit decoherence though, we thus can have decoherence without dissipation

Conversely however, we will see later that whenever there is dissipation, there also will be some decoherence. The time-scales on which these two phenomena occur, are typically very different, with decoherence happening a lot faster than dissipation.

II: Decoherence versus Classical Noise/ Dephasing
Decoherence introduced above and in section 1.2.1 arises through entanglement of the system and the environment. The symptoms, vanishing coherences in a density matrix, frequently also arise when averaging over multiple noisy realisation of an ensemble. Consider the ensemble of states

$$|\,\Psi_k\,\rangle = \frac{1}{\sqrt{2}}\big(|\!\uparrow\rangle + e^{i\varphi_k}|\!\downarrow\rangle\big) \otimes |\,\mathcal{E}\,\rangle, \tag{3.42}$$

for some spin system, with environmental state $|\,\mathcal{E}\,\rangle$. This is not entangled with the environment so for each member of the ensemble we would obtain a pure reduced density matrix for the spin.

However, if for whatever reason we now average these density matrices, we find:

$$\bar{\bar{\rho}} = \sum_k^N |\,\Psi_k\,\rangle\langle\,\Psi_k\,| = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow| + \big(\frac{1}{2N}\sum_k e^{i\varphi_k}\big)|\downarrow\rangle\langle\uparrow| + \big(\frac{1}{2N}\sum_k e^{-i\varphi_k}\big)|\uparrow\rangle\langle\downarrow|. \tag{3.43}$$

The average over lots of random phases is zero, hence for $N \to \infty$ we have $\bar{\bar{\rho}} = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow|$, which looks just like a mixed state.

- This is also called classical noise or dephasing.
- This example is meant to caution you that you always have to be careful which exact type and source of dephasing/decoherence/noise is referred to in any work.

3.3 Some Tricks and Tools

We finish section 3 with some useful techniques for the treatment of bi-partite quantum systems (e.g. split into system+environment) and representation of quantum states.

3.3.1 The Schmidt Decomposition

Consider two systems $\mathcal{A}$ and $\mathcal{B}$ with Hilbert-spaces $\mathcal{H}_\mathcal{A}$ and $\mathcal{H}_\mathcal{B}$. For a pure state of the combined system, we then have the

Schmidt decomposition theorem, that an arbitrary pure state of the composite system $\mathcal{AB}$ can be written in the form

$$|\,\Psi\,\rangle = \sum_n \lambda_n |\,a_n\,\rangle|\,b_n\,\rangle, \tag{3.44}$$

where $\{|\,a_n\,\rangle\}$ $[\{|\,b_n\,\rangle\}]$ form an orthonormal basis of $\mathcal{H}_\mathcal{A}$ $[\mathcal{H}_\mathcal{B}]$.

- The expansion coefficients $\lambda_n \in \mathbb{C}$ fulfill $\sum_n |\lambda_n|^2 = 1$.
- However any complex phase factors in λ_n can in fact be absorbed into the bases, such that we can chose $0 < \lambda_n \in \mathbb{R}$, hence

$$|\,\Psi\,\rangle = \sum_n \sqrt{p_n}|\,a_n\,\rangle|\,b_n\,\rangle. \tag{3.45}$$

- The Schmidt decomposition (3.45) is unique iff all the coefficients $\sqrt{p_n}$ are different from each other.

Proof and construction algorithm: The Schmidt decomposition directly follows from the singular value decomposition (SVD) of an $N \times M$ matrix. Let $\{|\,\phi_n\,\rangle\}$ and $\{|\,\varphi_m\,\rangle\}$ be arbitrary orthonormal bases of $\mathcal{H}_\mathcal{A}$ and $\mathcal{H}_\mathcal{B}$ respectively. We then certainly can write any state $|\,\Psi\,\rangle$ in $\mathcal{H}_\mathcal{A} \otimes \mathcal{H}_\mathcal{B}$ as

$$|\,\Psi\,\rangle = \sum_n^N \sum_m^M c_{nm} |\,\phi_n\,\rangle |\,\varphi_m\,\rangle. \tag{3.46}$$

We assumed $N = \dim(\mathcal{H}_\mathcal{A})$, and $M = \dim(\mathcal{H}_\mathcal{B})$. Let us interpret the coefficients c as a $N \times M$ matrix $\underline{\underline{C}}$.

Proof cont.: That matrix has a SVD

$$\underline{\underline{C}} = \underline{\underline{U}}\,\underline{\underline{\Lambda}}\,\underline{\underline{V}}, \tag{3.47}$$

with unitary matrices $\underline{\underline{U}}$ $(N \times N)$, $\underline{\underline{V}}$ $(M \times M)$, and a $N \times M$ matrix $\underline{\underline{\Lambda}}$ with d real and positive entries λ_k on the diagonal only.

In component notation, (3.47) becomes $c_{nm} = \sum_k^d u_{nk}\lambda_k v_{km}$, where u and v are matrix elements of $\underline{\underline{U}}$ and $\underline{\underline{V}}$.

Insertion into Eq. (3.46) gives

$$\begin{aligned} |\,\Psi\,\rangle &= \sum_n^N \sum_m^M \left(\sum_k^d u_{nk}\lambda_k v_{km} \right) |\,\phi_n\,\rangle |\,\varphi_m\,\rangle \\ &= \sum_k^d \lambda_k \underbrace{\left(\sum_n^N u_{nk} |\,\phi_n\,\rangle \right)}_{\equiv |\,a_k\,\rangle} \underbrace{\left(\sum_m^M v_{km} |\,\varphi_m\,\rangle \right)}_{\equiv |\,b_k\,\rangle}, \end{aligned} \tag{3.48}$$

which takes the form (3.44) after defining the new bases $\{|\,a_k\,\rangle\}$ $[\{|\,b_k\,\rangle\}]$. This thus also gives a recipe for the construction of these.

- You can see that for the case where $N = M$, (3.47) just represents the diagonalisation of the matrix $\underline{\underline{C}}$.
- It can be seen from (3.44), that the reduced density matrices in systems $\mathcal{A}$ and $\mathcal{B}$ are $\hat{\rho}_\mathcal{A} = \sum_n p_n |\,a_n\,\rangle\langle\,a_n\,|$ and $\hat{\rho}_\mathcal{B} = \sum_n p_n |\,b_n\,\rangle\langle\,b_n\,|$ respectively (proof: exercise/book). We can thus also find the decomposition by determining both these reduced density matrices directly from $|\,\Psi\,\rangle$, and diagonalising them.

Example 23, Example: We consider again a bi-partite spin system with state

$$|\,\Psi\,\rangle = \frac{1}{\sqrt{2}}|\downarrow\downarrow\rangle + \frac{1}{2}|\uparrow\rangle \otimes (|\uparrow\rangle + |\downarrow\rangle). \tag{3.49}$$

In terms of the basis ordering $\{|\downarrow\rangle, |\uparrow\rangle\}$ for rows and columns, this gives a matrix

$$\underline{\underline{C}} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{2} \\ 0 & \frac{1}{2} \end{bmatrix} = \underbrace{\begin{bmatrix} \frac{\sqrt{2+\sqrt{2}}}{2} & -\frac{1}{2}\sqrt{2-\sqrt{2}} \\ \frac{1}{\sqrt{2(2+\sqrt{2})}} & \frac{\sqrt{2+\sqrt{2}}}{2} \end{bmatrix}}_{=\underline{\underline{U}}} \underbrace{\begin{bmatrix} \frac{\sqrt{2+\sqrt{2}}}{2} & 0 \\ 0 & \frac{\sqrt{2-\sqrt{2}}}{2} \end{bmatrix}}_{=\underline{\underline{\Lambda}}} \underbrace{\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}}_{=\underline{\underline{V}}}, \tag{3.50}$$

where we also have already written its SVD.

Example 24, Example contd.: We thus can write

$$|\,\Psi\,\rangle = \frac{\sqrt{2+\sqrt{2}}}{2}|\,a_1\,\rangle \otimes |\,b_1\,\rangle + \frac{\sqrt{2}-\sqrt{2}}{2}|\,a_2\,\rangle \otimes |\,b_2\,\rangle, \tag{3.51}$$

with new bases $\{|\,a_1\,\rangle, |\,a_2\,\rangle\} = \left\{\frac{\sqrt{2+\sqrt{2}}}{2}|\downarrow\rangle + \frac{\sqrt{2+\sqrt{2}}}{2}|\uparrow\rangle,\ -\frac{1}{2}\sqrt{2-\sqrt{2}}|\downarrow\rangle + \frac{\sqrt{2+\sqrt{2}}}{2}|\uparrow\rangle\right\}$ and $\{|\,b_1\,\rangle, |\,b_2\,\rangle\} = \left\{\frac{1}{\sqrt{2}}|\downarrow\rangle + \frac{1}{\sqrt{2}}|\uparrow\rangle,\ -\frac{1}{\sqrt{2}}|\downarrow\rangle + \frac{1}{\sqrt{2}}|\uparrow\rangle\right\}$.
Thus even for an innocent looking example, the actual construction of (3.45) can be cumbersome.

3.3.2 The Wigner representation

Let us consider the specific example of a quantum particle moving in one dimension, e.g. the simple harmonic oscillator. The Wigner representation maps its density matrix $\hat{\rho}$ (or quantum state $|\,\Psi\,\rangle$) onto a function in phase-space $W(x,p)$.

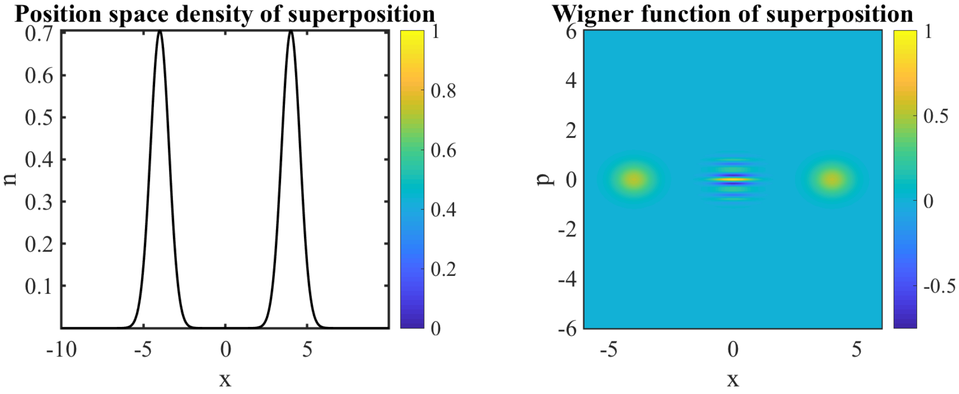
Consider the position-space density matrix elements $\rho(x,x') = \langle\, x\,|\hat{\rho}|\,x'\,\rangle$, where $|\,x\,\rangle$ are position "eigen-states". Thus if the position-space representation of $|\,\Psi\,\rangle$ is $\Psi(x) = \langle\, x\,|\,\Psi\,\rangle$, we have $\rho(x,x') = \Psi(x)\Psi^*(x')$. Then we define the

Wigner function

$$W(x,p) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dy\ e^{ipy}\ \rho(x - \frac{y}{2}, x + \frac{y}{2}) \tag{3.52}$$

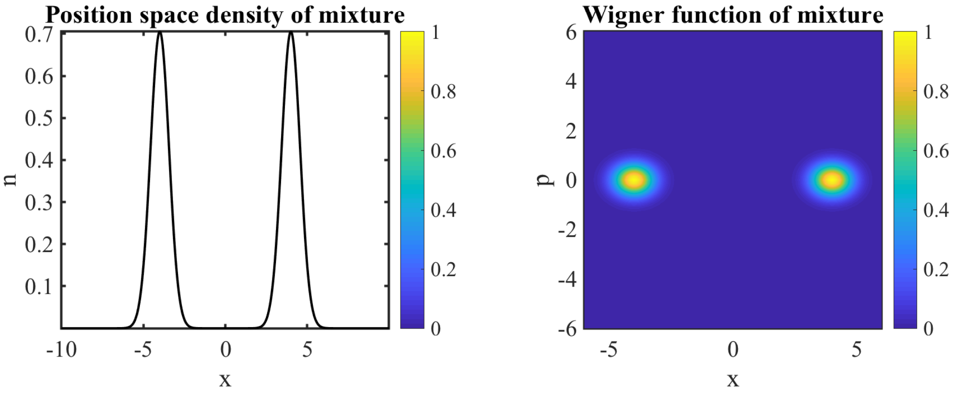
where p is the momentum of the particle.

Example 25, Example: Wigner function for a superposition of Gaussian wavepackets $\Psi(x) = \frac{\mathcal{N}}{\sqrt{2}}\left(e^{-\frac{(x-a)^2}{2\sigma^2}} + e^{-\frac{(x-b)^2}{2\sigma^2}}\right) \equiv \frac{1}{\sqrt{2}}\big(\varphi_a(x) + \varphi_b(x)\big)$, for $|a-b| \gg \sigma$, see figure below.



- The purpose of this is primarily to find the closest possible quantum-mechanical equivalent to the classical concept of a phase-space coordinate.
- Due to the uncertainty relation, we always have a distribution in phase space.
- Note, however, that $W(x,p)$ cannot be interpreted as a probability distribution, since it may take negative values.
- However, we can show $P(x) = \int dpW(x,p)$ and $P(p) = \int dxW(x,p)$ are the position- and momentum distributions in state ρ. For this reason, the Wigner function is called a quasi-probability distribution.

Example 26, Example: Wigner function for a mixture of Gaussian wavepackets $\rho(x,x') = \varphi_a(x)\varphi_a^*(x') + \varphi_b(x)\varphi_b^*(x')$.



- It is typically superpositions that give rise to the negative features in the Wigner function. These are just used to pinpoint non-classical effects.

- After getting some experience in the interpretation of Wigner functions, these can thus be used to visualize the evolution of quantum states from “quantum” (coherent) to “classical” (mixed).
- Using the inverse of (1.21), the definition (3.52) can straightforwardly be applied to states given in the number representation $|\, n\,\rangle$.
- Similar phase space distributions for spin-states exist.

3.3.3 Purifying the Environment

In section 3.1.3 we have seen how a reduced density matrix for the system can be obtained from a pure-state density matrix for system+environment, and may then in general contain mixed features.

We can also do this in the opposite direction. Suppose you are given an arbitrary system density matrix, which, after diagonalization, reads $\hat{\rho}_{\mathcal{S}} = \sum_n p_n |\, \phi_n \,\rangle\langle\, \phi_n \,|$. This can be viewed as reduced density matrix of a fictitious system+environment in a pure state

$$|\, \Psi \,\rangle = \sum_n p_n |\, \phi_n \,\rangle |\, \varphi_n \,\rangle, \tag{3.53}$$

where $\{|\, \varphi_n \,\rangle\}$ is an arbitrary basis of the environment. (convince yourself that $\hat{\rho}_{\mathcal{S}}$ is the corresponding reduced density matrix (3.13) for the system).

The main practical utility of this statement is that in all the following it makes sense to assume an initially pure state of the environment. If this was not the case we could simply enlarge the environment as above, and then do the math.

3.3.4 The operator sum formalism

The following technique is a useful tool to gain some formal insight, but typically not much use for actually solving the problem. Suppose we have a system+environment in an initial density matrix

$$\hat{\rho}(0) = \hat{\rho}(0)_{\mathcal{S}} \otimes \hat{\rho}(0)_{\mathcal{E}}, \tag{3.54}$$

where $\hat{\rho}(0)_{\mathcal{E}} = \sum_k p_k |\, E_k \,\rangle\langle\, E_k \,|$ is the initial density matrix of the environment expressed in the eigen basis $\{E_k\}$ of the density matrix. Further assume we actually know the total time-evolution of system+environment given by the total time evolution operator $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$. We can then formally write the time-evolving reduced density matrix of the system as

$$\hat{\rho}(t)_{\mathcal{S}} = \mathrm{Tr}_{\mathcal{E}} \left\{ \hat{U}(t) \left[\hat{\rho}(0)_{\mathcal{S}} \otimes \sum_k p_k |\, E_k \,\rangle\langle\, E_k \,| \right] \hat{U}^{\dagger}(t) \right\}. \tag{3.55}$$

Using the

Kraus operators defined as

$$\hat{E}_{ij}(t) = \sqrt{p_i} \langle\, E_j \,|\hat{U}(t)|\, E_i \,\rangle \tag{3.56}$$

we can rewrite (3.55) as

$$\hat{\rho}(t)_{\mathcal{S}} = \sum_{ij} \hat{E}_{ij}(t)\hat{\rho}(0)_{\mathcal{S}}\hat{E}^{\dagger}_{ij}(t). \tag{3.57}$$

- Calculation and more discussion see SD 2.15.4., and tutorial.
- There it is also shown, that due to the unitarity of $\hat{U}(t)$, the Kraus operators fulfill $\sum_{ij} \hat{E}_{ij}\hat{E}^{\dagger}_{ij} = \mathbb{1}_{\mathcal{S}}$, where $\mathbb{1}_{\mathcal{S}}$ is the unit operator in the system space. A direct consequence of this is $\mathrm{Tr}[\hat{\rho}(t)_{\mathcal{S}}] = \mathrm{Tr}[\hat{\rho}(0)_{\mathcal{S}}] = 1$, so a time evolution written down in terms of Kraus operators preserves the trace of the reduced density matrix.
- Note that the Kraus operators (3.56) act in the system only, no longer in the environment.
- The reason the utility is limited is that this technique still requires us to know the complete time evolution operator $\hat{U}(t)$.
- However (3.57) is useful to constrain the formal structure the time-evolution in the space of reduced density matrices has to take. We shall make use of that in the next section.
- Kraus operators directly map the system density matrix from some initial time $t = 0$ into some final time t, as in (3.57). We can use this to shortcut the evolution due to a van-Neumann measurement that we have seen in section 3.2.1, i.e. from $\hat{\rho}(0)$ over (3.21) into (3.41). For this we choose the Kraus operators as

  $$\hat{E}_{ij} = \delta_{ij} |\, \phi_j \,\rangle\langle\, \phi_j \,|, \tag{3.58}$$

  where ϕ_j are the eigenstates of the operator to be measured, and the operator on the right hand side is the projection operator used in (1.8). *Proof: Exercise.*

Week ⑥

PHY 435 / 635 Decoherence and Open Quantum Systems
Instructor: Sebastian Wüster, IISER Bhopal, 2021

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4 Markovian Open Quantum Systems

So far we had considered decoherence either via some simplistic state-mappings $|\,\Psi(0)\,\rangle \rightarrow |\,\Psi(t)\,\rangle$ or via solving the full many-body problem in some simple cases and then taking the partial trace over the environment to reduce dynamics onto the system:

$$\hat{\rho}_{\mathcal{S}}(t) = \text{Tr}_{\mathcal{E}}\{\hat{U}(t)\hat{\rho}_{tot}(0)\hat{U}^{\dagger}(t)\}, \tag{4.1}$$

where $\hat{\rho}_{tot}(0)$ is the initial system plus environment density matrix and $\hat{U}(t)$ the total time evolution operator.

The approach (4.1) is typically impractical because the environment will be to large or too complex to obtain $\hat{U}(t)$. We thus need to learn some techniques to circumvent having to obtain $\hat{U}(t)$ to know about $\hat{\rho}_{\mathcal{S}}(t)$.

$$\begin{tikzcd}
\hat{\rho}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_\mathcal{E} \arrow[r, "\text{unitary}", "\text{evolution}"'] \arrow[d, "tr_\mathcal{E}"'] & \hat{\rho}(t) = \hat{U}(t)[\hat{\rho}_S(0) \otimes \hat{\rho}_\mathcal{E}]\hat{U}^{\dagger}(t) \arrow[d, "tr_\mathcal{E}"] \\
\hat{\rho}_S(0) \arrow[r, "\text{dynamical map}"] & \hat{\rho}_S(t) = \underline{\hat{V}(t)}[\hat{\rho}_S(0)]
\end{tikzcd}$$

top: Instead we would wish to shortcut the process and find the object $\hat{V}(t)$ in the diagram above directly.

