Week ②

PHY 435 / 635 Decoherence and Open Quantum Systems
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2 System environment models

In this section we list mathematical system-environment models that could describe most of the examples in section 1.2. 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 <u>continuous</u> or a <u>discrete</u> 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 <u>four</u> 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.
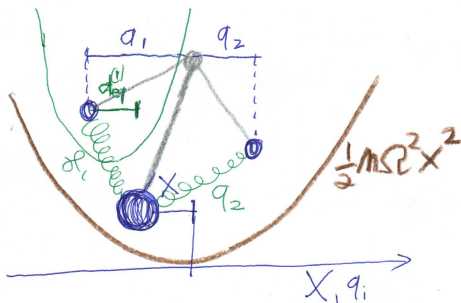
left: Consider a central (heavy) harmonic oscillator as the system, that is weakly coupled to a pool of other (light) oscillators, as shown in this figure. We schematically also show the presence of couplings, please refer to equations for the actual details.

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

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

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

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 (1.20), 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 (1.20) 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.

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.
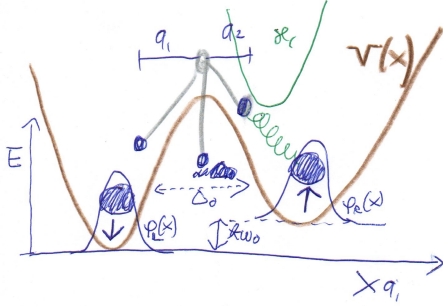
left: Damped double well system realization of the spin-boson model. The system particle (blue ball) couples to the environment oscillators (grey rods) as in section 2.1. However it now feels a different potential $V(x)$. We consider energies where it can only reside in the left well, with wavefunction $\varphi_L(x)$, 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 (1.16) 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.
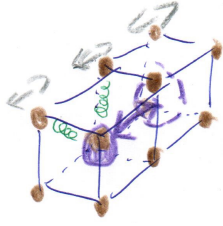
left: A physical system that realizes the above is a defect atom (violet) tunnelling in a solid crystal (brown), with crystal-phonons (green) as bath of oscillators.

> **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 $\Delta_0 = 0$, when the Hamiltonian Eq. (2.12) <u>does not include dissipation</u>. 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 (1.15) and (1.24). Thus $|\Psi(t)\rangle = \sum_{s,n} c_{sn}|sn\rangle$. 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 $|\uparrow\rangle$?", "$\cdots|\downarrow\rangle$?.

Numerical solution of single-spin, single-boson model: Consider an initial-state $|\Psi(0)\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \otimes |0\rangle$. We can guess the evolution directly from (2.7)-(2.7):
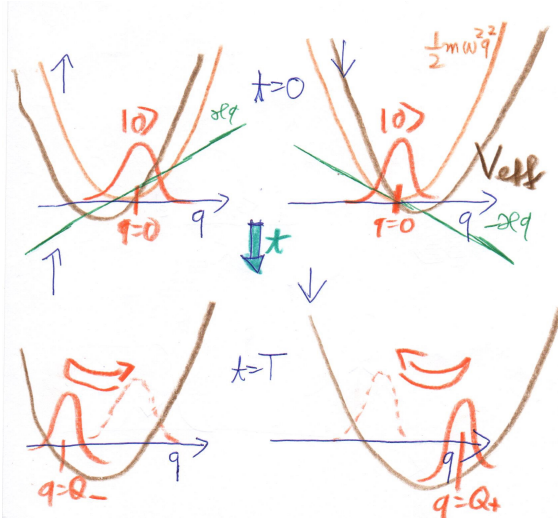
left: For spin in state $|\uparrow\rangle$ we have $\langle\uparrow|\hat{H}_{\text{int}}|\uparrow\rangle = \kappa\hat{q}$, while $\langle\downarrow|\hat{H}_{\text{int}}|\downarrow\rangle = -\kappa\hat{q}$. In either case the single oscillator feels a <u>shifted</u> harmonic potential $V_{\text{eff}} = \frac{1}{2}m\omega q^2 \pm \kappa q$ as shown in the figure. However the <u>shift direction depends on the spin</u>. 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 <u>depends on the state of the spin</u>.

