Week ①

PHY 435 / 635 Decoherence and Open Quantum Systems
Instructor: Sebastian Wüster, IISER Bhopal, 2018

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 "*
- Breuer and Petruccione, *"The theory of open quantum systems "*

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.

(iii) Assessment:

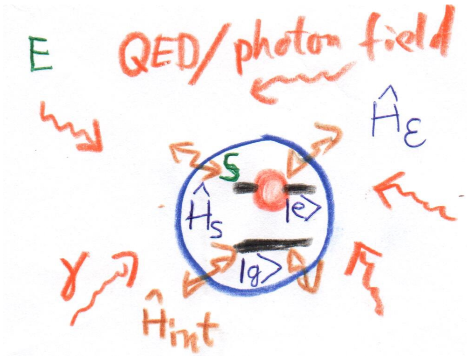
- **Three scheduled Quizzes with examineer: 15%** To supplement the exams, there will be three quizzes lasting one lecture hour, conducted using the examineer webpage . These are "open notes" quizzes, so bring a copy of your notes. Quizzes will be simpler than exams, intended to encourage you to continuously keep on top of the material. **Make sure to bring an internet capable phone/tablet/laptop on the days of the quizz. Please contact me if there is a problem with this. You also need some pen and paper for scrap notes on quiz days.**
  - Quiz 1: Thu 23rd August (in lecture)
  - Quiz 2: Tue 11th September
  - Quiz 3: Thu 1st November

- **Flipped classroom / Assignments: 10%** There will be about five 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. Additionally however the TA is asked to deduct marks for messy presentation and blatant copying.
- **Flipped classroom participation: 5%** In the middle of the two week assignment period we will make one ”flipped class”: I will record the lecture as video provided online and expect you to watch it in your usual ”homework time”. Instead of that lecture we will spend the time with you working with your team on the assignment/ asking questions/ reviewing material. Participation in this class will be taken.
- **Mid-Sem exam: 30%**
- **Final exam: 40%** The exams 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*.

1 Motivation and Review

1.1 What is an open quantum system?

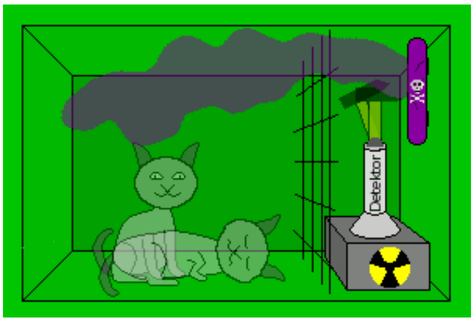
- Split the world into a ”system” of interest S and an environment E.
- Fundamentally, both ought to be described quantum mechanically.
- Frequently we have a system that is simple/ describable, but an environment that is too large to treat quantum mechanically (see section 2), and that we don’t even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

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

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

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

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[1] fortunately, for the cat.

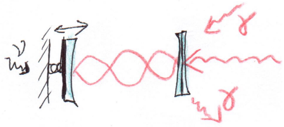
1.2 Most quantum systems are open

quantum technologies

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

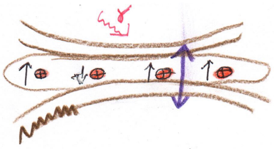
Opto-mechanics

- cavity with oscillating mirror
- Phonon and photon leakage



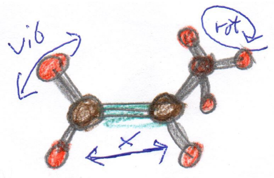
Quantum computers/
Quantum information

- 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.

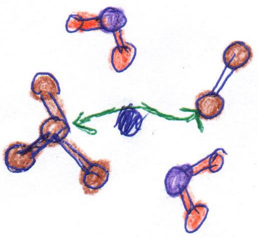
- Conceptually, we can make an open system closed by including the environment. "Openness" depends on the *choice* of S and E. The choice is however usually well motivated and constrainted by practicalities or interest.