4.1 Master-Equation formulation of open quantum systems

What we are after, is called a

Quantum Master equation, which is a <u>dynamical map</u>

$$\hat{\rho}_{\mathcal{S}}(t) = \hat{V}(t)[\hat{\rho}_{\mathcal{S}}(0)]. \tag{4.2}$$

- Here $\hat{V}(t)$ takes the role of the time-evolution operator, only it works on the level of the system density matrix only. Since $\hat{V}(t)$ is mapping an operator (the density matrix at $t = 0$) onto another operator (the density matrix at $t > 0$), it is also called a superoperator.

- If a Master equation is exact, we would have $\hat{V}(t)[\hat{\rho}_{\mathcal{S}}(0)] = \mathrm{Tr}_{\mathcal{E}}\{\hat{U}(t) \underbrace{\hat{\rho}_{tot}(0)}_{=\hat{\rho}_{\mathcal{S}}(0)\otimes\hat{\rho}_{\mathcal{E}}(0)} \hat{U}^{\dagger}(t)\}$, however typically this is only approximately the case.
- Caution: In the literature there are also classical Masterequations. These are rate equations describing physical processes via the evolution of some probability distributions.

In this section 4, we will ultimately be aiming for Master equations that are local in time. This means we want to write a

Markovian Master equation

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) = \hat{\mathcal{L}}[\hat{\rho}_{\mathcal{S}}(t)] = -\frac{i}{\hbar}\big[\hat{H}'_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)\big] + \hat{\mathcal{D}}[\hat{\rho}_{\mathcal{S}}(t)], \tag{4.3}$$

where again $\hat{\mathcal{L}}$ and $\hat{\mathcal{D}}$ are super-operators.

- In (4.3), the evolution of the reduced density matrix depends only on the current state of the density matrix, not on its history ($\hat{\rho}_{\mathcal{S}}(t')$, for $t' < t$). In the language of section 1.5.7, we can classify this evolution as Markovian.
- In terms of the superoperator $\hat{\mathcal{L}}(t)$, the requirement to have Markovian time evolution can also be expressed through the dynamical semi-group property:

  $$\hat{\mathcal{L}}(t_1 + t_2) = \hat{\mathcal{L}}(t_1)\hat{\mathcal{L}}(t_2), \tag{4.4}$$

  for $t_1, t_2 > 0$. We shall denote the superoperator $\hat{V}(t)$ by $\mathcal{L}(t)$ in the Markovian case. It is also called Liouvillian, since (4.3) resembles the Liouville equation encountered in classical physics.
- The first part in (4.3) corresponds to a von Neumann type equation just as in (3.2), as we would have for the unitary evolution of a closed system. Note, however, that the Hamiltonian $\hat{H}'_{\mathcal{S}}$ may not quite be the system Hamiltonian $\hat{H}_{\mathcal{S}}$, but can get slightly modified.
- We shall see that a new non-unitary dissipator $\hat{\mathcal{D}}$ can describe the onset of decoherence.

4.2 Born-Markov Master equation

In the previous section we have only formally introduced how a Master equation would look like. To use this concept, we have to be able to derive it from our open quantum system models, consisting of $\hat{H}_{\mathcal{S}}$, $\hat{H}_{\mathcal{E}}$ and $\hat{H}_{\mathrm{int}}$ as listed in section 2. The derivation is lengthy but so central to this course that we show it in almost full detail.

We assume that the interaction Hamiltonian takes the form

$$\hat{H}_{\text{int}} = \sum_{\alpha} \hat{S}_{\alpha} \otimes \hat{E}_{\alpha}, \tag{4.5}$$

where the $\hat{S}_{\alpha}$ act on the system only and $\hat{E}_{\alpha}$ on the environment only. This was the case for all examples in section 2. We now move to an interaction picture (see section 1.5.6 and QM books) with $\hat{H}_0 = \hat{H}_{\mathcal{S}} + \hat{H}_{\mathcal{E}}$ and $\hat{V} = \hat{H}_{\text{int}}$. In this section we set $\hbar = 1$ to compress notation.

Using the definitions in section 1.5.6 we then have the interaction operator and density matrix in the interaction-picture as

$$\hat{H}^{(I)}_{\text{int}}(t) = e^{i\hat{H}_0 t}\hat{H}_{\text{int}}e^{-i\hat{H}_0 t}, \tag{4.6}$$

$$\hat{\rho}^{(I)}(t) = e^{i\hat{H}_0 t}\hat{\rho}(t)e^{-i\hat{H}_0 t} = e^{i\hat{H}_0 t}e^{-i\hat{H}t}\hat{\rho}(0)e^{i\hat{H}t}e^{-i\hat{H}_0 t}. \tag{4.7}$$

Using these, we can start from (3.2) and derive the

Interaction-picture Liouville-von Neumann equation

$$\frac{d}{dt}\hat{\rho}^{(I)}(t) = -i\big[\hat{H}^{(I)}_{\text{int}}(t), \hat{\rho}^{(I)}(t)\big], \tag{4.8}$$

stating that in the interaction picture, evolution of the density matrix follows directly from the interaction Hamiltonian. This resembles Eq. (1.49), which was for a state vector.

- Proof: Assignment.
- Note, this differs from (1.50), since the density matrix is a special kind of operator.

We can now formally integrate the differential equation (4.8) over time from 0 to t and find

$$\hat{\rho}^{(I)}(t) = \hat{\rho}^{(I)}(0) - i\int_0^t dt' \,\big[\hat{H}^{(I)}_{\text{int}}(t'), \hat{\rho}^{(I)}(t')\big]. \tag{4.9}$$

We now insert (4.9) back into (4.8) and reach

$$\frac{d}{dt}\hat{\rho}^{(I)}(t) = -i\big[\hat{H}^{(I)}_{\text{int}}(t), \hat{\rho}(0)\big] - \int_0^t dt' \,\big[\hat{H}^{(I)}_{\text{int}}(t), \big[\hat{H}^{(I)}_{\text{int}}(t'), \hat{\rho}^{(I)}(t')\big]\big]. \tag{4.10}$$

We could repeat this step over and over, but stop here. This perturbative expansion makes sense if $\hat{H}_{\text{int}}$ is "small", see below. Next, using $\hat{\rho}^{(I)}_{\mathcal{S}}(t) = \text{Tr}_{\mathcal{E}}\{\hat{\rho}^{(I)}(t)\}$ (proof: assignment[6]), we find

$$\frac{d}{dt}\hat{\rho}^{(I)}_{\mathcal{S}}(t) = -i\text{Tr}_{\mathcal{E}}\big[\hat{H}^{(I)}_{\text{int}}(t), \hat{\rho}(0)\big] - \int_0^t dt' \,\text{Tr}_{\mathcal{E}}\big[\hat{H}^{(I)}_{\text{int}}(t), \big[\hat{H}^{(I)}_{\text{int}}(t'), \hat{\rho}^{(I)}(t')\big]\big]. \tag{4.11}$$

It turns out, that the first term in (4.11) can be set to zero. You will show in the assignment that if it was nonzero, we could redefine $\hat{H}_0$ and $\hat{H}_{\text{int}}$ to make it zero.

---

[6] The lhs. means <u>first</u> form reduced DM, then find its interaction picture evolution, hence this step is not immediately obvious.

So far we have mainly complicated things without gain, there are still two disadvantages to the right hand side of (4.11):

(A) It still depends on $\hat{\rho}^{(I)}(t')$, the entire density matrix (including the environment).

(B) It also depends on the density matrix at all earlier times $t' < t$, not only at time t.

Let us address problem (A) by invoking the

Born approximation, that the system environment coupling is "weak", and the environment so large that the system does not significantly affect it. Mathematically we express the latter by

$$\hat{\rho}(t) \approx \hat{\rho}_{\mathcal{S}}(t) \otimes \hat{\rho}_{\mathcal{E}}(0), \tag{4.12}$$

with $\hat{\rho}_{\mathcal{E}}(0) \approx const.$ the environmental initial state.

- We define "weak" operationally, as "the line (4.12) is valid, when inserted into (4.10)".
- The "≈" instead of "=" is important. We cannnot have "=" since this would imply a pure reduced system state at all times, and we want to describe decoherence which requires system-environment entanglement. We will thus only use (4.12) to simplify (4.11) and not assume that it actually preserves a separable system-environment state.

We have thus now reached:

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}^{(I)}(t) = -\int_0^t dt' \, \mathrm{Tr}_{\mathcal{E}}\big[\hat{H}_{\mathrm{int}}^{(I)}(t), \big[\hat{H}_{\mathrm{int}}^{(I)}(t'), \hat{\rho}_{\mathcal{S}}^{(I)}(t') \otimes \hat{\rho}_{\mathcal{E}}(0)\big]\big], \tag{4.13}$$

which no longer depends on the full environmental dynamics, solving problem (A) above.

However (B) is still there. To see the details of the $t' < t$ dependence better, let us rewrite the expression a bit. Note that

$$\begin{aligned}\hat{H}_{\mathrm{int}}^{(I)}(t') &= e^{i\hat{H}_0 t}\hat{H}_{\mathrm{int}}e^{-i\hat{H}_0 t} = \sum_\alpha \left(e^{i\hat{H}_{\mathcal{S}}t}\hat{S}_\alpha e^{-i\hat{H}_{\mathcal{S}}t}\right) \otimes \left(e^{i\hat{H}_{\mathcal{E}}t}\hat{E}_\alpha e^{-i\hat{H}_{\mathcal{E}}t}\right)\\ &= \sum_\alpha \hat{S}_\alpha^{(I)}(t) \otimes \hat{E}_\alpha^{(I)}(t),\end{aligned} \tag{4.14}$$

which allows us to write

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}^{(I)}(t) = -\int_0^t dt' \sum_{\alpha\beta} \mathrm{Tr}_{\mathcal{E}}\left[\hat{S}_\alpha^{(I)}(t)\otimes\hat{E}_\alpha^{(I)}(t), \left[\hat{S}_\beta^{(I)}(t')\otimes\hat{E}_\beta^{(I)}(t'), \hat{\rho}_{\mathcal{S}}^{(I)}(t')\otimes\hat{\rho}_{\mathcal{E}}(0)\right]\right] \tag{4.15}$$

$$= -\int_0^t dt' \sum_{\alpha\beta} \Big\{$$

$$\hat{S}_\alpha^{(I)}(t)\hat{S}_\beta^{(I)}(t')\hat{\rho}_{\mathcal{S}}^{(I)}(t')\mathrm{Tr}_{\mathcal{E}}\left\{\hat{E}_\alpha^{(I)}(t)\hat{E}_\beta^{(I)}(t')\hat{\rho}_{\mathcal{E}}(0)\right\} - \hat{S}_\beta^{(I)}(t')\hat{\rho}_{\mathcal{S}}^{(I)}(t')\hat{S}_\alpha^{(I)}(t)\mathrm{Tr}_{\mathcal{E}}\left\{\hat{E}_\beta^{(I)}(t')\hat{\rho}_{\mathcal{E}}(0)\hat{E}_\alpha^{(I)}(t)\right\}$$

$$-\hat{S}_\alpha^{(I)}(t)\hat{\rho}_{\mathcal{S}}^{(I)}(t')\hat{S}_\beta^{(I)}(t')\mathrm{Tr}_{\mathcal{E}}\left\{\hat{E}_\alpha^{(I)}(t)\hat{\rho}_{\mathcal{E}}(0)\hat{E}_\beta^{(I)}(t')\right\} + \hat{\rho}_{\mathcal{S}}^{(I)}(t')\hat{S}_\beta^{(I)}(t')\hat{S}_\alpha^{(I)}(t)\mathrm{Tr}_{\mathcal{E}}\left\{\hat{\rho}_{\mathcal{E}}(0)\hat{E}_\beta^{(I)}(t')\hat{E}_\alpha^{(I)}(t)\right\}.\Big\}$$

After the equality we have only expanded the two nested commutators and split everything into the system versus environment part of the tensor product.

Since it occurs repeatedly in (4.15), we now define the

Environment self-correlation functions,

$$\mathcal{C}_{\alpha,\beta}(t,t') \equiv \mathrm{Tr}_{\mathcal{E}}\left\{\hat{E}_\alpha^{(I)}(t)\hat{E}_\beta^{(I)}(t')\hat{\rho}_{\mathcal{E}}(0)\right\} = \mathrm{Tr}_{\mathcal{E}}\left\{\hat{E}_\alpha^{(I)}(t-t')\hat{E}_\beta^{(I)}(0)\hat{\rho}_{\mathcal{E}}(0)\right\} \equiv \mathcal{C}_{\alpha,\beta}(t-t') \tag{4.16}$$

- We can also write $\mathcal{C}_{\alpha,\beta}(t,t') = \langle\hat{E}_\alpha^{(I)}(t)\hat{E}_\beta^{(I)}(t')\rangle$, see Eq. (3.4).
- The $\mathcal{C}_{\alpha,\beta}(t,t')$ quantify to what extent the environmental operator $\hat{E}_\alpha^{(I)}(t)$ at time t is correlated with another such operator β at another time t', given the environmental state $\hat{\rho}_{\mathcal{E}}(0)$.
- This can be viewed as "memory" of the environment: Does the environment still know at time $t-t'$, what the system did to it at time 0? The time range $t-t'$ over which (4.16) significantly differs from 0 is called memory time or correlation time τ_{corr} of the environment.
- For the middle equality we assume that the environment is always in a stationary state and hence $\left[\hat{H}_{\mathcal{E}}, \hat{\rho}_{\mathcal{E}}\right] = 0$.[7] Since it is stationary, correlations cannot depend on the absolute time, only on time differences.

With (4.16) we can write (4.15) a bit more nicely as

---

[7] This implies a stationary state due to (3.2), taking into account that the system does not significantly affect the environment.

Quantum master equation in the second[a] **Born approximation**,

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}^{(I)}(t) = -\int_0^t dt' \sum_{\alpha\beta} \Big\{$$

$$\mathcal{C}_{\alpha,\beta}(t-t')\left[\hat{S}_\alpha^{(I)}(t), \hat{S}_\beta^{(I)}(t')\hat{\rho}_{\mathcal{S}}^{(I)}(t')\right] + \mathcal{C}_{\beta,\alpha}(t'-t)\left[\hat{\rho}_{\mathcal{S}}^{(I)}(t')\hat{S}_\beta^{(I)}(t'), \hat{S}_\alpha^{(I)}(t)\right]\Big\} \tag{4.17}$$

---

[a] This implies that it is second order in $\hat{H}_{\text{int}}$, as we see from (4.13).

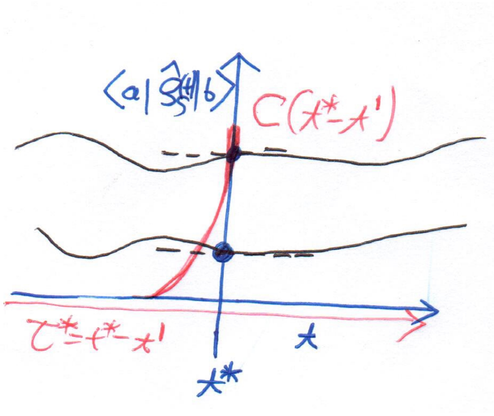
We used the cyclic property of the trace $\text{Tr}_{\mathcal{E}}\left\{\hat{E}_\alpha\hat{E}_\beta\hat{\rho}_{\mathcal{E}}\right\} = \text{Tr}_{\mathcal{E}}\left\{\hat{E}_\beta\hat{\rho}_{\mathcal{E}}\hat{E}_\alpha\right\} = \text{Tr}_{\mathcal{E}}\left\{\hat{\rho}_{\mathcal{E}}\hat{E}_\alpha\hat{E}_\beta\right\}$

Warning: A partial trace is only cyclic as long as operators within act in the space being traced over. Thus e.g. $\text{Tr}_{\mathcal{E}}\left\{\hat{S}_\alpha\hat{E}_\alpha\hat{\rho}\right\} \neq \text{Tr}_{\mathcal{E}}\left\{\hat{\rho}\hat{S}_\alpha\hat{E}_\alpha\right\}$, with full density matrix $(\mathcal{S}+\mathcal{E})$ $\hat{\rho}$.

- Proof of warning: Assignment.

So far we still did not address problem (B) (above Eq. (4.12)), hence let us finally also invoke the

Markov approximation, under which the environmental memory time τ_{corr} is much shorter than the characteristic time-scale for changes in the system τ_{S}, thus $\tau_{\text{corr}} \ll \tau_{\text{S}}$. τ_{S} is typically set by $\hat{H}_{\mathcal{S}}$, for example by the differences of energy eigenvalues of $\hat{H}_{\mathcal{S}}$, e.g. $\tau_{\text{S}} \sim |E_n - E_m|/h$. However τ_{S} may also be affected by relaxation due to the environment.



left: Sketch of the scenario where the Markov approximation is valid. The environment correlations decay substantially faster than $\hat{\rho}_{\mathcal{S}}$ evolves. $t = t^*$ is a reference timepoint (origin of x-axis) wwith respect to which we plot the correlation function $C(\tau^*)$.

The Markov approximation has two consequences:

(i) It allows us to replace $\hat{\rho}_{\mathcal{S}}^{(I)}(t') \to \hat{\rho}_{\mathcal{S}}^{(I)}(t)$ in the time integrals occuring in (4.17), corresponding to the dashed approximation in the figure above.

(ii) We now can extend the integral $\int_0^t \to \int_{-\infty}^t$ (since $\mathcal{C}_{\alpha,\beta}(t-t') = 0$ for large $|t-t'|$ anyway).f

Let us implement consequence (i) only for now, we then obtain the

Redfield equations,

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}^{(I)}(t) = -\sum_{\alpha}\Big\{\big[\hat{S}_{\alpha}^{(I)}(t), \hat{\Gamma}_{\alpha}(t)\hat{\rho}_{\mathcal{S}}^{(I)}(t)\big] + \big[\hat{\rho}_{\mathcal{S}}^{(I)}(t)\hat{\Gamma}_{\alpha}^{\dagger}(t), \hat{S}_{\alpha}^{(I)}(t)\big]\Big\} \tag{4.18}$$

With $\hat{\Gamma}_{\alpha}(t) = \int_0^t dt' \sum_{\beta} \mathcal{C}_{\alpha,\beta}(t-t')\hat{S}_{\beta}^{(I)}(t')$, and assuming Hermitian $\hat{S}$ and $\hat{E}$.

- The Redfield equation is on first sight already local in time, but it still depends "on the past" in a hidden way, since the definition of the time-dependent rate operators $\hat{\Gamma}_{\alpha}(t)$ refers to an initialisation (start of dynamics) at $=0$. Thus (4.18) it is not yet Markovian (BP).
- One has to be careful when using the Redfield equations, as it does not guarantee populations in $\rho_{\mathcal{S}}$ to remain positive. See discussion around Eq. (4.23) later.

After consequence (ii) following from the Markov approximation and the substitution $\tau = t - t'$ in the time integration, we have

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}^{(I)}(t) = -\int_0^{\infty} d\tau \sum_{\alpha\beta}\Big\{\ \mathcal{C}_{\alpha,\beta}(\tau)\big[\hat{S}_{\alpha}^{(I)}(t), \hat{S}_{\beta}^{(I)}(t-\tau)\hat{\rho}_{\mathcal{S}}^{(I)}(t)\big] + \mathcal{C}_{\beta,\alpha}(-\tau)\big[\hat{\rho}_{\mathcal{S}}^{(I)}(t)\hat{S}_{\beta}^{(I)}(t-\tau), \hat{S}_{\alpha}^{(I)}(t)\big]\Big\} \tag{4.19}$$

Now we can transform (4.19) back into the Schrödinger picture for the density matrix. The steps are technical and can be found in SD. We see

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) = -i\big[\hat{H}_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)\big] - \int_0^{\infty} d\tau \sum_{\alpha\beta}\Big\{\ \mathcal{C}_{\alpha,\beta}(\tau)\big[\hat{S}_{\alpha}^{(I)}(0), \hat{S}_{\beta}^{(I)}(-\tau)\hat{\rho}_{\mathcal{S}}(t)\big] + \mathcal{C}_{\beta,\alpha}(-\tau)\big[\hat{\rho}_{\mathcal{S}}(t)\hat{S}_{\beta}^{(I)}(-\tau), \hat{S}_{\alpha}^{(I)}(0)\big]\Big\} \tag{4.20}$$

Note the changes in the time-arguments of system operators on the rhs. In a final step we define

$$\begin{aligned}
\hat{B}_{\alpha} &= \int_0^{\infty} d\tau \sum_{\beta} \mathcal{C}_{\alpha,\beta}(\tau)\hat{S}_{\beta}^{(I)}(-\tau),\\
\hat{C}_{\alpha} &= \int_0^{\infty} d\tau \sum_{\beta} \mathcal{C}_{\beta,\alpha}(-\tau)\hat{S}_{\beta}^{(I)}(-\tau),
\end{aligned} \tag{4.21}$$

and write the

Born-Markov Masterequation as

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) = -i\big[\hat{H}_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)\big] - \sum_{\alpha}\Big\{\big[\hat{S}_{\alpha}, \hat{B}_{\alpha}\hat{\rho}_{\mathcal{S}}(t)\big] + \big[\hat{\rho}_{\mathcal{S}}(t)\hat{C}_{\alpha}, \hat{S}_{\alpha}\big]\Big\} \tag{4.22}$$

- The essential difference between (4.18) and (4.22) is that we integrate over <u>all time delays</u> τ in (4.21). Thus the operators $\hat{B}_\alpha$ and $\hat{C}_\alpha$ are time-independent and we have finally reached a Markovian Master equation.

4.3 Lindblad Master equation

One of the shortcomings of the Born-Markov equation (4.22), is that it does not guarantee the positivity (positive definite-ness) of the evolving reduced density matrix:

$$\langle \Psi(t) | \hat{\rho}_{\mathcal{S}}(t) | \Psi(t) \rangle \geq 0, \tag{4.23}$$

for any pure state $|\Psi(t)\rangle$ of the system. We need this so that when we diagonalize the density matrix, $\hat{\rho}_{\mathcal{S}}(t) = \sum_k p_k |\varphi_k\rangle\langle\varphi_k|$, all its eigenvalues are positive $p_k \geq 0$. Only then can they be interpreted as a probability, and we have a physical density matrix. In terms of the map $\hat{V}(t)$, we say that it has to be CPTP (completely positive trace preserving), meaning it ensures $\mathrm{Tr}[\hat{\rho}_{\mathcal{S}}(t)] = 1$ and (4.23) at all times. While this of course must be true for $\hat{V}(t)$ based on the system+environment $\hat{U}(t)$, one can show counter examples where it is not fulfilled by (4.22), because the approximations we have used broke the feature. To the rescue comes the

Lindblad theorem The most general Master equation that guarantees (4.23) must take the form

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) = -i\big[\hat{H}_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)\big] + \frac{1}{2}\sum_{\alpha\beta}\gamma_{\alpha\beta}\Big\{\big[\hat{S}_\alpha, \hat{\rho}_{\mathcal{S}}(t)\hat{S}^\dagger_\beta\big] + \big[\hat{S}_\alpha\hat{\rho}_{\mathcal{S}}(t), \hat{S}^\dagger_\beta\big].\Big\} \tag{4.24}$$

Here the coefficients $\gamma_{\alpha\beta}$ control all processes to do with the environmental coupling, and $\hat{S}$ are some operators (not necessarily Hermitian).

- We will present a proof shortly.
- (4.24) is a special case of a Born-Markov ME (4.22), but not equivalent.
- We can frequently derive such a form from (4.22) under the additional secular (or rotating wave-approximation), which neglects all terms in the Master equation that rotate fastest (i.e. contain a $e^{i\omega t}$ with the largest ω).

We can simplify (4.24) somewhat by diagonalising the coefficient matrix $\gamma_{\alpha\beta}$ and then reach the

Lindblad Masterequation in the standard form

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) = -i\big[\hat{H}'_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)\big] - \frac{1}{2}\sum_{\mu}\kappa_\mu\Big\{\hat{L}^\dagger_\mu\hat{L}_\mu\hat{\rho}_{\mathcal{S}}(t) + \hat{\rho}_{\mathcal{S}}(t)\hat{L}^\dagger_\mu\hat{L}_\mu - 2\hat{L}_\mu\hat{\rho}_{\mathcal{S}}(t)\hat{L}^\dagger_\mu\Big\} \tag{4.25}$$

- Already (4.24) is also called "Lindblad Masterequation".

- $\hat{H}'_{\mathcal{S}}$ is called the Lamb shifted Hamiltonian, and contains the original $\hat{H}_{\mathcal{S}}$ plus some energy shifts arising due to the coupling to the environment.
- The $\hat{L}_\mu$ are called Lindblad operators and encapsulate any decoherence process. They are obtained as linear combinations of the original $\hat{S}_\alpha$ operators.
- For $\kappa_\mu \; in\mathbb{R}$ one usually absorbs κ_μ into the Lindblad operators by defining $\sqrt{\kappa_\mu}\hat{L}_\mu \to \hat{L}_\mu$, so we can skip writing κ_μ in Eq. (4.25).
- Comparing (4.25) with (4.3), this now defines the dissipator $\hat{D}[\hat{\rho}]$ we set out to find.
- The Eq. (4.25) only contains the density matrix at time $t = 0$ and time-independent operators, so is manifestly Markovian.
- If the $\hat{L}_\mu$ are Hermitian (observables), which may not be the case, we can write (4.25) as

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) = -i\big[\hat{H}'_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)\big] - \frac{1}{2}\sum_\mu \kappa_\mu \big[\hat{L}_\mu, \big[\hat{L}_\mu, \hat{\rho}_{\mathcal{S}}(t)\big]\big]. \tag{4.26}$$

- Lindblad Masterequations are the kind you will most frequently encounter in practice, e.g.:

Example 27, Dephasing Lindblad equation: Consider a two-level system (described as a pseudo spin-1/2) with Hamiltonian

$$\hat{H} = \frac{\Omega}{2}\hat{\sigma}_x - \frac{\Delta}{2}\hat{\sigma}_z, \tag{4.27}$$

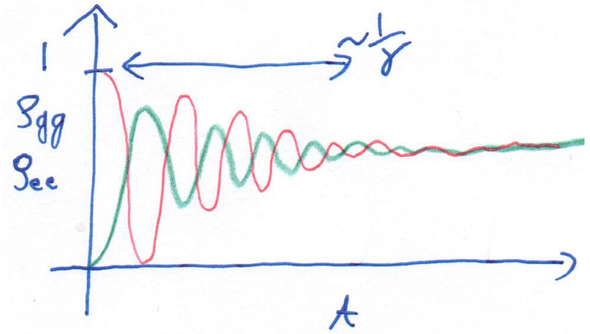
and Lindblad operator $\sqrt{\kappa}\hat{L} = \sqrt{\frac{\gamma}{2}}\hat{\sigma}_z$, with dephasing rate γ. By comparison with Eq. (4.24) and Eq. (4.22), we can see that this physically could be caused by fluctuations of the transition energy $\sim \hat{\sigma}_z$ of the pseudo-spin due to interactions with the environment.
By insertion into Eq. (4.25), we can find the components of the Masterequation as

$$\begin{aligned}
\dot{\rho}_{\uparrow\uparrow} &= +i\frac{\Omega}{2}(\rho_{\uparrow\downarrow} - \rho_{\downarrow\uparrow}), \\
\dot{\rho}_{\downarrow\downarrow} &= -i\frac{\Omega}{2}(\rho_{\uparrow\downarrow} - \rho_{\downarrow\uparrow}), \\
\dot{\rho}_{\uparrow\downarrow} &= -\gamma\rho_{\uparrow\downarrow} + i\Delta\rho_{\uparrow\downarrow} + i\frac{\Omega}{2}(\rho_{\uparrow\uparrow} - \rho_{\downarrow\downarrow}).
\end{aligned} \tag{4.28}$$

One way to solve this coupled differential equation system is to first change variables to the population imbalance $\Delta N = \rho_{\uparrow\uparrow} - \rho_{\downarrow\downarrow}$ and the combined coherences $\rho_\pm = \rho_{\uparrow\downarrow} \pm \rho_{\downarrow\uparrow}$. For $\Delta = 0$ we can then simplify (4.28) into $\frac{\partial}{\partial t}\Delta N(t) = i\Omega\rho_-(t)$ and $\frac{\partial}{\partial t}\rho_-(t) = -\gamma\rho_-(t) + i\Omega\Delta N(t)$, $\frac{\partial}{\partial t}\rho_+(t) = -\gamma\rho_+(t)$. Using initial conditions $N(0) = 1$ and $\rho_- = \rho_+(0) = 0$, standard methods for the solution of two coupled ODEs then give us:

$$\begin{aligned}
\rho_-(t) &= \frac{\Omega}{\Omega_{\text{eff}}} e^{-\frac{\gamma}{2}t} \sin(\Omega_{\text{eff}} t), \quad \rho_+(t) = 0, \\
\Delta N(t) &= e^{-\frac{\gamma}{2}t}\left(\cos(\Omega_{\text{eff}} t) + \frac{\gamma}{2\Omega_{\text{eff}}}\sin(\Omega_{\text{eff}} t)\right)
\end{aligned} \tag{4.29}$$

with $\Omega_{\text{eff}} = \sqrt{\Omega^2 - (\gamma/2)^2}$.
We see that for $\gamma = 0$, the system undergoes coherent Rabi oscillations where the population periodically transfers from $|\uparrow\rangle$ to $|\downarrow\rangle$.



left: If $\gamma > 0$, these oscillations dephase such that populations no longer reach 1. Long after the dephasing time $t \gg 1/\gamma$, $\Delta N(t) \approx 0$, which implies $\rho_{\uparrow\uparrow} \approx \rho_{\downarrow\downarrow} = 1/2$, and $\rho_\pm = 0$.

Decomposing the two-level system purity as $P(t) = \left(1 + \Delta N(t)^2 + \rho_+(t)^2 + \rho_-(t)^2\right)/2$, we see that it continuously evolves from $P = 1$ at $t = 0$ to $P = 1/2$ at $t \gg 1/\gamma$. We thus have just seen our first example of decoherence calculated in the system space only, as we had seen in section 3.2 based on solutions of the entire system, which are typically impractical in realistic settings.

Proof of Lindblad's theorem: We had seen after (3.57) hat evolution via Kraus operators preserves the trace of $\hat{\rho}_{\mathcal{S}}$, and in the same way you can show that it preserves the condition (4.23) if it was true at $t = 0$. For this reason, let us start from (3.57) . Using (4.4) with $t_1 = t$ and $t_2 = dt$ (infinitesimal) and compressing indices ij into a single index k in (3.57), we can write

$$\hat{\rho}(t + dt)_{\mathcal{S}} = \sum_k \hat{E}_k(dt)\hat{\rho}(t)_{\mathcal{S}}\hat{E}_k^\dagger(dt). \tag{4.30}$$

Let us compare this with an infinitesimal expansion of (4.3):

$$\hat{\rho}(t + dt)_{\mathcal{S}} = \hat{\rho}_{\mathcal{S}}(t) + dt\hat{\mathcal{L}}[\hat{\rho}_{\mathcal{S}}(t)], \tag{4.31}$$

and then ask which structure has to be contained in the $\hat{E}_k(dt)$ to make (4.30) agree with (4.31) to order dt.
Since in the limit $dt \to 0$ we need something leftover on the rhs, at least one Kraus operator must contain an identity. Let us take that one to be $k = 0$ and write its infinitesimal form as $\hat{E}_0(dt) = \mathbb{1} + \hat{G}dt$, where $\hat{G}$ is an arbitrary operator that we shall split as $\hat{G} = \hat{K} - i\hat{H}$ into two Hermitian pieces $\hat{K}$ and $\hat{H}$. For the remaining Kraus operators with $k \neq 0$ we write $\hat{E} = \sqrt{dt}\hat{L}_k$, for again arbitrary $\hat{L}_k$.

Starting from the condition $\mathbb{1}_{\mathcal{S}} = \sum_k \hat{E}_k\hat{E}_k^\dagger$ (see after Eq. (3.57)) and inserting the above infinitesimals we reach

$$\begin{aligned}\mathbb{1}_{\mathcal{S}} &= \hat{E}_0\hat{E}_0^\dagger + \sum_{k\neq 0}\hat{E}_m\hat{E}_m^\dagger = (\mathbb{1} + \hat{G}^\dagger dt)(\mathbb{1} + \hat{G}dt) + dt\sum_{k\neq 0}\hat{L}_k^\dagger\hat{L}_k \\ &= \mathbb{1} + (\hat{G}^\dagger + \hat{G})dt + dt\sum_{k\neq 0}\hat{L}_k^\dagger\hat{L}_k + \mathcal{O}(dt^2).\end{aligned} \tag{4.32}$$

Since (4.32) should remain $\mathbb{1}$ to order dt, we require $\hat{G}^\dagger + \hat{G} = 2\hat{K} = -\frac{1}{2}\sum_{k\neq 0}\hat{L}_k^\dagger\hat{L}_k$. Finally inserting our $\hat{E}_k$ into (4.30) we reach up to order dt(exercise)

$$\hat{\rho}(t + dt)_{\mathcal{S}} = \hat{\rho}(t) - i\,dt\big[\hat{H}, \hat{\rho}\big] + dt\sum_{k\neq 0}\left(\hat{L}_k\hat{\rho}\hat{L}_k^\dagger - \frac{1}{2}\left\{\hat{L}_k^\dagger\hat{L}_k, \rho\right\}\right). \tag{4.33}$$

We recognize this as the infinitesimal version of (4.25), which completes the proof.

- For a different style proof, using an operator-space basis for the $\hat{E}_k$, see BP.

We finally supply one option for the missing step from (4.22) to (4.24).

Derivation of Lindblad equation from Born-Markov ME: Let us assume the memory time of the environment is so short, that we can write $\mathcal{C}_{\alpha,\beta}(\tau) = \gamma_{\alpha,\beta}\delta(\tau)$ in Eq. (4.21). Using $\int_0^\infty \delta(\tau)f(\tau) = f(0)/2$, we find $\hat{B}_\alpha = \sum_\beta \gamma_{\alpha,\beta}\hat{S}_\beta$ and $\hat{C}_\alpha = \sum_\beta \gamma_{\beta,\alpha}\hat{S}_\beta$.
Inserting this into (4.22) gives

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) = -i\big[\hat{H}_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)\big] - \frac{1}{2}\sum_{\alpha,\beta}\Big\{\gamma_{\alpha,\beta}\big[\hat{S}_\alpha, \hat{S}_\beta\hat{\rho}_{\mathcal{S}}(t)\big] + \gamma_{\beta,\alpha}\big[\hat{\rho}_{\mathcal{S}}(t)\hat{S}_\beta, \hat{S}_\alpha\big]\Big\} \tag{4.34}$$

Changing the sign by turning $\big[\hat{A}, \hat{B}\big] = -\big[\hat{B}, \hat{A}\big]$, exchanging the two terms in {} and renaming dummy indices vigorously, we can see that we can move this into:

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) = -i\big[\hat{H}_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)\big] + \frac{1}{2}\sum_{\alpha\beta}\gamma_{\alpha\beta}\Big\{\big[\hat{S}_\alpha, \hat{\rho}_{\mathcal{S}}(t)\hat{S}_\beta\big] + \big[\hat{S}_\alpha\hat{\rho}_{\mathcal{S}}(t), \hat{S}_\beta\big].\Big\} \tag{4.35}$$

If the $\hat{S}_\alpha$ are Hermitian, this already is Eq. (4.24). If they are not, then note that $\hat{H}_{\text{int}}$ in Eq. (4.5) also needs to contain another term $\hat{S}_\alpha^\dagger \otimes \hat{E}_\alpha^\dagger$, for the interaction Hamiltonian to be Hermitian as a whole. In this case we can reach Eq. (4.24) only with one additional approximation, see dotpoint below.

- If the $\hat{S}_\alpha$ are not Hermitian, for the interaction Hamiltonian to be Hermitian as a whole we need $\hat{H}_{\text{int}} = \sum_{\alpha=1}^{2N}\hat{S}_\alpha \otimes \hat{E}_\alpha$, where if we call $\hat{S}_\alpha = \hat{L}_\alpha$ for $1 \leq \alpha \leq N$ then $\hat{S}_\alpha = \hat{L}_\alpha^\dagger$ for $N+1 \leq \alpha \leq 2N$. When we expand this in (4.35), we get four parts of the sums ($\alpha, \beta \leq N$, $\alpha, \beta > N$, $\alpha \leq N, \beta > N$ and $\alpha > N, \beta \leq N$). Some of this gives us the structure Eq. (4.24) and for the "undesired" parts we have to invoke what is called the rotating wave approximation (or secular approximation), which essentially neglects terms in the final master equation that are proportional to $\exp[i\omega t]$ for some very large ω. We do not do this explicitly here, due to excess technicalities involved, but you can find the details in books, e.g. BP.
- Importantly, at least for system-environment couplings with e.g. only single term, we can see from the origin of (4.35) that the Lindblad operators (e.g. in example 27) will be related to the original $\hat{S}_\alpha$ (system part of system-environment interaction).

4.4 Section conclusion

We have now achieved a central goal of this course, all the equations (4.17), (4.18), (4.22) and (4.25) allow us to deal with the evolution of the system in $\hat{\rho}_{\mathcal{S}}$ only, without having to explicitly model the environment. This only enters indirectly, when we are using (4.22) through the environment correlation functions $\mathcal{C}(\tau)$, defined in (4.16), and when we are using (4.25) even more abstractly through the Lindblad operator $\hat{L}_\mu$ and rates κ_μ.

The equations starting from section 4.3 additionally ensure that we have CPTP and Markovian dynamics in the system only, which is frequently sufficient to describe decoherence.

We will devote section 5 later to non-Markovian techniques, based on (4.16).

Week ⑦

PHY 435 / 635 Decoherence and Open Quantum Systems
Instructor: Sebastian Wüster, IISER Bhopal, 2021

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In the remaining parts of section 4 on "Markovian OQS", we apply the Master equation concept to most of the system-environment models introduced in section 2. In this section, we mostly set $\hbar = 1$.

4.5 Quantum Brownian Motion

Example 28, Classical Brownian Motion: First checkout the classical version . See this video .

We begin with a central harmonic oscillator coupled to an environment of oscillators, please revise the complete Hamiltonian $\hat{H}$ and setup in section 2.1. Our objective is to derive the Born-Markov Master equation (4.22), following from $\hat{H}$.

Returning to the system-environment coupling term (2.3) we see that we had written it as

$$\hat{H}_{\text{int}} = \hat{X} \otimes \sum_i \kappa_i \hat{q}_i \equiv \underbrace{\hat{X}}_{\equiv \hat{S}} \otimes \hat{E}, \tag{4.36}$$

thus in our starting point (4.5) we get away with using only a single coupling term $\alpha = 0$ and hence can drop the indices α, β that we used throughout section 4 so far.

In order to assemble (4.22) we now need to calculate four pieces

- (i) The environmental self correlation functions $\mathcal{C}(\tau)$.
- (ii) The interaction picture evolution $\hat{S}^{(I)}(\tau)$ of the system part of $\hat{H}_{\text{int}}$.
- (iii) The decoherence operators $\hat{B}$, $\hat{C}$ [they follow from (i) and (ii)].
- (iv) The usual unitary system evolution $\left[\hat{H}_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)\right]$.