Really closed systems:

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

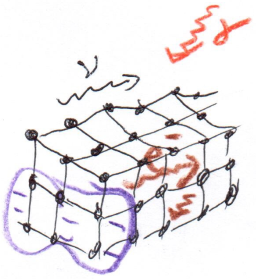
Quantum chemistry

- Chemical reactions
- Solvent influence



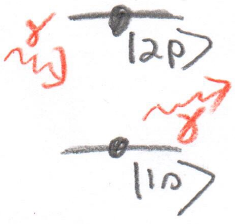
Material science

- Quasi-particle damping
- Dissipation



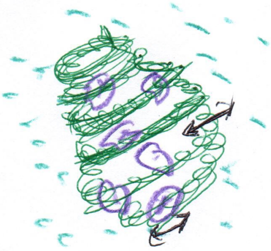
Atomic physics

- Spont. decay
- QED vacuum



(Quantum-?)-biology

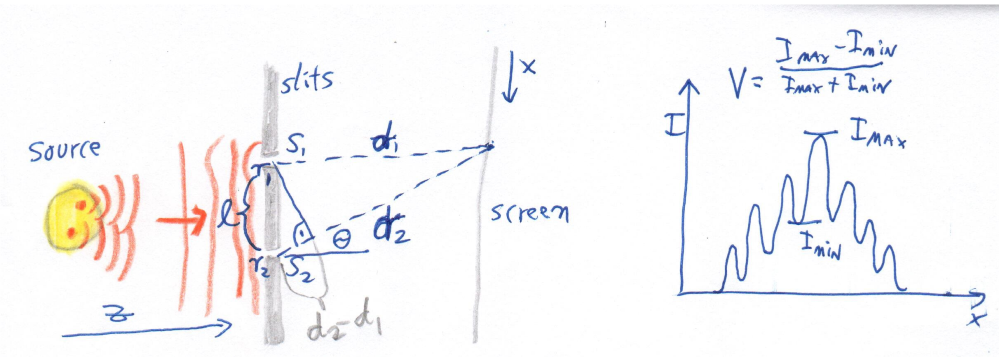
- Mag-field sensing
- Sense of smell
- Photosynthesis?



1.3 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 $\{\exp\left[i(\omega_n t - k_n x + \varphi_n)\right]\}$ is termed coherent if it will show spatial or temporal interference patterns after averaging over the ensemble.
- 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

$$E(\mathbf{x}, t) = E_1(\mathbf{x}, t) + E_2(\mathbf{x}, t), \text{ with}$$

$$E_n(\mathbf{x}, t) = E\left(\mathbf{r}_n, t - \frac{d_n}{c}\right) \frac{1}{d_n} e^{i(k - \frac{\omega}{c}) d_n} \tag{1.2}$$

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.

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

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

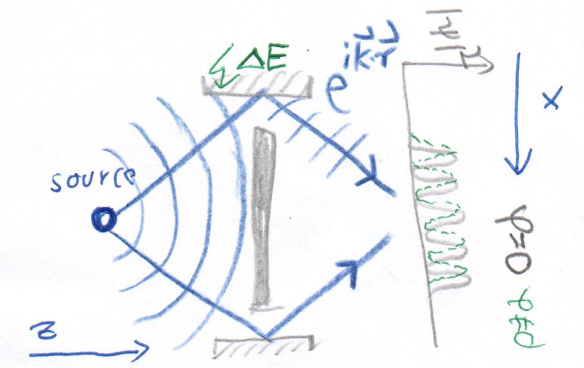
which enters the last line in (1.4) and thus the fringe visibility V. It measures to what extent the electric field at position $\mathbf{r}_1$ and time t_1 will have on average the same phase as that at position $\mathbf{r}_2$ and time t_2

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.