4.5.1 Environmental correlation functions and spectral densities

The correlation functions are defined in (4.16). Since we have only one environment operator in (4.36), namely $\hat{E}$, there are no indices α, β (or they are both $= 0$). We thus require $\mathcal{C}(\tau) =$

$\mathrm{Tr}_{\mathcal{E}}\left\{\hat{E}^{(I)}(\tau)\hat{E}^{(I)}(0)\hat{\rho}_{\mathcal{E}}(0)\right\} = \langle\hat{E}^{(I)}(\tau)\hat{E}^{(I)}(0)\rangle_{\mathcal{E}}$, where we have used (3.4). To evaluate this, we have to crucially assume a state $\hat{\rho}_{\mathcal{E}}(0)$ for the environment. We pick the

Thermal State for the Environment: In analogy to what you know from thermodynamics, we can write the environmental density matrix in thermal equilibrium as

$$\hat{\rho}_{\mathcal{E}} = \frac{1}{Z}e^{-\beta\hat{H}_{\mathcal{E}}}, \quad Z = \mathrm{Tr}[e^{-\beta\hat{H}_{\mathcal{E}}}], \tag{4.37}$$

using $\beta = 1/k_BT$ and $\hat{H}_{\mathcal{E}}$ the environmental Hamiltonian. For this section we take $\hat{H}_{\mathcal{E}}$ from Eq. (2.5)). Decomposed into individual oscillators, (4.37) then becomes

$$\hat{\rho}_{\mathcal{E}} = \bigotimes_n \hat{\rho}_n = \bigotimes_n \left(\sum_k p_{kn}\left[|\,k\,\rangle\langle\,k\,|\right]_n\right), \quad p_{kn} = \frac{e^{-\beta\omega_n k}}{\sum_m e^{-\beta\omega_n m}}. \tag{4.38}$$

- Since we write (4.38) as a product of density matrices for each oscillator, the individual oscillators are <u>uncorrelated</u>. This means that all $\langle\hat{O}_a\hat{O}_b\rangle - \langle\hat{O}_a\rangle\langle\hat{O}_b\rangle = 0$ for $a \neq b$, where $\hat{O}_a$ is an operator acting on oscillator a only (proof: excercise).
- We see that each possible state $|\,k\,\rangle$ for an oscillator is occupied with probability given by the Boltzmann factor $e^{-\beta E_{kn}}$, where $E_{kn} = \omega_n k$ is the energy of oscillator number n being excited by k quanta. All these density matrices, for each oscillator and the joint one, are <u>mixed</u> (see section 3.1.2).

We can now calculate the environmental correlation function. In a first step we note:

$$\mathcal{C}(\tau) \overset{\text{insert } \hat{E}}{=} \sum_{ij}\kappa_i\kappa_j\langle\hat{q}_i(\tau)\hat{q}_j(0)\rangle = \sum_j \kappa_j^2\langle\hat{q}_j(\tau)\hat{q}_j(0)\rangle. \tag{4.39}$$

• The last step follows, because in (4.37) all the individual oscillators are uncorrelated and the individual $\langle\hat{q}_j(\tau)\rangle = 0$.

In the assignment we have solved the interaction picture evolution for $\hat{a}$, $\hat{a}^\dagger$ (governed by $\hat{H}_{\mathcal{E}}$ only), which allows us to use the inverse of (1.21) and write the interaction picture time evolution of each oscillator's position operator as:

$$\hat{q}_j(\tau) = \frac{1}{\sqrt{2m_j\omega_j}}\big(\hat{a}_j(0)e^{-i\omega_j\tau} + \hat{a}_j^\dagger(0)e^{i\omega_j\tau}\big). \tag{4.40}$$

Inserting (4.40) into (4.39) gives (because terms $\langle\hat{a}_j(0)\hat{a}_j(0)\rangle = \langle\hat{a}_j^\dagger(0)\hat{a}_j^\dagger(0)\rangle = 0$ since the thermal density matrix is a sum of number states)

$$\mathcal{C}(\tau) = \sum_j \kappa_j^2\left\{\frac{1}{2m_j\omega_j}\left(\underbrace{\langle\hat{a}_j(0)\hat{a}_j^\dagger(0)\rangle}_{=\hat{a}_j^\dagger(0)\hat{a}_j(0)+1} e^{-i\omega_j\tau} + \langle\hat{a}_j^\dagger(0)\hat{a}_j(0)\rangle \underbrace{e^{i\omega_j\tau}}_{\cos(\omega_j\tau)+i\sin(\omega_j\tau)}\right)\right\} \tag{4.41}$$

In the state (4.38), we have the mean thermal occupation $N_j(T) = \langle \hat{a}_j^\dagger(0)\hat{a}_j(0)\rangle = 1/(e^{\beta\omega_j} - 1)$ (exercise), and hence

$$\begin{aligned}\mathcal{C}(\tau) &= \sum_j \kappa_j^2 \left\{ \frac{1}{2m_j\omega_j} \Big([1 + 2N_j(T)] \cos(\omega_j \tau) - i \sin(\omega_j \tau) \Big) \right\} \\ &= \sum_j \kappa_j^2 \left\{ \frac{1}{2m_j\omega_j} \left(\coth\left(\frac{\omega_j}{2k_B T}\right) \cos(\omega_j \tau) - i \sin(\omega_j \tau) \right) \right\} \\ &\equiv \nu(\tau) - i\eta(\tau). \end{aligned} \tag{4.42}$$

With the last line we have defined the

Noise Kernel:

$$\nu(\tau) = \sum_j \frac{\kappa_j^2}{2m_j\omega_j} \coth\left(\frac{\omega_j}{2k_B T}\right) \cos(\omega_j \tau) = \frac{1}{2} \sum_j \kappa_j^2 \langle \{\hat{q}_j(\tau), \hat{q}_j(0)\} \rangle \tag{4.43}$$

and **Dissipation Kernel:**

$$\eta(\tau) = \sum_j \frac{\kappa_j^2}{2m_j\omega_j} \sin(\omega_j \tau) = \frac{i}{2} \sum_j \kappa_j^2 \langle [\hat{q}_j(\tau), \hat{q}_j(0)] \rangle \tag{4.44}$$

- For the form using commutators you can re-follow the steps before (4.42).

Finally we define the

Spectral Density:

$$J(\omega) \equiv \sum_j \frac{\kappa_j^2}{2m_j\omega_j} \delta(\omega - \omega_j). \tag{4.45}$$

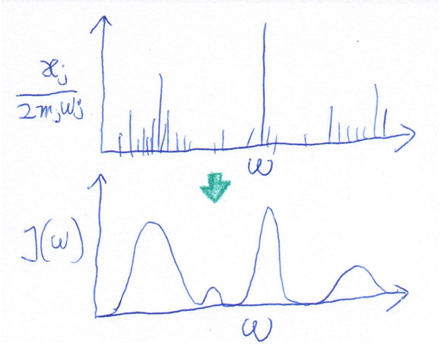
with which we can write

$$\begin{aligned}\nu(\tau) &= \int_0^\infty d\omega J(\omega) \coth\left(\frac{\omega}{2k_B T}\right) \cos(\omega\tau), \\ \eta(\tau) &= \int_0^\infty d\omega J(\omega) \sin(\omega\tau). \end{aligned} \tag{4.46}$$

- The reason for the Kernel names in (4.43) and (4.43) will become clear later.
- The influence of the environment onto the system in the Born Markov ME (4.22) is fully hidden in the environment correlations $\mathcal{C}(\tau)$. From the manipulations above we see that this in turn can be fully expressed via the spectral density of the environment.

- At zero temperature we can write (4.46) as $C(\tau) = \nu(\tau) - i\eta(\tau) = \int_0^\infty d\omega J(\omega) e^{-i\omega\tau}$, so that the spectral density is the (half-sided) Fourier Transform of the environment correlation function $\mathcal{C}(\tau)$. We can invert the relation to give: $J(\omega) = (2\pi)^{-1} \int_0^\infty d\tau \mathcal{C}(\tau) e^{i\omega\tau}$
- Note that we derived the relations between $J(\omega)$ and $C(\tau)$ above strictly only for a thermal bath of uncoupled harmonic oscillator. However they are then frequently also used for more general baths, with some caution.

Example 29, Interpretation of spectral density: The spectral density allows us to move from an explicitly numbered collection of environmental oscillators to a continuous distribution of them.



left: Consider the collection of oscillators on the left. We have drawn sticks of length $L_j = \frac{\kappa_j^2}{2m_j\omega_j}$ at frequencies ω_j. If there is a dense collection of sticks, their impact on the system will be well captured by $J(\omega)$.[a]

---

[a] In other words, any sum over sticks (4.43) or integral over J (4.46) for any small frequency interval $\Delta\omega$ will be the same.

We have now completed item (i) of the list after Eq. (4.36). As a final step, we see that using the definitions of the Kernels (4.42), we can now specify (4.22) for the present case as

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) = -i\big[\hat{H}_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)\big] - \int_0^\infty d\tau \; \Big\{ \nu(\tau)\big[\hat{S}(0), \big[\hat{S}^{(I)}(-\tau), \hat{\rho}_{\mathcal{S}}(t)\big]\big] - i\eta(\tau)\big[\hat{S}(0), \{\hat{S}^{(I)}(-\tau), \hat{\rho}_{\mathcal{S}}(t)\}\big]\Big\}. \tag{4.47}$$

4.5.2 Assembling Master equation for Brownian motion

Proceeding further we require $\hat{S}^{(I)}(\tau)$, which in our case is $\hat{X}^{(I)}(\tau)$. Recall that an interaction picture operator evolves according to $\hat{H}_0 = \hat{H}_{\mathcal{S}} + \hat{H}_{\mathcal{E}}$, according to (1.50). From $\hat{H}_{\mathcal{S}} = \hat{P}^2/2M + M\Omega^2\hat{X}^2/2$ we find (still $\hbar$=1)

$$\begin{aligned} i\frac{\partial}{\partial t}\hat{X}_I(t) &= \big[\hat{X}_I(t), \hat{H}_{0I}(t)\big] = \frac{1}{M} i\hat{P}_I(t), \\ i\frac{\partial}{\partial t}\hat{P}_I(t) &= \big[\hat{P}_I(t), \hat{H}_{0I}(t)\big] = -iM\Omega^2\hat{X}_I(t). \end{aligned} \tag{4.48}$$

The second equalities above use that also $[\hat{X}_I(t), \hat{P}_I(t)] = i\hbar$, i.e. the commutation relations are preserved (this follows directly from (1.48)).

The equations (4.48) have the solution

$$\hat{X}_I(\tau) = \hat{X}(0)\cos(\Omega\tau) + \frac{1}{M\Omega}\hat{P}(0)\sin(\Omega\tau),$$
$$\hat{P}_I(\tau) = \hat{P}(0)\cos(\Omega\tau) - M\Omega\hat{X}(0)\sin(\Omega\tau). \tag{4.49}$$

- Proof: Substitute (4.49) into (4.48).

Inserting $\hat{S}^{(I)}(\tau) = \hat{X}_I(\tau)$ from (4.49) into (4.21) using (4.42) we obtain

$$\hat{B} = \int_0^\infty d\tau\ \mathcal{C}(\tau)\hat{S}^{(I)}(-\tau) = \int_0^\infty d\tau\ \big(\nu(\tau) + i\eta(\tau)\big)\big(\hat{X}(0)\cos(-\Omega\tau) + \frac{1}{M\Omega}\hat{P}(0)\sin(-\Omega\tau)\big),$$
$$\hat{C} = \int_0^\infty d\tau\ \mathcal{C}(-\tau)\hat{S}^{(I)}(-\tau) = \int_0^\infty d\tau\ \big(\nu(-\tau) + i\eta(-\tau)\big)\big(\hat{X}(0)\cos(-\Omega\tau) + \frac{1}{M\Omega}\hat{P}(0)\sin(-\Omega\tau)\big). \tag{4.50}$$

In a final step we insert (4.50) into the general expression for a Born-Markov ME (4.22) or (4.47), then extensively re-arrange terms (exercise), to write the

Master equation for Quantum Brownian Motion (QBM)

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) = -i\big[\hat{H}_{\mathcal{S}} + \frac{1}{2}M\tilde{\Omega}^2\hat{X}^2, \hat{\rho}_{\mathcal{S}}(t)\big] - i\gamma\big[\hat{X}, \{\hat{P}, \hat{\rho}_{\mathcal{S}}(t)\}\big]$$
$$- D\big[\hat{X}, [\hat{X}, \hat{\rho}_{\mathcal{S}}(t)]\big] - f\big[\hat{X}, [\hat{P}, \hat{\rho}_{\mathcal{S}}(t)]\big]. \tag{4.51}$$

where all operators without time argument are at time $t = 0$. The coefficients are

$$\tilde{\Omega}^2 = -\frac{2}{M}\int_0^\infty d\tau\ \eta(\tau)\cos(\Omega\tau), \tag{4.52}$$
$$\gamma = \frac{1}{M\Omega}\int_0^\infty d\tau\ \eta(\tau)\sin(\Omega\tau), \tag{4.53}$$
$$D = \int_0^\infty d\tau\ \nu(\tau)\cos(\Omega\tau), \tag{4.54}$$
$$f = -\frac{1}{M\Omega}\int_0^\infty d\tau\ \nu(\tau)\sin(\Omega\tau). \tag{4.55}$$

- We have now achieved the goal to describe the central oscillator in terms of $\hat{\rho}_{\mathcal{S}}(t)$ and $\hat{X}$, $\hat{P}$ only, even for a very large number of environmental oscillators.
- The time-evolution depends on constant coefficients $\tilde{\Omega}^2$, γ, D, f, that can fully be calculated from the original environmental coupling κ_j, frequency ω_j, and state $\hat{\rho}_{\mathcal{E}}$.

We will provide the physical meaning of the coefficients (4.52)-(4.55) in section 4.5.3. To that end, it will help to also look at (4.51) in the position basis. For this we first have to write the density matrix in the position basis as

$$\hat{\rho}_{\mathcal{S}} = \int dX \int dX' \rho_{\mathcal{S}}(X, X') |\, X \,\rangle\langle\, X' \,|. \tag{4.56}$$

Using further that that$\langle\, X \,|\hat{P}\hat{\rho}_{\mathcal{S}}|\, X' \,\rangle = -i\frac{\partial}{\partial X}\langle\, X \,|\hat{\rho}_{\mathcal{S}}|\, X' \,\rangle$, we then reach the

QBM Master equation in position space

$$\begin{aligned}\frac{d}{dt}\rho_{\mathcal{S}}(X, X', t) = \Big\{ &- \frac{i}{2M}\left(\frac{\partial^2}{\partial X'^2} - \frac{\partial^2}{\partial X^2}\right) - \frac{i}{2}M(\Omega^2 + \tilde{\Omega}^2)(X^2 - X'^2) \\ &+ \gamma(X - X')\left(\frac{\partial}{\partial X'} - \frac{\partial}{\partial X}\right) - D(X - X')^2 \\ &+ i\, f(X - X')\left(\frac{\partial}{\partial X'} + \frac{\partial}{\partial X}\right)\Big\}\rho_{\mathcal{S}}(X, X', t).\end{aligned} \tag{4.57}$$

We now proceed to infer the consequences of all the ”new terms” using both, (4.51) and (4.57).

4.5.3 Decoherence and Dissipation in Quantum Brownian motion

part $\sim \tilde{\Omega}^2$: The contribution by the $\tilde{\Omega}^2$ term is easiest. It occurs in exactly the same place and way as the system oscillator frequency Ω^2, and hence corresponds to an environmentally induced shift of the oscillator frequency. We had called that a Lamb shift in section 4.3. Recall from your Atomic-Molecular Physics course, that the Lamb-shift of atomic spectral lines is due to the quantized electromagnetic field. This field can be viewed as a collection of quantum oscillators forming an environment for the atom, so the origin of both Lamb-shifts is mathematically the same. We will follow this viewpoint further shortly.

part $\sim \gamma$: Consider the evolution of the mean momentum $\langle\hat{P}\rangle$, that follows from (4.51). We find that the γ term gives rise to

Momentum damping or friction, according to

$$\frac{d}{dt}\langle\hat{P}\rangle = -M(\Omega^2 + \tilde{\Omega}^2)\langle\hat{X}\rangle - 2\gamma\langle\hat{P}\rangle. \tag{4.58}$$

- The first term is just usually oscillatory motion in the Lamb-shifted oscillator potential.
- The second term alone would result in $\langle\hat{P}\rangle = e^{-2\gamma t}\langle\hat{P}\rangle_{t=0}$, i.e. exponential damping.

Mean values from Master equation: Deriving Eq. (4.58) is a good exercise. For example considering only the friction term $\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) = \cdots - i\gamma\big[\hat{X}, \big\{\hat{P}, \hat{\rho}_{\mathcal{S}}(t)\big\}\big]$, we can write ($\hbar = 1$)

$$\begin{aligned}\frac{d}{dt}\langle\hat{P}\rangle &= \frac{d}{dt}\mathrm{Tr}_{\mathcal{S}}\Big\{\hat{\rho}_{\mathcal{S}}(t)\hat{P}\Big\} = \mathrm{Tr}_{\mathcal{S}}\Big\{\frac{d\hat{\rho}_{\mathcal{S}}(t)}{dt}\hat{P}\Big\} = -i\gamma\mathrm{Tr}_{\mathcal{S}}\Big\{\big[\hat{X}, \{\hat{P}, \hat{\rho}_{\mathcal{S}}(t)\}\big]\hat{P}\Big\} \\ &= -i\gamma\mathrm{Tr}_{\mathcal{S}}\Big\{\Big(\hat{X}(\hat{P}\hat{\rho}_{\mathcal{S}}(t) + \hat{\rho}_{\mathcal{S}}(t)\hat{P}) - (\hat{P}\hat{\rho}_{\mathcal{S}}(t) + \hat{\rho}_{\mathcal{S}}(t)\hat{P})\hat{X}\Big)\,\hat{P}\Big\} \\ &= -i\gamma\mathrm{Tr}_{\mathcal{S}}\Big\{\hat{\rho}_{\mathcal{S}}(t)\big(\hat{P}\hat{X}\hat{P} + \underbrace{\hat{P}\hat{P}\hat{X} - \hat{X}\hat{P}\hat{P}}_{=\left[\hat{P}^2,\hat{X}\right]=-2i\hat{P}} - \hat{P}\hat{X}\hat{P}\big)\Big\} = -2\gamma\mathrm{Tr}_{\mathcal{S}}\Big\{\hat{\rho}_{\mathcal{S}}(t)\hat{P}\Big\} = -2\gamma\langle\hat{P}\rangle.\end{aligned} \tag{4.59}$$

- Exercise: Using similar steps, convince yourself that the D and f terms in (4.51) do not contribute to Eq. (4.58).
- Note that the friction coefficient γ depends only on the spectral density and not on temperature (only on $\eta(\tau)$, not on $\nu(\tau)$).

part $\sim D$: This terms has two consequences. The first is best seen from (4.57), from where we infer the

Spatial decoherence evolution

$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(X, X', t) = \cdots - D(X - X')^2\rho_{\mathcal{S}}(X, X', t), \tag{4.60}$$

which implies that spatial coherences in the reduced density matrix at a separation $|X - X'|$ are decaying with a decoherence timescale $\tau = 1/[D(X - X')^2]$. [this means $\hat{\rho}_{\mathcal{S}}(X, X', t) \sim e^{-t/\tau}\hat{\rho}_{\mathcal{S}}(X, X', 0)$]

The second role can be seem by inspecting the

Momentum diffusion

$$\frac{d}{dt}\langle\hat{P}^2\rangle = -M(\Omega^2 + \tilde{\Omega}^2)\langle\hat{X}\hat{P} + \hat{P}\hat{X}\rangle - 4\gamma\langle\hat{P}^2\rangle + 2D, \tag{4.61}$$

which means that just via the D-term, the variance of momentum[a] grows as $\langle\hat{P}^2\rangle \sim Dt$.

---

[a] Assuming $\langle\hat{P}\rangle = 0$.

- D is thus also referred to as normal diffusion coefficient
- The derivation of (4.61) is analogous to that of Eq. (4.58), see (4.59).

- Also position space uncertainty scales as $\Delta X^2 \sim Dt$.
- D depends on the spectral density and on the temperature.

part $\sim f$: The f is called anomalous diffusion coefficient. It is usually much less important than the D coefficient. See SD for some more information.

4.5.4 Types of spectral density, Ohmic Decoherence and Dissipation

The discussion of the previous section already contained all effects that occur for our oscillator in contact with the environment. To characterise the physics of these effects, it was sufficient to know the system part of the system-environment coupling $\hat{S}^{(I)}(\tau) = \hat{X}_I(\tau)$, the (operator) form of which then decides which terms occur in Eq. (4.51).

However to find out about the strength of these effects, i.e. value of the coefficients (4.52)-(4.55), we finally have to specify a spectral density. Often ones does not take the path via the definition $J(\omega) = \sum_j \frac{\kappa_j^2}{2m_j\omega_j}\delta(\omega - \omega_j)$, for example because individual κ_j are not known. Instead one directly takes some of a frequently used

List of spectral densities

Ohmic spectral density:

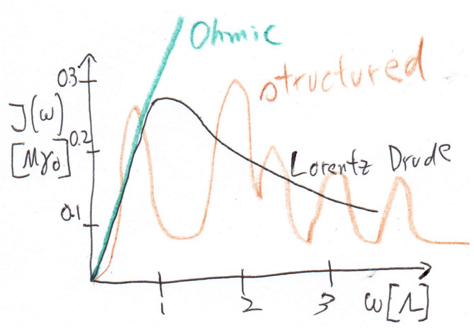
$$J(\omega) = \frac{2M\gamma_0}{\pi}\omega. \tag{4.62}$$

Lorentz-Drude spectral density:

$$J(\omega) = \frac{2M\gamma_0}{\pi}\omega\frac{\Lambda^2}{\Lambda^2 + \omega^2}. \tag{4.63}$$

Structured spectral density: All the above have a very simple shape as seen below. Anything with more detail, such as multiple peaks, is called "structured spectral density".

- More generally, spectral densities with $J(\omega) \sim \omega^\alpha$ are called *Ohmic* for $\alpha = 1$, sub-ohmic for $\alpha < 1$ and super-ohmic for $\alpha > 1$.
- A purely Ohmic spectral density typically cannot be right, since it diverges at large ω. This is cured by the cutoff Λ in the Lorentz-Drude form.



left: Sketch of all the spectral densities discussed above. The Lorentz-Drude spectral density is the Ohmic one with a high frequency cut-off Λ.

We will focus now only on the Lorentz-Drude spectral density (4.63), which has the nice feature that all the coefficients in the previous section can be relatively easily evaluated.

We find

$$\gamma = \frac{2}{\pi}\frac{1}{M\Omega}J(\Omega) = \gamma_0 \frac{\Lambda^2}{\Lambda^2+\Omega^2}, \tag{4.64}$$

$$D = \frac{2}{\pi}J(\Omega)\coth\left(\frac{\Omega}{2k_BT}\right) = M\gamma_0\Omega\frac{\Lambda^2}{\Lambda^2+\Omega^2}\coth\left(\frac{\Omega}{2k_BT}\right), \tag{4.65}$$

$$\tilde{\Omega}^2 = -2\gamma_0\frac{\Lambda^3}{\Lambda^2+\Omega^2}. \tag{4.66}$$

- We skipped f, it is not so important in this case.
- The first relation for γ and D is valid in general and expresses the coefficients via the spectral density evaluated at the frequency of the system oscillator. To see this for γ we gather its definition (4.53) and that of the dissipation Kernel $\eta(\tau)$ (4.44) occuring in it, to see that γ is essentially the double Fourier sine-transform of the spectral density. This returns the original (odd) function.: $\frac{2}{\pi}\int_0^\infty dk\, \sin(x'k)\int_0^\infty dx\, g(x)\sin(kx) = g(x')$. Similarly, for D we use that the double cosine transform returns the original (even) function.
- Note that $\gamma = \gamma_0$ for system frequencies far below the cut-off ($\Omega \ll \Lambda$).
- In the limit $k_BT \gg \Omega$ (high temperatures) and $\Omega \ll \Lambda$, we can write $D = 2M\gamma_0 k_BT$ and using the thermal de-Broglie wavelength for the system oscillator $\lambda_{dB} = 1/\sqrt{2Mk_BT}$ the spatial decoherence time-scale τ after (4.60) then becomes $\tau^{-1} = \gamma_0\left(\frac{X-X'}{\lambda_{dB}}\right)^2$. This tells us that any spatial superpositions with an extent $|X-X'|$ much larger than λ_{dB} will decohere much faster than the system dissipates (the rate for which is γ_0).

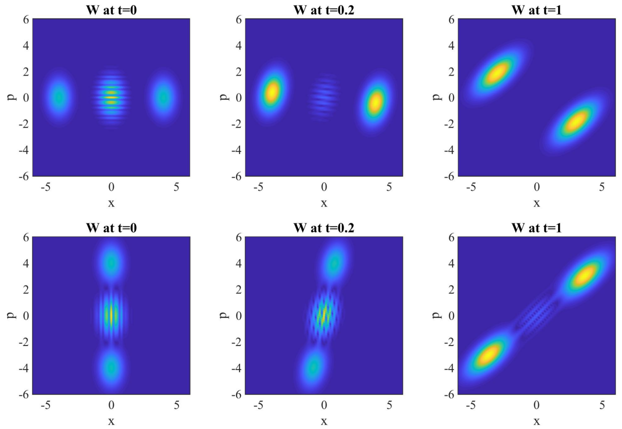
4.5.5 Dynamics of Quantum Brownian motion

The previous discussion already allowed us to "guess" all physical effects relevant to QBM and their time-scales. However equations like (4.51) and (4.57) allow us to investigate the dynamics of these effects in much more detail.

Example 30, Numerical Quantum Brownian motion: by a solution in position-space (of Eq. (4.57)). Let us consider two different (pure) initial states for our system oscillator

$$|\,\Psi_A(x)\,\rangle = \mathcal{N}\left(e^{-\frac{(x-x_0)^2}{2\sigma^2}} + e^{-\frac{(x+x_0)^2}{2\sigma^2}}\right), |\,\Psi_B(x)\,\rangle = \mathcal{N}e^{-\frac{x^2}{2\sigma^2}}\left(e^{ip_0x/\hbar} + e^{-ip_0x/\hbar}\right), \quad (4.67)$$

where $|\,\Psi_A(x)\,\rangle$ is a superposition of two Gaussians in position space, and $|\,\Psi_B(x)\,\rangle$ a superposition of two Gaussians in momentum space.



left: Evolution of the Wigner function (3.52) for the reduced density matrix $\rho(x, x', t)$ evolving according to Eq. (4.57). The top row starts from the initial state $|\,\Psi_A(x)\,\rangle$, the bottom one from $|\,\Psi_B(x)\,\rangle$. We see that the interference features in the centre of phase space, indicating a superposition (see section 3.3.2) are damped out faster when starting in $|\,\Psi_A(x)\,\rangle$.

- We can use (4.57) including all the terms, to study for which density matrices the average decrease in purity (Eq. (3.10)) is smallest. Such states would be deemed most robust against decoherence. It turns out that these are precisely coherent states (1.27). In terms of our discussion in section 3.2.4, these would be the pointer states of the system.
- It makes sense that the spatial superposition $|\,\Psi_A(x)\,\rangle$ in the example above decoheres faster than the momentum superposition $|\,\Psi_B(x)\,\rangle$. That is because the system part of $\hat{H}_{\text{int}}$ is $\hat{X}$, thus the "environment measures X".

Week ⑧

PHY 435 / 635 Decoherence and Open Quantum Systems
Instructor: Sebastian Wüster, IISER Bhopal, 2021

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4.6 Spin Decoherence

In section 4.5 we have applied the concepts of section 4 to the oscillator-oscillators model of section 2. We now do the same for the spin-oscillators model / Spin-Boson model.

4.6.1 Master equation for Spin-Boson model

Compared to our earlier treatment in section 2.2.1 we will at first not be making the simplification $\Delta_0 = 0$, but instead set $\omega_0 = 0$. The complete Hamiltonian is then ($\hbar = 1$):

$$\hat{H} = \underbrace{-\frac{1}{2}\Delta_0\hat{\sigma}_x + \sum_i \omega_i \left(\hat{a}_i^\dagger \hat{a}_i + \frac{1}{2}\right)}_{=\hat{H}_0} + \hat{\sigma}_z \otimes \sum_i \bar{\kappa}_i \left(\hat{a}_i + \hat{a}_i^\dagger\right), \tag{4.68}$$

Since the environment of the Spin-Boson model is the same as that for quantum Brownian motion, our results from section 4.5 regarding environmental correlations functions and noise Kernels, e.g. Eq. (4.42) and (4.46), can all be used here too.

What changes is mainly the system evolution, which we require in order to assemble the $\hat{S}^{(I)}(\tau)$ piece of the Master equation. We have $\hat{S} = \hat{\sigma}_z$ and hence

$$\begin{aligned}\hat{S}^{(I)}(\tau) = \hat{\sigma}_z(\tau) &= e^{i\hat{H}_S\tau}\hat{\sigma}_z e^{-i\hat{H}_S\tau} = e^{-i\Delta_0\hat{\sigma}_x\tau/2}\hat{\sigma}_z e^{i\Delta_0\hat{\sigma}_x\tau/2} \\ &\overset{Eq.\ (4.70)}{=} \hat{\sigma}_z(0)\cos\left(\Delta_0\tau\right) - \hat{\sigma}_y(0)\sin\left(\Delta_0\tau\right). \end{aligned} \tag{4.69}$$

Expression such as (4.69) occur frequently in the quantum dynamics involving spins and can be dealt with by evaluating $e^{-i\Delta_0\hat{\sigma}_x\tau/2}$ etc. using Matrix exponentials in mathematica or evaluating the operator power series. Alternatively one can use the

Spin rotation formula: (related to Rodrigues' rotation formula)

$$e^{ia(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})}\boldsymbol{\sigma}e^{-ia(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})} = \boldsymbol{\sigma}\cos(2a) + (\hat{\mathbf{n}}\times\boldsymbol{\sigma})\sin(2a) + \hat{\mathbf{n}}(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})(1-\cos(2a)), \tag{4.70}$$

where $\hat{\mathbf{n}}$ is a unit vector that can be thought of as a rotation axis, and $2a$ a number that can be thought of as a rotation angle around that axis. $\boldsymbol{\sigma} = [\underline{\underline{\sigma}}_x, \underline{\underline{\sigma}}_y, \underline{\underline{\sigma}}_z]^T$ is a vector of Pauli matrices. The formula then gives the effect of that rotation on the cartesian spin components.

- To apply (4.70) to (4.69) (exercise) we only look at the z component of the transformed Pauli-vector, and set $a = -\Delta_0\tau/2$ and $\hat{\mathbf{n}} = \hat{\mathbf{i}}$ (unit vector along x axis).

We can also recycle (4.47) from section 4.5 and just replace $\hat{S}$ with $\hat{\sigma}_z$. Then we insert (4.69) do some extensive re-arrangements, and reach the

Born-Markov master equation for the Spin-Boson model (with $\omega_0 = 0$):

$$\begin{aligned}\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) = &-i\big(\hat{H}'_{\mathcal{S}}\hat{\rho}_{\mathcal{S}}(t) - \hat{\rho}_{\mathcal{S}}(t)\hat{H}'^{\dagger}_{\mathcal{S}}\big) - \tilde{D}\big[\hat{\sigma}_z, \big[\hat{\sigma}_z, \hat{\rho}_{\mathcal{S}}(t)\big]\big] \\ &+ \zeta\hat{\sigma}_z\hat{\rho}_{\mathcal{S}}(t)\hat{\sigma}_y + \zeta^*\hat{\sigma}_y\hat{\rho}_{\mathcal{S}}(t)\hat{\sigma}_z,\end{aligned} \tag{4.71}$$

where all operators without time argument are at $t = 0$. The Lamb-shifted Hamiltonian is

$$\hat{H}'_{\mathcal{S}} = \left(-\frac{1}{2}\Delta_0 - \zeta^*\right)\hat{\sigma}_x, \tag{4.72}$$

and the coefficients are

$$\zeta = \tilde{f} - i\tilde{\gamma}, \tag{4.73}$$

$$\tilde{D} = \int_0^\infty d\tau\ \nu(\tau)\cos(\Delta_0\tau), \tag{4.74}$$

$$\tilde{f} = \int_0^\infty d\tau\ \nu(\tau)\sin(\Delta_0\tau), \tag{4.75}$$

$$\tilde{\gamma} = \int_0^\infty d\tau\ \eta(\tau)\sin(\Delta_0\tau). \tag{4.76}$$

- We use $\tilde{\dots}$ on the coefficients to make apparent that they are not quite the same as we had for quantum Brownian motion.
- Since $\zeta \in \mathbb{C}$ in general, $\hat{H}'_{\mathcal{S}}$ may no longer be Hermitian.
- The $\tilde{D}$ term already explicitly takes the Lindblad form as in Eq. (4.26), with a dephasing Lindblad operator $\hat{L} = \sqrt{\tilde{D}}\hat{\sigma}_z$ as in example 27. We have thus now justified the dephasing model used there. This is the most important term when the bath memory time is much

shorter than the system period: $\tau_{mem} \ll 2\pi/\Delta_0$, as you can see from Eq. (4.74)-Eq. (4.76). Thus, let's look at its function in detail once more:

4.6.2 Decoherence in the Spin-Boson model

Luckily, with the simplification $\Delta_0 = 0$ all coefficients in (4.71) drastically simplify, and we find $\tilde{f} = \tilde{\gamma} = 0$ and $\tilde{D} = \int_0^\infty d\tau\, \nu(\tau) = \int_0^\infty d\tau \int_0^\infty d\omega J(\omega) \cos(\omega\tau)$ (for $T = 0$). Using similar arguments about repeated cosine transform as we did below Eq. (4.66), we finally can write $\tilde{D} = \frac{\pi}{2} J(0)$. Since e.g. for the Ohmic spectral density this would be zero, let's rather take it as "lowest frequency contributions to the spectral density".

The Eq. (4.71) becomes

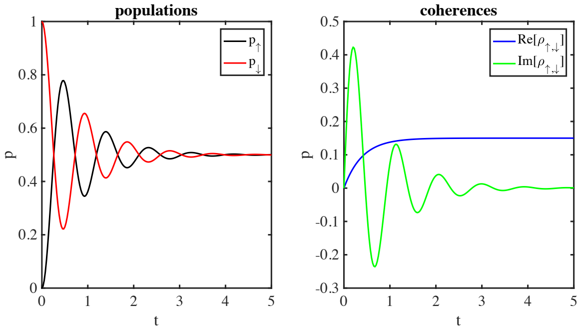
$$\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) = -i\big[\hat{H}_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)\big] - \tilde{D}\big[\hat{\sigma}_z, \big[\hat{\sigma}_z, \hat{\rho}_{\mathcal{S}}(t)\big]\big]. \tag{4.77}$$

For $\hat{H}_{\mathcal{S}} = 0$, we an write the entire (4.77) in 2×2 matrix notation, and find:

$$\frac{d}{dt}\begin{bmatrix} \rho_{\uparrow\uparrow}(t) & \rho_{\uparrow\downarrow}(t) \\ \rho_{\downarrow\uparrow}(t) & \rho_{\downarrow\downarrow}(t) \end{bmatrix} = -4\tilde{D}\begin{bmatrix} 0 & \rho_{\uparrow\downarrow}(t) \\ \rho_{\downarrow\uparrow}(t) & 0 \end{bmatrix}, \tag{4.78}$$

which immediately yields $\rho_{\uparrow\downarrow}(t) = \rho_{\uparrow\downarrow}(0)\exp[-\tilde{D}t]$. We thus see that that coherences are exponentially damped with rate $\tilde{D}$. We can interpret this decoherence as arising because the environment "measures" the observable $\hat{S}_z$ via dynamics as shown in the example of section 2.2.1. Thus coherences in the basis $|\uparrow\rangle$, $|\downarrow\rangle$ are exponentially damped.

Example 31, Numerical solution of Spin-Boson ME: without any simplifications. We can use a matrix representation $\rho_{\mathcal{S},nm}$ for the reduced density matrix $\hat{\rho}_{\mathcal{S}}(t) = \sum_{nm} \rho_{\mathcal{S},nm}(t)|\,n\,\rangle\langle\,m\,|$ of the spin, where $|\,n\,\rangle$ and $|\,m\,\rangle \in \{|\uparrow\rangle, |\downarrow\rangle\}$, and derive equations of motion $\frac{\partial}{\partial t}\rho_{\mathcal{S},nm}(t) = \cdots$ from (4.71) (assignment). These can then be solved without any further simplifications.



left: Results of Eq. (4.71) for $\Omega_0 = (2\pi)$, $\tilde{D} = (2\pi)/10$ and $\zeta = (2\pi)(0.05 + i0.03)$. We see initially coherent spin-oscillations due to $\Omega_0 > 0$, which are progressively decohering, governed by $4\tilde{D}$.

We can do the same explicit expansion for the remaining terms in (4.71) and find:

$$\frac{d}{dt}\begin{bmatrix} \rho_{\uparrow\uparrow}(t) & \rho_{\uparrow\downarrow}(t) \\ \rho_{\downarrow\uparrow}(t) & \rho_{\downarrow\downarrow}(t) \end{bmatrix} = \cdots + \begin{bmatrix} 0 & -2i[\zeta\rho_{\uparrow\uparrow}(t) + \zeta^*\rho_{\downarrow\downarrow}(t)] \\ -2i[\zeta\rho_{\downarrow\downarrow}(t) + \zeta^*\rho_{\uparrow\uparrow}(t)] & 0 \end{bmatrix}, \tag{4.79}$$

where $\cdots$ stands for pieces already discussed earlier. The effect of these terms is less obvious, they may even counteract decoherence.

4.7 Spontaneous decay

Now let us shift our attention to the two level atom interacting with a quantized photon field, that we had introduced in section 2.2.2. Since each photon mode is mathematically equivalent to a harmonic oscillator, and our two-level atom is equivalent to a spin-1/2 system, this falls into the category of system: spin - environment: oscillator.

We had already decomposed the Hamiltonian appropriately in (2.18)-(2.20). We do a slight modification (see changed version) and then let us only cast the interaction Hamiltonian into our usual form ($\hbar = 1$):

$$\hat{H}_{\text{int}} = \underbrace{\sum_{n\nu} \left(g_{n\nu} \hat{a}_{n\nu} + g^*_{n\nu} \hat{a}^\dagger_{n\nu} \right)}_{=\hat{E}} \underbrace{(\hat{\sigma}_+ + \hat{\sigma}_-)}_{=\hat{S}} \tag{4.80}$$

We follow the usual steps to obtain a Born-Markov ME, so we first require the environmental correlation function. We shall assume the photon-field to be in the thermal state (4.37), which can describe the vacuum for $T \to 0$ and otherwise incorporates black-body radiation at temperature T.

As before, the ladder operators in the interaction picture are simply $\hat{a}^{(I)}_{n\nu}(t) = \hat{a}_{n\nu}(0) e^{-i\omega_{n\nu} t}$. This yields the correlation function

$$\begin{aligned}
\mathcal{C}(\tau) = \langle \hat{E}^{(I)}(\tau) \hat{E}^{(I)}(0) \rangle &= \sum_{n\nu, n'\nu'} \langle \left(g_{n\nu} \hat{a}_{n\nu}(0) e^{-i\omega_{n\nu}\tau} + g^*_{n\nu} \hat{a}^\dagger_{n\nu}(0) e^{i\omega_{n\nu}\tau} \right) \left(g_{n'\nu'} \hat{a}(0)_{n'\nu'} + g^*_{n'\nu'} \hat{a}^\dagger_{n'\nu'}(0) \right) \rangle \\
&= \sum_{n\nu} |g_{n\nu}|^2 \left(\langle \hat{a}_{n\nu}(0) \hat{a}^\dagger_{n\nu}(0) \rangle e^{-i\omega_{n\nu}\tau} + \langle \hat{a}^\dagger_{n\nu}(0) \hat{a}_{n\nu}(0) \rangle e^{i\omega_{n\nu}\tau} \right) \\
&= \sum_{n\nu} |g_{n\nu}|^2 \left([N_{n\nu}(T) + 1] e^{-i\omega_{n\nu}\tau} + N_{n\nu}(T) e^{i\omega_{n\nu}\tau} \right),
\end{aligned} \tag{4.81}$$

which really is the same as we had seen in (4.41), expect for a renaming of coupling constants and more complex indexing of the oscillators.