1.3.1 Quantum coherence

- Also in quantum mechanics, coherence controls the degree of visibility of interference effects.
- As we shall see, the concept of quantum coherence crucially involves a large environment. Interferences we like to measure in a quantum system, then are affected by 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.

Example: 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 (mo-

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

mentum 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 $\varphi = -\Delta E T/(2\hbar)$. 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.

1.4 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):

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

(2) 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:

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

(3) 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).

(4) The quantum state obeys the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\,\Psi(t)\,\rangle = \hat{H}|\,\Psi(t)\,\rangle, \tag{1.8}$$

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 (3) is fundamentally unsatisfactory (we see later why, in section 3.2.2).

1.5.2 Single particle quantum mechanics

To study open quantum systems, a recurring approach is to consider a system based on a single object (particle), with environment composed of many. We want to frequently describe a single particle in a basis made of eigenstates of the

Time-independent Schrödinger equation(TISE)

$$\hat{H}_0|\varphi_n\rangle = E_n|\varphi_n\rangle. \tag{1.9}$$

- 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
- E_n are single particle energies

Examples:
(i) Free particles in Volume V

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} = -\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m}, \qquad E_n = \frac{\hbar^2 \mathbf{k}^2}{2m} = \frac{\mathbf{p}^2}{2m}, \tag{1.10}$$

$$|\,\varphi_n\,\rangle \rightsquigarrow |\phi_k\rangle \;=\; \frac{1}{\sqrt{\mathcal{V}}} e^{i\mathbf{kx}}. \tag{1.11}$$

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

$$\hat{\mathbf{S}}^2 |\,\chi_{s,m_s}\,\rangle = \hbar^2 s(s+1) |\,\chi_{s,m_s}\,\rangle, \tag{1.12}$$

$$\hat{S}_z |\,\chi_{s,m_s}\,\rangle = \hbar m_s |\,\chi_{s,m_s}\,\rangle, \quad m_s = -s \cdots s. \tag{1.13}$$

$$\tag{1.14}$$

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

$$|\,\varphi_n\,\rangle \rightsquigarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix} \cong |\uparrow\rangle = |\,\chi_{\frac{1}{2},+\frac{1}{2}}\,\rangle \text{ or } \begin{bmatrix} 0 \\ 1 \end{bmatrix} \cong |\downarrow\rangle = |\,\chi_{\frac{1}{2},-\frac{1}{2}}\,\rangle. \tag{1.15}$$

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

$$\mathbb{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{1.16}$$

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).

$$\hat{H}_0 = \Delta E \;\; \hat{\sigma}_3, \qquad E_{\uparrow\downarrow} = \pm\Delta E, \tag{1.17}$$

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

(iii) Simple Harmonic oscillator. Hamiltonian:

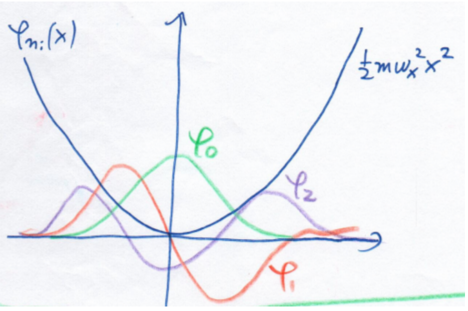
$$H_0 = \frac{\mathbf{p^2}}{2m} + \frac{1}{2} m\omega^2 x^2. \tag{1.18}$$

Examples cont.:

Spatial wave function /States:

$$\varphi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}\sigma}} e^{-\frac{x^2}{2\sigma^2}} H_n\left(\frac{x}{\sigma}\right), \tag{1.19}$$

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



left: Sketch of first few oscillator wave-functions.