For the second line we used that photon modes with $n\nu \neq n'\nu'$ are uncorrelated in state (4.37), and that it is a mixture of number states. For the last line we have again made use of the thermal population $N_{n\nu}(T)$ of mode $n\nu$ at temperature T.

Next also we require the interaction picture evolution of the system operators, and find:

$$i \frac{\partial}{\partial t} \hat{\sigma}_\pm = \left[\hat{\sigma}_\pm, \hat{H}_{\mathcal{S}} \right] = \mp \omega_{ge} \hat{\sigma}_\pm, \tag{4.82}$$

and hence $\hat{S}^{(I)}(t) = \hat{\sigma}_+(0) e^{-i\omega_{ge} t} + \hat{\sigma}_-(0) e^{+i\omega_{ge} t}$.

In a final step, we combine the correlation function and $\hat{S}^{(I)}(t)$ into decoherence operators $\hat{B}$, $\hat{C}$

and find:

$$\begin{aligned}\hat{B} &= \int_0^\infty d\tau\, \mathcal{C}(\tau)\hat{S}^{(I)}(-\tau)\\ &= \int_0^\infty d\tau \sum_{n\nu} |g_{n\nu}|^2 \left([N_{n\nu}(T)+1]e^{-i\omega_{n\nu}\tau} + N_{n\nu}(T)e^{i\omega_{n\nu}\tau}\right) \times \left(\hat{\sigma}_+(0)e^{+i\omega_{ge}\tau} + \hat{\sigma}_-(0)e^{-i\omega_{ge}\tau}\right)\end{aligned} \tag{4.83}$$

We now use the

Cauchy principal value:

$$\int_0^\infty d\tau\, e^{-i\omega\tau} = \pi\delta(\omega) + i\mathcal{P}\left(\frac{1}{\omega}\right). \tag{4.84}$$

This expression has to be thought of being applied onto a test function $f(\omega)$ and then integrated over, then $\int_{-\infty}^{\infty} d\omega \mathcal{P}\left(\frac{1}{\omega}\right) f(\omega) \equiv \lim_{\epsilon\to 0}\left(\int_{-\infty}^{-\epsilon} d\omega \frac{f(\omega)}{\omega} + \int_{\epsilon}^{\infty} d\omega \frac{f(\omega)}{\omega}\right)$

We also convert $\sum_{n\nu} \to \int_0^\infty d\omega \rho(\omega)$, where $\rho(\omega)$ is the photon density of states [i.e. the number of photon modes in a small frequency interval $[\omega, \omega + d\omega]$]. Ignoring the principal value part for the moment, we then arrive at

$$\begin{aligned}\hat{B} &= \int_0^\infty d\tau\, \mathcal{C}(\tau)\hat{S}^{(I)}(-\tau)\\ &= \pi \int_0^\infty d\omega \rho(\omega)|g(\omega)|^2 \left([N_\omega(T)+1]\hat{\sigma}_-\delta(\omega-\omega_{eg}) + N_\omega(T)\hat{\sigma}_+\delta(\omega-\omega_{eg})\right) + \mathcal{P}\text{ part}\\ &= \underbrace{\pi\rho(\omega_{eg})|g(\omega_{eg})|^2}_{\equiv\gamma/2}\left([N_{\omega_{eg}}(T)+1]\hat{\sigma}_- + N_{\omega_{eg}}(T)\hat{\sigma}_+\right) + \mathcal{P}\text{ part}\end{aligned} \tag{4.85}$$

In the second line we have already discarded two terms containing a delta function like $\delta(\omega + \omega_{ge})$ that cannot be fulfilled since all frequencies are positive, and in the third applied the remaining delta-functions. Similarly we find:

$$\hat{C} = \frac{\gamma}{2}\left([N_{\omega_{eg}}(T)+1]\hat{\sigma}_+ + N_{\omega_{eg}}(T)\hat{\sigma}_-\right) + \mathcal{P}\text{ part} \tag{4.86}$$

We finally insert (4.85) and (4.86) into (4.22), calculate lots of commutators and re-arrange. After the dust settles, we have the

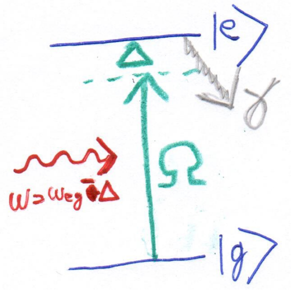
Master equation for a two-level atom in a quantum radiation field

$$\begin{aligned}\frac{d}{dt}\hat{\rho}_{\mathcal{S}}(t) &= -i\left[\hat{H}'_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)\right] + \frac{\gamma}{2}[N_{\omega_{eg}}(T)+1]\Big(2\hat{\sigma}_-\hat{\rho}_{\mathcal{S}}(t)\hat{\sigma}_+ - \hat{\sigma}_+\hat{\sigma}_-\hat{\rho}_{\mathcal{S}}(t) - \hat{\rho}_{\mathcal{S}}(t)\hat{\sigma}_+\hat{\sigma}_-\Big)\\ &\quad + \frac{\gamma}{2}N_{\omega_{eg}}(T)\Big(2\hat{\sigma}_+\hat{\rho}_{\mathcal{S}}(t)\hat{\sigma}_- - \hat{\sigma}_-\hat{\sigma}_+\hat{\rho}_{\mathcal{S}}(t) - \hat{\rho}_{\mathcal{S}}(t)\ \hat{\sigma}_-\hat{\sigma}_+\Big)\end{aligned} \tag{4.87}$$

$\hat{H}'_{\mathcal{S}} = \left(\frac{\hbar\omega_{eg}}{2} + \Delta E\right)\sigma_z$, where ΔE is a Lamb-shift from the $\mathcal{P}$ parts glossed over above.

- Eq. (4.87) is of the Lindblad form (4.25), with two operators $\hat{L}_\mu \in \{\hat{\sigma}_+, \hat{\sigma}_-\}$.
- The first line, where $\hat{L} = \hat{\sigma}_-$, describes spontaneous decay and stimulated emission of the atom. The term is non-zero even in vacuum $T = 0$, and detailed inspection of Eq. (4.87) (in the example below), reveals that this part redistributes population from the upper to the lower state.
- Hence the second line, where $\hat{L} = \hat{\sigma}_+$ is due to absorption of the incoherent black-body radiation.
- In Eq. (4.87) only the radiation density exactly on resonance affects the atom. This cannot be the full story and is an artefact of the Markov approximation used.

Example 32, Decoherence of Rabi oscillations / Optical Bloch equations:



left: Consider an additional coherent laser field driving transitions from $|\,g\,\rangle$ to $|\,e\,\rangle$ as shown on the left. It turns out (PHY402), this can be described by an effective system (atom) Hamiltonian (the same as in example 27)

$$\hat{H}_{\mathcal{S}} = \frac{\Omega}{2}\hat{\sigma}_x - \frac{\Delta}{2}\hat{\sigma}_z, \tag{4.88}$$

with $\hat{\sigma}_z = |\,e\,\rangle\langle\,e\,| - |\,g\,\rangle\langle\,g\,|$ and $\hat{\sigma}_x = |\,e\,\rangle\langle\,g\,| + |\,g\,\rangle\langle\,e\,|$. Since the atom can spontaneously decay while being illuminated by the laser, we solve (4.87) for $T = 0$ using[a] the Hamiltonian (4.90).

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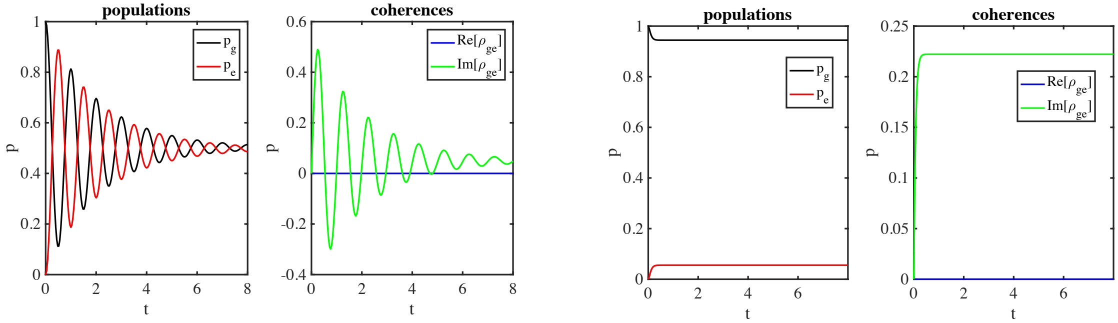
[a] Technically, since we changed the system Hamiltonian, we also ought to re-derive the ME, since the system operator evolution (4.82) will be different now. We don't, since spontaneous decay involves the energy/time scale defined by $\omega_{ge} \sim 500$THz, which is much larger/faster than Ω, $\Delta \sim$ MHz, GHz. So we can first find the effect of spontaneous decay as discussed in section 4.7, and then add the slow system evolution later.

Writing (4.87) explicitly in terms of elements of the density matrix, we then find:

$$\begin{aligned}\frac{\partial}{\partial t}\begin{bmatrix}\rho_{gg} & \rho_{ge}\\ \rho_{eg} & \rho_{ee}\end{bmatrix} &= \begin{bmatrix} i\frac{\Omega}{2}(\rho_{ge}-\rho_{eg}) & i\frac{\Omega}{2}(\rho_{gg}-\rho_{ee}) - i\Delta\rho_{ge}\\ i\frac{\Omega}{2}(\rho_{ee}-\rho_{gg}) + i\Delta\rho_{eg} & -i\frac{\Omega}{2}(\rho_{ge}-\rho_{eg})\end{bmatrix}\\ &+ \gamma[N_{\omega_{eg}}(T)+1]\begin{bmatrix}\rho_{ee} & -\frac{1}{2}\rho_{ge}\\ -\frac{1}{2}\rho_{eg} & -\rho_{ee}\end{bmatrix} + \gamma N_{\omega_{eg}}(T)\begin{bmatrix}-\rho_{gg} & -\frac{1}{2}\rho_{ge}\\ -\frac{1}{2}\rho_{eg} & \rho_{gg}\end{bmatrix}\end{aligned} \tag{4.89}$$

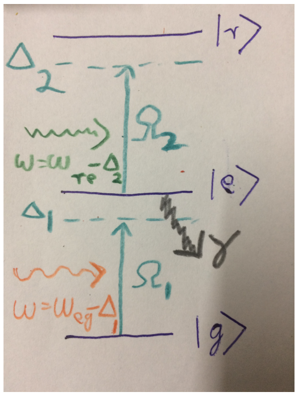
On the rhs, we have separated off the unitary part from $-i\big[\hat{H}_{\mathcal{S}}, \hat{\rho}_{\mathcal{S}}(t)\big]$ from the part related to spontaneous decay. We see that (4.91) can simultaneously describe coherent driving and incoherent decay of the atom, as well as incoherent excitation by BBR. The second line corroborates our interpretation given earlier. For $T = 0$, (4.91) are called the optical Bloch equations.

Example continued:



Two exemplary numerical solutions of (4.91) for $\Delta = 0$ and $N_{\omega_{eg}}(T) = 0$ are shown on the top. The left one has $\Omega = (2\pi)$, $\gamma = (2\pi)/10$, so Rabi oscillations are seen but decohere on a time-scale $2\pi/\gamma$. The right one is for $\Omega = (2\pi)$, $\gamma = 4(2\pi)$, where no oscillations are visible but some equilibrium is reached quickly.

Example 33, Coherent versus incoherent two-photon transition to Rydberg states:



left: Now we extend the earlier example by a second follow-up laser transition from the excited state $|\, e\, \rangle$ to an even higher excited state $|\, r\, \rangle$. If $|\, r\, \rangle$ is a Rydberg state (e.g. principal quantum number $n = 80$, see PHY 402), it makes sense to assume that $|\, r\, \rangle$ does *not* spontaneously decay, only $|\, e\, \rangle$ does, as shown in the figure.

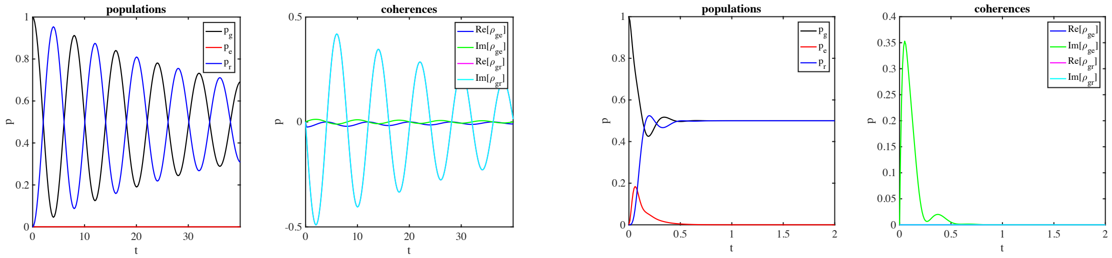
The effective system (atom) Hamiltonian for this case is

$$\hat{H}_{\mathcal{S}} = \frac{\Omega_1}{2}(|\, e\, \rangle\langle\, g\,| + |\, g\, \rangle\langle\, e\,|) - \Delta_1 |\, e\, \rangle\langle\, e\,| + \frac{\Omega_2}{2}(|\, r\, \rangle\langle\, e\,| + |\, e\, \rangle\langle\, r\,|) - (\Delta_1 + \Delta_2)|\, r\, \rangle\langle\, r\,|. \tag{4.90}$$

If we include the decay of the middle level $|\, e\, \rangle$ (we now take $N(T) = 0$, i.e. $T = 0$) via the derived Lindblad operator $\hat{\sigma}_- \rightarrow |\, g\, \rangle\langle\, e\,|$, we find the three-level optical Bloch equations:

$$\begin{aligned}
\dot{\rho}_{gg} &= \gamma\rho_{ee} + i\frac{\Omega_1}{2}(\rho_{ge} - \rho_{eg}), \\
\dot{\rho}_{ee} &= -\gamma\rho_{ee} - i\frac{\Omega_1}{2}(\rho_{ge} - \rho_{eg}) - i\frac{\Omega_2}{2}(\rho_{re} - \rho_{er}), \\
\dot{\rho}_{rr} &= +i\frac{\Omega_2}{2}(\rho_{re} - \rho_{er}), \\
\dot{\rho}_{ge} &= -\frac{\gamma}{2}\rho_{ge} + i\frac{\Omega_1}{2}(\rho_{gg} - \rho_{ee}) + i\frac{\Omega_2}{2}\rho_{gr} - i\Delta_1\rho_{ge}, \\
\dot{\rho}_{gr} &= -i\frac{\Omega_1}{2}\rho_{er} + i\frac{\Omega_2}{2}\rho_{ge} - i(\Delta_1 + \Delta_2)\rho_{gr}, \\
\dot{\rho}_{er} &= -\frac{\gamma}{2}\rho_{er} - i\frac{\Omega_1}{2}\rho_{gr} - i\frac{\Omega_2}{2}(\rho_{rr} - \rho_{ee}) - i\Delta_2\rho_{er}.
\end{aligned} \tag{4.91}$$

Example continued:
As before we can solve these numerically:



(left two panels) Populations and coherences for $\Omega_1 = \Omega_2 = (2\pi)5$ and $\Delta_1 = -\Delta_2 = (2\pi)100$. Hence $\Delta_1 + \Delta_2 = 0$ and the *two-photon* transition is resonant for $|\,g\,\rangle \leftrightarrow |\,r\,\rangle$. However since $|\Delta_k| \gg |\Omega_k|$, we say that this transitions is proceeding *off-resonantly* via $|\,e\,\rangle$. Thus population in $|\,e\,\rangle$ and thus spontaneous decay and decoherence can be kept small. This is used in experiments in practice to create coherent transitions between ground- and Rydberg states using two lasers.
(right two panels) Populations and coherences for $\Omega_1 = \Omega_2 = (2\pi)5$ and $\Delta_1 = \Delta_2 = 0$. Now we proceed *resonantly* via the middle level. As a result excitation is strongly decohered by spontaneous decay.

Example 34, Adiabatic Elimination:
Let us understand the coherent coupling in example II using adiabatic elimination. In the equations for $\dot{\rho}_{ge}$ the by far largest term on the rhs is $-i\Delta_1\rho_{ge}$. This will cause the complex number ρ_{ge} to very quickly rotate. If we coarse grain in time, this allows us to actually set $\dot{\rho}_{ge} = 0$. *Warning: The implication is confusingly not that it varies too slowly, but rather too fast.* We can then solve the resultant *algebraic equation*, using also $\Delta_1 \gg \gamma$ to yield:

$$\rho_{ge} \approx \frac{\Omega_1}{2\Delta_1}(\rho_{gg} - \rho_{ee}) + \frac{\Omega_2}{2\Delta_1}\rho_{gr}. \tag{4.92}$$

Similarly for $\dot{\rho}_{er}$ we find

$$\rho_{er} \approx -\frac{\Omega_2}{2\Delta_2}(\rho_{rr} - \rho_{ee}) - \frac{\Omega_1}{2\Delta_2}\rho_{gr}. \tag{4.93}$$

Inserting these into the remaining equations gives (assuming $\rho_{ee} \approx 0$)

$$\begin{aligned}
\dot{\rho}_{gg} &= +i\frac{\Omega_{\text{eff}}}{2}(\rho_{gr} - \rho_{rg}), \\
\dot{\rho}_{rr} &= +i\frac{\Omega_{\text{eff}}}{2}(\rho_{rg} - \rho_{gr}), \\
\dot{\rho}_{gr} &= i\frac{\Omega_{\text{eff}}}{2}(\rho_{gg} - \rho_{rr}),
\end{aligned} \tag{4.94}$$

where $\Omega_{\text{eff}} = \frac{\Omega_1\Omega_2}{2\Delta_1}$ takes the place of an *effective Rabi frequency* of our coherent two-photon transition. The corresponding Rabi period is $T_{\text{rab}} = 2\pi/\Omega_{\text{eff}} = 8$ for example II, matching the observation in the left-most panel.

4.8 Steady states of a Master equation

The second example above shows a phenomenon that frequently happens when dealing with Master equations: At some time the dissipative or decohering terms have established a steady state, where none of the density matrix element change any more. Often this is of major interest, particularly if the time it takes to establish it (called the “transient“) is too short to be interesting for us. Mathematically we can define a

Steady state of a Master equation simply by demanding

$$\frac{d}{dt}\hat{\rho}(t) = 0, \text{ and } \mathrm{Tr}[\hat{\rho}^{(ss)}] = 1. \tag{4.95}$$

We call the solution of this $\hat{\rho}^{(ss)}$, for “steady state“.

This can often be solved much easier than the actual ME, since it is just an algebraic equation.

Example 35, Steady state of the driven atom:
Let us apply the concept to the example earlier. We combine Eq. (35) with Eq. (4.91), hence we just set the lhs of Eq. (4.91) to zero and solve the resultant system of algebraic equations including $\rho_{gg}^{(ss)} + \rho_{ee}^{(ss)} = 1$. We find (for $\Delta = 0$)

$$\begin{aligned} \rho_{gg}^{(ss)} &= \frac{\gamma^2 + \Omega^2}{\gamma^2 + 2\Omega^2}, & \rho_{ee}^{(ss)} &= \frac{\Omega^2}{\gamma^2 + 2\Omega^2}, \\ \rho_{ge}^{(ss)} &= \frac{i\gamma\Omega}{\gamma^2 + 2\Omega^2}, & \rho_{eg}^{(ss)} &= \frac{-i\gamma\Omega}{\gamma^2 + 2\Omega^2}. \end{aligned} \tag{4.96}$$

These values match with the steady simulation results found in example 32 earlier.
The same could be applied to example-II, right panels, to find the equilibrium populations of all the levels (exercise).