Raising and lowering operators We define,

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

$$\hat{b}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - i\sqrt{\frac{1}{2m\omega\hbar}}\hat{p} \tag{1.20}$$

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 (1.18) using raising and lowering operators as

$$\hat{H}_0 = \hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right) \tag{1.21}$$

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

Function of raising and lowering Operators

$$\hat{b}|\varphi_n\rangle = \sqrt{n}|\varphi_{n-1}\rangle \qquad \hat{b}|\varphi_0\rangle = 0 \tag{1.22}$$

$$\hat{b}^\dagger|\varphi_n\rangle = \sqrt{n+1}|\varphi_{n+1}\rangle \tag{1.23}$$

- 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 (1.19).

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

$$\hat{N}|\,n\,\rangle = n|\,n\,\rangle \tag{1.24}$$

The states (1.19) 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

$$\hat{D}(\alpha)|\,0\,\rangle = e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}. \tag{1.25}$$

We can then derive the explicit number state representation:

$$|\,\alpha\,\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |\,n\,\rangle. \tag{1.26}$$

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 $|\,\varphi_0\,\rangle$.

1.5.3 Many-particle quantum mechanics

When including the environment, most of the examples in section 1.2 are many-body systems.

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

$$q = \{\mathbf{r}, m_s, \cdots\}. \tag{1.27}$$

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.

An exemplary Hamiltonian for two equal mass particles that interact (with interaction potential U) would be written as

$$\hat{H} = -\frac{\hbar^2}{2m}(\nabla^2_{\mathbf{r}_1} + \nabla^2_{\mathbf{r}_2}) + V(\mathbf{r}_1) + V(\mathbf{r}_2) + U(\mathbf{r}_1, \mathbf{r}_2). \tag{1.28}$$

Self-exercise: Write a many-body state example for three spin-1/2 particles. Or for five harmonic oscillators.

As for single particle states we will use $\phi_k(\mathbf{x}_1, \mathbf{x}_2)$ to denote specific many-body *eigenstates* (typically of the Hamiltonian). We use $\Psi(\mathbf{x}_1, \mathbf{x}_2)$ for a general state, which can always be expanded as $\Psi(\mathbf{x}_1, \mathbf{x}_2) = \sum_k c_k \phi_k(\mathbf{x}_1, \mathbf{x}_2)$ in eigenfunctions of a Hermitian operator.

1.5.4 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 statesA many body state is called separable, if it can be written as a product of states for each particle

$$\Psi_{sep}\left(\mathbf{x_1},\mathbf{x_2},\cdots,\mathbf{x_n}\right)=\prod_{i=1}^{N}\phi_{n_i}\left(\mathbf{x}_i\right) \tag{1.29}$$

All states that are not separable are called entangled.

Examples:
Separable:

$$|\Psi\rangle=|\uparrow\uparrow\rangle=|\uparrow\rangle\otimes|\uparrow\rangle \tag{1.30}$$

$$|\Psi\rangle=\frac{1}{2}\left(|\uparrow\rangle+|\downarrow\rangle\right)\otimes\left(|\uparrow\rangle+|\downarrow\rangle\right)=\frac{1}{2}\left(|\uparrow\uparrow\rangle+|\downarrow\downarrow\rangle+|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle\right) \tag{1.31}$$

$$\Psi\left(x_1,x_2\right)=\frac{1}{\sqrt{\mathcal{V}}}\exp\left[ik_1x_1\right]\mathcal{N}\exp\left[-x_2^2/(2\sigma^2)\right]. \tag{1.32}$$

Entangled :

$$|\Psi\rangle=\frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle+|\downarrow\downarrow\rangle\right) \tag{1.33}$$

$$\Psi\left(x_1,x_2\right)=\mathcal{N}\exp\left[-\frac{\left(x_1-x_2\right)^2}{2\sigma_\perp^2}-\frac{\left(x_1+x_2\right)^2}{2\sigma_\parallel^2}\right] \tag{1.34}$$

Tensor product: We used the notation $|\uparrow\rangle\otimes|\uparrow\rangle$, where $\otimes$ denotes a tensor product.

1.5.5 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. (1.8), 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 $c(t)=c(0)e^{-iE_nt/\hbar}$. We can also define the time evolution operator

$$\hat{U}(t)=\exp\left[-i\hat{H}t/\hbar\right], \tag{1.35}$$

and use it to write $|\,\Psi(t)\,\rangle=\hat{U}(t)|\,\Psi(0)\,\rangle$. The simple expression (1.36) is valid for *time-independent* Hamiltonians only. Otherwise we need to use

$$\hat{U}(t)=\mathcal{T}\left\{\exp\left[-i\int_0^t\hat{H}(t')dt'/\hbar\right]\right\}, \tag{1.36}$$

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

$$\bar{O}(t) = \langle\, \Psi(t)\, |\hat{O}|\, \Psi(t)\,\rangle = \langle\, \Psi(0)\, |\hat{U}^\dagger(t)\hat{O}\hat{U}(t)|\, \Psi(0)\,\rangle = \langle\, \Psi(0)\, |\hat{O}(t)|\, \Psi(0)\,\rangle. \tag{1.37}$$

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 $|\,\Psi_I(t)\,\rangle = \hat{U}_I(t)|\,\Psi\,\rangle$ with

$$\hat{U}_I(t) = \exp{[-i\hat{H}_0 t/\hbar]}. \tag{1.38}$$

The subscript I denote interaction picture quantity, states and operators without I are in the Schrödinger picture. Operators are defined as

$$\bar{O}_I(t) = \hat{U}_I^\dagger(t)\hat{O}_S\hat{U}_I(t) \tag{1.39}$$

We can then show the evolution equations

$$i\hbar\frac{\partial}{\partial t}|\,\Psi_I(t)\,\rangle = \hat{V}_I|\,\Psi_I(t)\,\rangle, \tag{1.40}$$

$$i\hbar\frac{\partial}{\partial t}\hat{O}_I(t) = \left[\hat{O}_I, \hat{H}_0\right], \tag{1.41}$$

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.

1.5.6 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

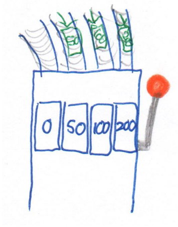
$$p(x_1, t_1; x_2, t_2, x_3, t_3, \cdots) \tag{1.42}$$

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

$$p(x_1, t_1; x_2, t_2, x_3, t_3, \cdots | y_1, \tau_1; y_2, \tau_2, y_3, \tau_3) \equiv \frac{p(x_1, t_1; x_2, t_2, x_3, t_3, \cdots, y_1, \tau_1; y_2, \tau_2, y_3, \tau_3)}{p(y_1, \tau_1; y_2, \tau_2, y_3, \tau_3)} \quad (1.43)$$

to have recorded that sequence given already earlier having recorded values y_1, y_2, y_3, $\cdots$ at times $\tau_1 > \tau_2 > \tau_3 > \cdots$.

Example I: Money gained from an infinite slot machine:



left: Suppose when pulling the level 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. (1.43) we can define a

Markov processas a stochastic process for which

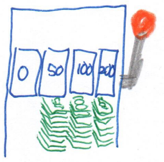
$$p(x_1, t_2; x_2, t_2, x_3, t_3, \cdots | y_1, \tau_1; y_2, \tau_2, y_3, \tau_3) = p(x_1, t_2; x_2, t_2, x_3, t_3, \cdots | y_1, \tau_1) \quad (1.44)$$

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 happens during $n = 1, \cdots, 9$ is irrelevant.

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

$$\Psi(x, t=0) = \frac{1}{\left(\sqrt{\pi}\sigma_0\right)^{1/2}} \exp\left[-\frac{x^2}{2\sigma_0^2}\right], \tag{1.45}$$

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:

$$|\Psi(x,t)|^2 = \frac{1}{\sqrt{\pi}\sigma(t)} \exp\left[-\frac{x^2}{\sigma(t)^2}\right], \tag{1.46}$$

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!.