Week ⑨

PHY 435 / 635 Decoherence and Open Quantum Systems
Instructor: Sebastian Wüster, IISER Bhopal, 2021

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5 Non-Markovian Open Quantum Systems

In section 1.5.7 we had seen that a stochastic process $X(t)$ can be classified as "Markovian" if the probabilities for the next step depend only on its currents state at time t. It is classified as "Non-Markovian", if the probabilities for the next step also can depend on the entire history including times $t' < t$. The same nomenclature applies to the underlying evolution of a probability distribution $P(X, t)$. Since (the diagonal of) a density matrix also represents a probability distribution, we use the terminology for open quantum systems as well: A

Markovian Open Quantum System is one for which the evolution of the reduced density matrix $\frac{\partial}{\partial t}\hat{\rho}_S(t)$ depends only on the present density matrix $\hat{\rho}_S(t)$, and not on its past $\hat{\rho}_S(t')$, $t' < t$.

Consequently a

Markovian Master equation is one in which the right-hand side in $\frac{\partial}{\partial t}\hat{\rho}_S(t) = RHS$, does not contain any explicit dependencies on $\hat{\rho}_S(t')$ at $t' < t$, nor requires knowledge of the environmental history.

- We distinguish the two statements due to some subtleties: For example a seemingly Non-Markovian Master equation where the RHS does contain $\hat{\rho}_S(t')$ at $t' < t$ may still give rise to Markovian dynamics (if those dependencies happen to be negligible or unimportant).
- According to the definitions above, "Non-Markovian" implies the negation of the statement.
- We will now supply some first examples of Non-Markovianity, building on section 4, and then explore a bit more what the definitions above imply.

The starting point for this section is the Quantum Master equation in the second Born approximation (4.17).

- That equations also already deals with only the reduced DM of the system $\hat{\rho}_{\mathcal{S}}^{(I)}(t)$ all information about the environment is neatly encapsulated in the correlation functions $\mathcal{C}_{\alpha,\beta}(t-t')$.
- However since we have not made the Markov approximation, the RHS still explicitly depends on $\hat{\rho}_S(t')$ at $t' < t$ (see time integration limits).
- Conceptually, this constitutes an integro-differential equation, posing additional challenges in its solution. It is typically the case, that methods for tackling non-Markovian OQS dynamics are substantially more involved than for Markovian ones.

5.1 Redfield Formalism

As a first example of a fairly simple to use Non-Markovian ME, we revisit the Redfield equations (4.18), which had popped up in section 4.2 mainly as a step in the derivation of the Born-Markov ME. However at this point we had not yet made the Markov approximation. Firstly, note that (4.18) can be rewritten as

Redfield equation in tensor notation,

$$\frac{d}{dt}\rho_{\mathcal{S},ab}^{(I)}(t) = -\sum_{cd} R_{ab;cd}\ \rho_{\mathcal{S},cd}^{(I)}(t) \tag{5.1}$$

where matrix elements are defined as usual $\rho_{\mathcal{S},ab}^{(I)}(t) = \langle\, a\,|\hat{\rho}_{\mathcal{S}}^{(I)}(t)|\, b\,\rangle$. We will use states $|\, n\,\rangle$ to denote basis states of the system, and then define the Redfield Relaxation Tensor

$$R_{ab;cd} = \delta_{a,c}\sum_{e}\Gamma^{*}_{be,de} + \delta_{b,d}\sum_{e}\Gamma_{ae,ec} - \Gamma^{*}_{ca,bd} - \Gamma_{db,ac}. \tag{5.2}$$

where the new symbol $\Gamma_{ab,cd} = \sum_\alpha \langle\, a\,|\hat{S}_\alpha^{(I)}(t)|\, b\,\rangle\langle\, c\,|\Gamma_\alpha(t)|\, d\,\rangle$. We assume $\hat{S}$ is Hermitian but $\hat{\Gamma}$ may not be.

- To show (5.1) from (4.18), we first take matrix elements $\langle\, a\,|\cdots|\, b\,\rangle$ of (4.18) and then insert the system unit operator in the form of $\mathbb{1} = \sum_n |\, n\,\rangle\langle\, n\,|$, between any two of operators ($\hat{\rho}$, $\hat{S}$, $\hat{\Gamma}$).
- In section 5.1.1 we now apply the Redfield formalism to the (first, simplified) Spin-Boson model, for which we had found the complete evolution pictorially in section 2.2.1 and mathematically in assignment 1. We can then compare the open quantum system approach with the full solution in section 5.1.2.

5.1.1 Simplified Spin-Boson model with the Redfield method

To apply Eq. (5.1) to (2.10)-(2.12), we have to go through the tedious task of assembling all the ingredients $\hat{\Gamma}$, $\hat{S}^I(t)$, $\Gamma_{ab,cd}$, $R_{ab;cd}$. Luckily there are only two states in the system basis $|\, n\,\rangle \in \{|\uparrow\rangle, |\downarrow\rangle\}$.

Using (4.69) with $\Delta_0 = 0$ (Simplified SBM), we find $\hat{S}^I(\tau) = \sigma_z(0)$, so the system part of $\hat{H}_{\text{int}}$ does not evolve in the interaction picture, and its matrix elements are

$$\langle\, a \,|\hat{S}^I(\tau)|\, b \,\rangle = \delta_{ab}(\delta_{a\uparrow} - \delta_{a\downarrow}). \tag{5.3}$$

Similar to Eq. (4.36) we define $\hat{H}_{\text{int}} = \hat{\sigma}_z \otimes \underbrace{\sum_i \bar{\kappa}_i \left(\hat{a}_i + \hat{a}_i^\dagger\right)}_{=\hat{E}}$, so there is only a single environmental operator $\hat{E}$ and we can also skip the index α. Thus as final piece to find $\Gamma_{ab,cd}$ we look at $\hat{\Gamma}_\alpha(t) = \int_0^t dt' \sum_\beta \mathcal{C}_{\alpha,\beta}(t-t')\hat{S}_\beta^{(I)}(t')$ from Eq. (4.18) and simplify this here to $\hat{\Gamma}(t) = \int_0^t d\tau \;\; \mathcal{C}(\tau)\sigma_z(0)$. Since we have the same oscillator environment as in section 4.5, we can use Eq. (4.42) for the bath correlation, assuming zero temperature $T \to 0$ and taking into account our slightly different definition of $\hat{E}$ here, which involves $\bar{\kappa}_i$ instead of κ_i. We find

$$\mathcal{C}(\tau) = \sum_j \bar{\kappa}_j^2 e^{-i\omega_j \tau}. \tag{5.4}$$

which we can straightforwardly integrate over time to find

$$\hat{\Gamma}(t) = \int_0^t d\tau \;\; \mathcal{C}(\tau)\sigma_z(0) = \underbrace{i\sum_j \frac{\bar{\kappa}_j^2}{\omega_j}\left(e^{-i\omega_j t} - 1\right)}_{\equiv -\gamma(t)} \sigma_z(0). \tag{5.5}$$

and hence

$$\langle\, c \,|\hat{\Gamma}(t)|\, d \,\rangle = -i\gamma(t)\delta_{cd}(\delta_{c\uparrow} - \delta_{c\downarrow}). \tag{5.6}$$

Now we combine (5.3) and (5.6) to write

$$\Gamma_{ab,cd} = -i\gamma(t)\delta_{ab}(\delta_{a\uparrow} - \delta_{a\downarrow})\delta_{cd}(\delta_{c\uparrow} - \delta_{c\downarrow}), \tag{5.7}$$

from which we find[8]

$$R_{ab,cd} = 2\,\mathrm{Im}[\gamma(t)]\big[1 - (\delta_{a\uparrow} - \delta_{a\downarrow})(\delta_{b\uparrow} - \delta_{b\downarrow})\big]\delta_{ac}\delta_{bd}. \tag{5.8}$$

Plugging these into (5.1) we finally reach the now surprisingly simple

Redfield equations for the simplified Spin-Boson model in the interaction picture

$$\begin{aligned} \frac{d}{dt}\rho_{\uparrow\uparrow}(t) &= 0, & \frac{d}{dt}\rho_{\uparrow\downarrow}(t) &= -4\mathrm{Im}[\gamma(t)]\rho_{\uparrow\downarrow}(t), \\ \frac{d}{dt}\rho_{\downarrow\downarrow}(t) &= 0, & \frac{d}{dt}\rho_{\downarrow\uparrow}(t) &= -4\mathrm{Im}[\gamma(t)]\rho_{\downarrow\uparrow}(t). \end{aligned} \tag{5.9}$$

Note: we have simplified notation $\rho_{\mathcal{S},\uparrow\uparrow}^{(I)}(t) \to \rho_{\uparrow\uparrow}(t)$

---

[8] Use e.g. $(\delta_{a\uparrow} - \delta_{a\downarrow})(\delta_{a\uparrow} - \delta_{a\downarrow}) = 1$.

- We can compare (5.9) with our Markovian treatment of the SBM in (4.71), if we set $\Delta_0 = 0$ in the latter, resulting in (4.79). We notice a very similar structure, with the crucial difference that in the present non-Markovian scenario, the dephasing rate $\gamma(t)$ is time dependent instead of constant. This manifests the fact that the environment has a memory, and damps the system differently depending on how long ago it was first perturbed.

Variation of constants/parameters: From mathematics courses we know that the ODE $f'(t) = g(t)f(t)$ has the general solution

$$f(t) = Ce^{\int dt\ g(t)} \tag{5.10}$$

where C is set by the initial conditions.

Using the result above, we can solve (5.9) to give $\rho_{\uparrow\uparrow}(t) = \rho_{\uparrow\uparrow}(0)$, $\rho_{\downarrow\downarrow}(t) = \rho_{\downarrow\downarrow}(0)$ and

$$\rho_{\uparrow\downarrow}(t) = \rho_{\uparrow\downarrow}(0)e^{-4\sum_j \frac{\bar{\kappa}_j^2}{\omega_j^2}\left(1-\cos\left(\omega_j t\right)\right)} \tag{5.11}$$

while $\rho_{\uparrow\downarrow}(t) = \rho_{\downarrow\uparrow}(t)^*$. Let's keep this result aside for a while and first revisit our earlier solution of the full problem (without using open system techniques / Master equations).

5.1.2 Reduced dynamics of the Spin

The simplified Spin-Boson model with $\Delta_0 = 0$ can be analytically solved (see section 2.2.1, the assignment and SD). In the assignment, you have found the solution

$$|\,\Psi(t)\,\rangle = c_1|\downarrow\rangle|\,\mathcal{E}_-\,\rangle + c_2|\uparrow\rangle|\,\mathcal{E}_+\,\rangle, \tag{5.12}$$

for the time dependent wave function following from the initial state $|\,\Psi(0)\,\rangle = (c_1|\downarrow\rangle + c_2|\uparrow\rangle)|\,0,\cdots,0\,\rangle$, where $|\,0,\cdots,0\,\rangle$ denotes all oscillators in the ground-state (hence the environment is at $T = 0$). Here $|\,\mathcal{E}_+\,\rangle$ is an environment state that is a tensor product of coherent states $|\,\mathcal{E}_+\,\rangle = |\,\lambda_1(t)/2\,\rangle \otimes |\,\lambda_2(t)/2\,\rangle \otimes \ldots$, where each amplitude

$$\lambda_i(t) \equiv 2\frac{\bar{\kappa}_i}{\omega_i}(1 - e^{i\omega_i t}) \tag{5.13}$$

will in general be different for the various environment oscillators. For $|\,\mathcal{E}_-\,\rangle$ we flip the sign of all $\lambda_i(t) \to -\lambda_i(t)$.

Since we managed to solve the whole model (4.68) for the simple case $\Delta_0 = 0$, we can construct the density matrix $\hat{\rho}(t) = |\,\Psi(t)\,\rangle\langle\,\Psi(t)\,|$, and then calculate the reduced density matrix for the spin only, using Eq. (3.13). Since Eq. (5.12) takes the bi-partite form Eq. (3.18) (treating the environment as just one"part" which is fine), we can directly use Eq. (3.19) for this and reach:

$$\hat{\rho}_S = |c_1|^2|\downarrow\rangle\langle\downarrow| + |c_2|^2|\uparrow\rangle\langle\uparrow| + c_1^* c_2|\downarrow\rangle\langle\uparrow|\underbrace{\langle\,\mathcal{E}_-\,|\,\mathcal{E}_+\,\rangle}_{=r(t)} + c_2^* c_1|\uparrow\rangle\langle\downarrow|\langle\,\mathcal{E}_+\,|\,\mathcal{E}_-\,\rangle\Big). \tag{5.14}$$

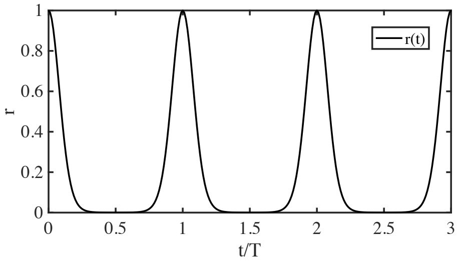
We call $r(t)$ the decoherence factor. Since we have an explicit expression for $|\,\mathcal{E}_\pm\,\rangle$ we can evaluate $r(t)$ directly. We use that the overlap of two coherent states

$$\langle\,\lambda\,|\,\mu\,\rangle = \exp\left[-|\lambda|^2/2 - |\mu|^2/2 + \lambda^*\mu\right], \tag{5.15}$$

which can be shown from the definition (1.27), and find:

$$\begin{aligned} r(t) = \langle\,\mathcal{E}_-\,|\,\mathcal{E}_+\,\rangle = \prod_i \langle\,-\lambda_i(t)/2\,|\,\lambda_i(t)/2\,\rangle &\overset{Eq.\ (5.15)}{=} \prod_i \exp\left[-|\lambda_i(t)|^2/2\right] \\ \overset{Eq.\ (5.13)}{=} \exp\left[-4\sum_i \frac{\bar{\kappa}_i{}^2}{\omega_i^2}\big(1-\cos(\omega_i t)\big)\right]&. \end{aligned} \tag{5.16}$$

Example 36, Compare full and ME solutions of the Spin Boson model: We can now directly extract the coherence factor $r(t)$ from (5.16) with that obtained in (5.11) ($\rho_{\uparrow\downarrow}(0) = c_1^* c_2$ so $r(t)$ is just the part with the exponential). We find the same expression in both cases. For just a *single* environmental oscillator (not really a bath), this is plotted in the figure below. We see strong periodic revivals of coherence, corresponding to the times where the oscillator has returned to its initial state. Since whether this happens depends on exactly when the oscillator has "started" its motion, this now *depends* on the history of the bath. Revival features of coherence as shown are characteristic of non-Markovian systems.



left: Coherence factor $r(t)$ for a single environmental oscillator with $\kappa = \omega = 2\pi$, and period $T = 2\pi/\omega$.

- We have now explicitly validated the general idea to derive an evolution equation for the system only, taking into account the environment effectively via its correlation functions, by comparison with the complete solution.
- The non-Markovian Redfield equation is capable to capture the revival features shown in the graph above, which would not be the case for a Markov treatment.
- See SD for some additional discussion of decoherence in the Spin-Boson model, such as a non-zero temperature environment.

5.1.3 Full Spin-Boson model with the Redfield method

We finally drop the simplification $\Delta_0 = 0$, solving the complete Spin-Boson model. We thus have to re-evaluate $\hat{S}^I(\tau)$ and all quantities where it appears, since the system evolution will now be different. As in section 4.6.1 we use $\omega_0 = 0$ however, and thus again can write

$$\hat{S}^{(I)}(\tau) = \hat{\sigma}_z(0)\cos(\Delta_0\tau) - \hat{\sigma}_y(0)\sin(\Delta_0\tau), \tag{5.17}$$

with

$$\langle\, a\,|\hat{S}^{I}(\tau)|\, b\,\rangle = \delta_{ab}(\delta_{a\uparrow} - \delta_{a\downarrow})\cos{(\Delta_0\tau)} - (i\delta_{c\uparrow}\delta_{d\downarrow} - i\delta_{c\downarrow}\delta_{d\uparrow})\sin{(\Delta_0\tau)}. \tag{5.18}$$

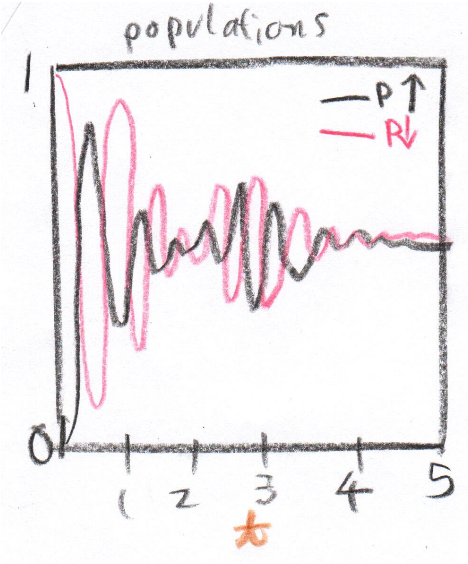
This changes (5.5) according to Eq. (4.69) into

$$\begin{aligned}\hat{\Gamma}(t) &= \int_0^t d\tau\ \mathcal{C}(\tau)\hat{S}^{(I)}(\tau) = \int_0^t d\tau\ \sum_j \bar{\kappa}_j^2 e^{-i\omega_j\tau}\left(\hat{\sigma}_z(0)\cos{(\Delta_0\tau)} - \hat{\sigma}_y(0)\sin{(\Delta_0\tau)}\right)\\ &= \underbrace{\sum_j \bar{\kappa}_j^2 \frac{i\omega_j + e^{-i\omega_j\tau}\left(\Delta_0\sin{(\Delta_0\tau)} - i\omega_j\cos{(\Delta_0\tau)}\right)}{\Delta_0^2 - \omega_j^2}}_{=\gamma_z(t)}\hat{\sigma}_z(0)\\ &+ \underbrace{\sum_j \bar{\kappa}_j^2 \frac{-\Delta_0 + e^{-i\omega_j\tau}\left(\Delta_0\cos{(\Delta_0\tau)} + i\omega_j\sin{(\Delta_0\tau)}\right)}{\Delta_0^2 - \omega_j^2}}_{=\gamma_y(t)}\hat{\sigma}_y(0).\end{aligned} \tag{5.19}$$

Matrix elements are thus $\langle\, c\,|\hat{\Gamma}(t)|\, d\,\rangle = \gamma_z(t)\delta_{cd}(\delta_{c\uparrow} - \delta_{c\downarrow}) + \gamma_y(t)(i\delta_{c\uparrow}\delta_{d\downarrow} - i\delta_{c\downarrow}\delta_{d\uparrow})$. We again assemble $\Gamma_{ab,cd}$ and $R_{ab,cd}$ and convert back to the Schrödinger picture as in section 4.2.

This time the equations would be much more complicated than Eq. (5.9), where each equation for ρ_{ab} contains most of the other ρ_{cd} on the rhs., together with time dependent functions stemming from the interplay of bath and system evolution, such as $\sin{(\Delta t)}$, $\sin{(\omega_j t)}$.

Example 37, Redfield equations for the full Spin-Boson model:



left: We sketched the expected dynamics on the left hands side. The time dependence of the Redfield rate coefficients on the rhs. yields to oscillations that are damped faster during some times than others, and can even show partial revivals of coherent oscillations. Compare this with the monotonous damping in section 4.6.2.

- WARNING: The Redfield equation suffers from the same potential problems, discussed in section 4.3, as the Born-Markov master equation. It does not guarantee populations to remain positive. In the next section we will briefly review some Non-Markovian OQS methods that do not have this problem.

Week ⑩

PHY 435 / 635 Decoherence and Open Quantum Systems
Instructor: Sebastian Wüster, IISER Bhopal, 2021

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In the previous section we had seen that revival features of coherences (or Purity) can correctly be captured by non-Markovian methods, but not with Markovian ones. The Redfield method used there is conceptually simple to derive, but not very efficient for larger systems (the Refield tensor $R_{ab;cd}$ has N^4 components for N system basis states).

In the next section we thus list several advanced methods that can be used to tackle challenging non-Markovian open quantum problems. The purpose is merely to provide you with keywords for further reading when needed.

5.2 Methods for Non-Markovian Open Quantum System Dynamics

Further reading: "Dynamics of non-Markovian open quantum systems", I. de Vega and D. Alonso, Rev. Mod. Phys. **89** 015001 (2017).

5.2.1 Stochastic Schrödinger equations (Markovian + Non-Markovian)

A fairly basic problem that already arises for Markovian open quantum systems, is that even if we restrict ourselves to a small number M of basis states in the Hilbert-space, the density matrix $\hat{\rho}$ has $M \times M$ elements, compared to M elements in a quantum state $|\Psi\rangle$, which complicated numerical solutions. For intermediate system sizes, this problem can efficiently be overcome using the

Quantum Jump Monte Carlo Method
Consider the Lindblad Master equation (4.25). Instead of it, we evolve a Schrödinger equation with a *non-Hermitian* effective Hamiltonian $\hat{H}_{\text{eff}}$:

$$i\hbar\frac{d}{dt}|\Psi_{\mathcal{S}}\rangle = \hat{H}_{\text{eff}}|\Psi_{\mathcal{S}}\rangle \equiv \left(\hat{H}_{\mathcal{S}} - i\hbar\sum_{\mu}\hat{L}_{\mu}^{\dagger}\hat{L}_{\mu}\right)|\Psi_{\mathcal{S}}\rangle. \tag{5.20}$$

After one numerical time-step δt, the wavefunction will have norm $\langle\Psi_{\mathcal{S}}|\Psi_{\mathcal{S}}\rangle = 1-\sum_{\mu}\delta p_{\mu} < 1$, for very small δp_{μ}. The latter are given by $\delta p_{\mu} = \delta t\langle\Psi_{\mathcal{S}}|\hat{L}_{\mu}^{\dagger}\hat{L}_{\mu}|\Psi_{\mathcal{S}}\rangle$.

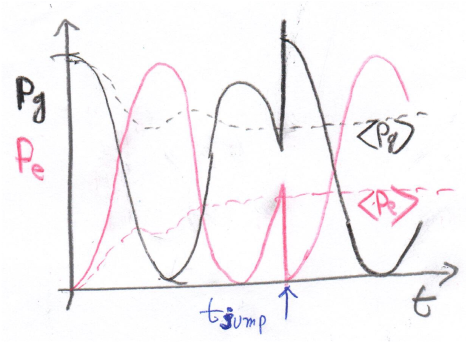
Using random numbers, we then perform a quantum jump with probability $p = \sum_\mu \delta p_\mu$, by projecting the wavefunction onto any of the states $\hat{L}_\mu | \Psi_{\mathcal{S}} \rangle$ with probability δp_μ, and then renormalizing the state to unity.
The density matrix in the end is obtained by averages over many realisations of this procedure, according to

$$\hat{\rho} = \overline{| \Psi_{\mathcal{S}} \rangle \langle \Psi_{\mathcal{S}} |}, \tag{5.21}$$

where $\overline{\cdots}$ is the stochastic average. Explicitly expanding the state in a basis $| \Psi_{\mathcal{S}} \rangle = \sum_n c_n(t) | n \rangle$, this implies density matrix elements $\rho_{nm} = \overline{c_n^*(t) c_m(t)}$.
See: K. Molmer, Y. Castin, and J. Dalibard, J. Opt. Soc. Am. B **10**, 524 (1993).

- The decohering effects of the environment enter here through the randomness of the jumps.
- Solving the evolution of the probability distributions underlying the density matrix through actual stochastic processes is called unravelling of the Master equation. Note that there may be multiple differing unravellings of any given Master equation.
- While they are mainly mathematical tricks, unravelling still also can give additional intuitive ideas of the physical origin of some decoherence phenomena, see below.

Example 38, Quantum Jump trajectories for driven two-level atom: left: Let us revisit example 32 on spontaneous decay of a two level atom (T=0). In that case there is only one Lindblad operator $\hat{L} = \sqrt{\gamma} | g \rangle \langle e |$ and then $\hat{L}^\dagger \hat{L} = \gamma | e \rangle \langle e |$.



The sketch on the left shows how the populations in the ground and excited state would look in a single trajectory (realisation) of quantum jump Monte Carlo (solid lines). The atom tries to undergo the usual Rabi oscillations, which are interrupted and reset at random moments t_{jump}. Averaging over many of those oscillations which are reset at random time causes a loss of all the oscillatory features (dotted lines are those averages). Compare dotted lines with RHS panels in example 32.

Tricksy use of classical random noise also allows efficient tackling of non-Markovian scenarios, such as in

Non-Markovian Quantum State Diffusion (NMQSD)
Here the system evolves according to the stochastic differential equation (SDE) ($\hbar = 1$, single μ)

$$\frac{d}{dt}|\,\Psi_{\mathcal{S}}\,\rangle = -i\hat{H}_{\mathcal{S}}|\,\Psi_{\mathcal{S}}\,\rangle + \hat{S}|\,\Psi_{\mathcal{S}}\,\rangle z(t) - \hat{S}^{\dagger}\int_0^t ds\;\, C(t,s)\hat{O}(t,s,z)ds|\,\Psi_{\mathcal{S}}\,\rangle. \tag{5.22}$$

Here $z(t)$ is a complex random process that has correlations $\overline{z^*(t)z(s)} = C(t,s)$, $\overline{z(t)s(t)}$, where $C(t,s)$ is the bath correlation function (4.16). $\hat{O}$ is an additional operator to be determined from some complicated procedure. See: L. Diósi, N. Gisin, and W. T. Strunz, Phys. Rev. A **58, 1699 (1998).**

- Non-Markovian effects can enter through the bath correlation function $C(t)$.
- As before, the density matrix is obtained through stochastic averaging.

5.2.2 Path Integral Methods

There are a couple of advanced methods based on Feynman's Path Integral (see advanced QM lectures), which we list here only in order for you to be able to place the abbreviations when you encounter them. See the review for references.

- Quasiadiabatic propagator path integral (QUAPI)
- Path integral Monte Carlo schemes (PIMC)
- Hierarchical Equation of Motion (HEOM)

5.3 Non-Markovian Dynamics and Information Flow

Further reading: "Colloquium: Non-Markovian dynamics in open quantum systems", H.-P. Breuer *et. al*, Rev. Mod. Phys. **88** 021002 (2016).

It turns out that information theoretic concepts can offer some interesting insight into Non-Markovian Dynamics. We have to first generalize the concepts of distinguishable states and overlap to density matrices.

Orthogonal density matrices Open quantum system "states" (density matrices) are called orthogonal, if their support is orthogonal. Diagonalizing the density matrix $\hat{\rho} = \sum_n p_n|\,n\,\rangle\langle\,n\,|$, the support is spanned by the vectors $\{|\,n\,\rangle, p_n \neq 0\}$, that is all eigenvectors with non-zero eigenvalue.

We introduce the

Trace distance of two density matrices $\hat{\rho}_1$, $\hat{\rho}_2$ as

$$D(\hat{\rho}_1, \hat{\rho}_2) \equiv \frac{1}{2}||\hat{\rho}_1 - \hat{\rho}_2||, \tag{5.23}$$

where we define the norm of an operator as $||\hat{O}|| = \mathrm{Tr}[\sqrt{\hat{O}^\dagger \hat{O}}](= \sum_j |o_j|)$. The expression as sum over mod-squares of eigenvalues o_j of $\hat{O}$ requires a Hermitian $\hat{O}$.

- One can show that $D(\hat{\rho}_1, \hat{\rho}_2) = 0$ iff $\hat{\rho}_1 = \hat{\rho}_2$ and $D(\hat{\rho}_1, \hat{\rho}_2) = 1$ iff $\hat{\rho}_1$ and $\hat{\rho}_2$ are orthogonal. In this sense the trace distance is a measure of the distinguishability of two density matrices.

Returning to the concept of reduced system evolution as a dynamical map (4.2), where $\hat{\rho}_{\mathcal{S}}(t) = \hat{V}(t,0)[\hat{\rho}_{\mathcal{S}}(0)]$ (we introduced the extra label 0, indicating time propagation from $t = 0$ to t), one can see that in the Markovian case we have

Divisible maps: For times $t > s > 0$, we have

$$\hat{\rho}_{\mathcal{S}}(t) = \hat{V}(t,0)[\hat{\rho}_{\mathcal{S}}(0)] = \hat{V}(t,s)[\hat{V}(s,0)[\hat{\rho}_{\mathcal{S}}(0)]]. \tag{5.24}$$

The dynamical map $\hat{V}(t,0)$ is then called divisible.

One (=mathematicians) can further show that under a trace preserving positive map[9], the trace distance between any two density matrices can only be reduced. This implies

$$D(\hat{\rho}_1(t), \hat{\rho}_2(t)) \leq D(\hat{\rho}_1(0), \hat{\rho}_2(0)) \tag{5.25}$$

for Markovian evolution (where $\hat{\rho}_1(t) = \hat{V}(t,0)[(\hat{\rho}_1(0)]$ etc.).

We now interpret the distinguishability (and hence the trace distance) of two density matrices as the level of information content of the system. Since D must decrease for Markovian evolution, information always flows one way from the system to the environment in that case. In contrast, in the non-Markovian case it can also flow back into the system.

These concepts than allow the definition of a "measure" of non-Markovianity, that can *quantify* to what degree a system is non-Markovian. One defines the

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[9] This means any physically reasonable map.

Measure for the "Non-Markovianity" of the time evolution of some open quantum systems:

$$\mathcal{NM} = \max_{\rho_{\mathcal{S}(1,2)}} \left[\int_{\sigma>0} dt\, \sigma(t) \right], \tag{5.26}$$

where $\sigma(t) = \frac{d}{dt} D(\hat{\rho}_1(t), \hat{\rho}_2(t))$.

- In words the above definition implies this algorithm: (i) Start with all possible pairs of density matrices $\hat{\rho}_1(0)$, $\hat{\rho}_2(0)$ in the system. Evolve these in time (or measure their time evolution), and determine the time evolution of the trace distance. (iii) Only for those time intervals where it is increasing we integrate this up. (iv) The measure $\mathcal{NM}$ is finally the maximal result for all initial states.
- Since we typically cannot really maximise over all possible pairs of initial states, just maximising over many pairs should already give us a solid lower bound.
- Different measures for this also exist in the literature.

6 Applications of Decoherence

For those interested I recommend reading chapters 6,7 of SD, "decoherence in action" and "decoherence and quantum computing" as a "reward" for the effort put into following this lecture. These contain interesting descriptions of real world experiments and technologies where the concepts learnt are absolutely crucial.

Week ⑪

PHY 435 / 635 Decoherence and Open Quantum Systems
Instructor: Sebastian Wüster, IISER Bhopal, 2021

These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

7 Extensions of Quantum Mechanics

We had seen since section 3.2, that the theory of decoherence in the framework of open quantum system does help a lot in addressing the "measurement problems" discussed in section 3.2. Note that everything we covered was strictly in the framework the usual quantum mechanics. We had also already stated that decoherence theory does *not* really offer a solution to the dissatisfactory need to *postulate* the collapse of the wave function and hence the existence of definite outcomes of measurements in quantum theory [measurement problem III, problem of outcomes].

We now briefly mention a few speculative[10] ideas in which the collapse problem is addressed *within the mathematical framework*. This means that the proposals actually attempt to change the laws of quantum mechanics, rather than just their interpretation. These changes are tightly constrained, since they must not contradict the multitude of successful and accurate verifications of quantum mechanics.

7.1 Physical collapse models

The final result of the von Neumann measurement in the presence of decoherence was $\hat{\rho}_S(t_f) = \sum_n |c_n|^2 |\, s_n \rangle |\, a_n \rangle \langle\, s_n \,| \langle\, a_n \,|$, see Eq. (3.41) and Eq. (3.21). Recall that chosen basis $\langle\, a_n \,|$ had to be the pointer basis of the apparatus in the presence of the environment.

Collapse models try to augment the measurement process, by changing the time evolution of $\hat{\rho}_S$ (or $|\, \Psi \,\rangle$), such that the final state is actually only $\hat{\rho}_S(t_f) = |\, s_k \,\rangle |\, a_k \,\rangle \langle\, s_k \,| \langle\, a_k \,|$, for one specific k. However the k has to be random such that it occurs with probability $|c_k|^2$ (defined by the initial state). To this end, different theories modify the Schrödinger equation by (i) random noise terms, turning it into a stochastic differential equation (SDE), (ii) non-linear terms[11] or the occasional random projection onto more localised wavefunctions. The latter process is sketched in the figure below.

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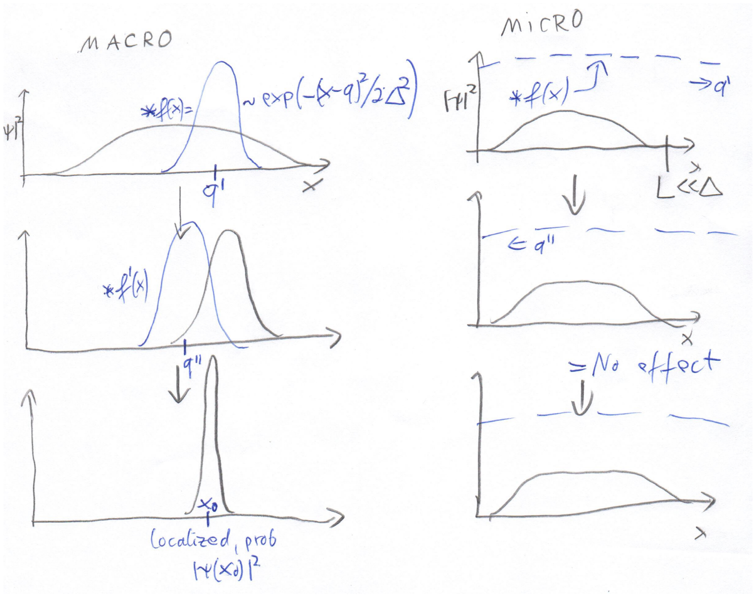
[10] This means that to our knowledge there were no experiments that support these ideas compared to others.

[11] Note that the entire von-Neumann measurement chain relies on the *linearity* of the SE, so non-linearities are a logical way out.



left: continuous spontaneous localisation Sketch of wave function evolution in the continous spontanous localisation model. Spatially delocalized states on scales $x \ll \Delta$ (microscopic ones) are not much affected so that the usual QM works there. Macroscopically delocalized wavefunctions will localize dynamically in this way.

One motivation for interference experiments with larger and larger molecules (^{60}C, Biomolecules) such as mentioned in section 3.2.3, is to verify or exclude such collapse models. It turns out that this is very hard, since the special predictions of these are very similar to the effects of decoherence. So the interfering buckyball has to be exceptionally well shielded form decoherence (possible in principle but hard in practice) to see the effect of spontaneous localisation (which would be un-avoidable if it exists).

For example a master equation can also be derived for continuous spontaneous localisation, and then annoyingly has the same form as Eq. (4.57), with a term $\frac{d}{dt}\rho(x,x') \sim -\Lambda(x-x')^2\rho(x,x')$ that destroys spatial coherences. The advantage of collapse models though, is that in the end the sytem really is only in one location, not in a superposition state.

Further reading: "Dynamical reduction models", A. Bassia and G. Ghirardi, Phys. Rep. **379** 257 (2003).

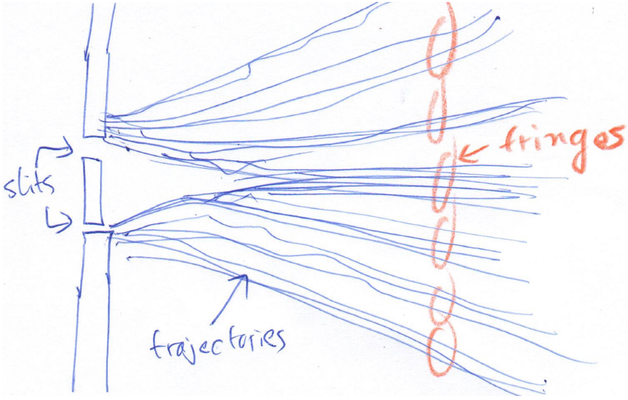
7.2 Bohmian Mechanics

Bohmian mechanics attempts to re-establish the concept of particles at specific positions and momenta, that we had to abandon to construct quantum mechanics. To reconcile the two, the positions of these particles are guided by their matter wave. We assume the position of the particle is $\mathbf{q}$. It will then move according to

$$\frac{d\mathbf{q}}{dt} = \mathbf{v} = \frac{1}{m}\mathrm{Im}\left(\frac{\Psi^*\boldsymbol{\nabla}\Psi}{|\Psi|^2}\right)(\mathbf{q}), \tag{7.1}$$

where Ψ is the usual wave function that obeys Schrödinger's equation. The construction makes sure that experimental observations regarding the probabilities of particle positions would be consistent with the usual quantum mechanics. Compare (7.1) with the hydro-dynamics formulation of quantum mechanics (density, velocity).

The difference to the usual interpretation is, that the particle initially *does have* a fixed position $\mathbf{q}(t=0)$, which is however unknown. We could use an equation such as Eq. (7.1) for particles with lots of different random initial positions passing through a double slit, and draw their tracks. This is shown below:



left: Double slit interference in Bohmian Mechanics For a large number of initial conditions, we realize the usual double slit inteference pattern as regions with many ending trajectories (orange). Following an individual trajectory shows some irritating non-Newtonian behavior. See also SD for better picture.

- Particle physics / relativistic quantum mechanics actually requires the concept of quantum fields rather than particles. Quantum fields are a more advanced version of a wave function. The requirements arise from elementary conditions such as causality and Lorentz invariance. For these reasons a forced return to the particle concept as above is not very popular.
- Since Bohmian Mechanics reproduces quantum mechanics through the assumption of precise but unknown initial particle positions, it is an example of a *hidden variable theory.* These attribute all the randomness of quantum mechanics to unknown variables (i.e. we simply don't know the real, deterministic, theory yet).

7.3 Many Worlds theory

We can continue the von-Neumann chain, by including ourselves as the observer into the superposition:

$$|\,\psi\,\rangle \otimes |\,a_r\,\rangle \otimes |\,b_r\,\rangle = \left(\sum_n c_n |\,s_n\,\rangle\right) \otimes |\,a_r\,\rangle |\,b_r\,\rangle \to \sum_n c_n \big(|\,s_n\,\rangle \otimes |\,a_n\,\rangle |\,b_n\,\rangle\big), \tag{7.2}$$

Here $|\,b_r\,\rangle$ denotes the state of your brain when you are ready to do the experiment and $|\,b_n\,\rangle$ that after you have seen that the apparatus has indicated $|\,a_n\,\rangle$.

The many worlds theory tries to embrace that simply all components of the superposition in fact happen, only since we are part of one branch we cannot experience the other branches. Essentially, whenever any quantum evolution takes place, the universe splits up into further universes (multiverse). Each possible result of a measurement would happen in some of them.

- It is clear from the discussion that this has now more to do with philosophy than physics. I leave it up to you which viewpoint (e.g. many worlds or problem of outcomes) you find more irritating. Since we can per definition not make experiments in another universe, the idea is also difficult to disprove.

- As an intermediate step, some of the early researchers on quantum theory had speculated that it is our consciousness $|\, b_n \,\rangle$, which ultimately collapses the superposition.

The End