- 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 "turning point" T shown in the figure the overall state is

$$|\Psi(T)\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |\alpha_{Q-}\rangle + |\downarrow\rangle \otimes |\alpha_{Q+}\rangle). \tag{2.13}$$

- 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).

- The creation of an entangled state (2.13) 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 <u>entangling</u> quantum evolution discussed above. We will refer to the evolution by

$$\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \otimes |0\rangle \rightarrow \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |\alpha_{Q-}\rangle + |\downarrow\rangle \otimes |\alpha_{Q+}\rangle), \tag{2.14}$$

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

- See assignment 1 for many more details.

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

$$\hat{\mathbf{A}}(\mathbf{x},t) = \sum_{n,\nu} \sqrt{\frac{\hbar}{2\epsilon_0 \omega_n \mathcal{V}}} \mathbf{e}_{n\nu} \left(e^{i(\mathbf{k}_n \mathbf{x} - \omega_n t)} \hat{a}_{n\nu} + e^{-i(\mathbf{k}_n \mathbf{x} - \omega_n t)} \hat{a}_{n\nu}^\dagger \right). \tag{2.15}$$

QED continued: 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 $\hat{a}_{n\nu}$, $\hat{a}_{n\nu}^\dagger$ 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 $|g\rangle \to |\downarrow\rangle$ and some excited state $|e\rangle \to |\uparrow\rangle$. 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

$$\mathbf{d}_{eg} = \langle e | \hat{\mathbf{A}}(\mathbf{x},t) \cdot \boldsymbol{\nabla} | g \rangle. \tag{2.16}$$

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 (2.15) as:

$$\hat{H}_S = \frac{\hbar \omega_{eg}}{2} \hat{\sigma}_z, \tag{2.17}$$

$$\hat{H}_{\mathcal{E}} = \sum_{n\nu} \hbar \omega_n \hat{a}_{n\nu}^\dagger \hat{a}_{n\nu}, \tag{2.18}$$

$$\hat{H}_{\text{int}} = \hbar \sum_{n\nu} \left(g_{n\nu} \hat{a}_{n\nu} \hat{\sigma}_+ + g_{n\nu}^* \hat{a}_{n\nu}^\dagger \hat{\sigma}_- \right), \tag{2.19}$$

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 $\hat{\sigma}_+ = \hat{\sigma}_x + i\hat{\sigma}_y = |\uparrow\rangle\langle\downarrow|$, $\hat{\sigma}_- = \hat{\sigma}_x - i\hat{\sigma}_y = |\downarrow\rangle\langle\uparrow|$.

- 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 (2.17)-(2.19) 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.
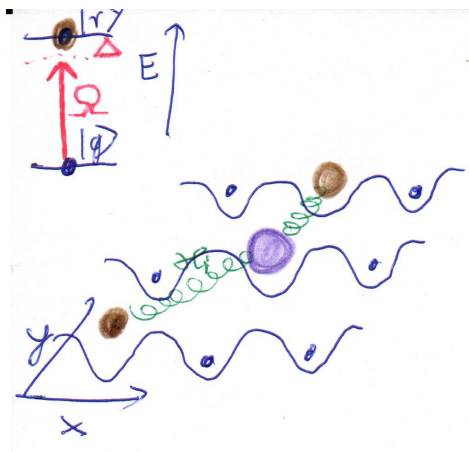
left: Spin-spin environment model realized by an array of optically trapped Rydberg atoms. Each atom is trapped on a single 2D lattice site, so position dynamics is fully suppressed. Atoms can be in a ground state $|g\rangle$ or Rydberg state $|r\rangle$. Under certain conditions (see PHY402) a laser 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 with: $\hat{V} = \kappa_{nm}[|r\rangle\langle r|]^{(n)} \otimes [|r\rangle\langle r|]^{(m)}$ (operator $[\cdots]^{(n)}$ acts on atom n only.).

In such a case we can write a

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

$$\hat{H}_S = \frac{1}{2}\omega_0\hat{\Sigma}_z - \frac{1}{2}\Delta_0\hat{\Sigma}_x, \tag{2.20}$$

$$\hat{H}_{\mathcal{E}} = \sum_i^N \frac{1}{2}\omega_i\hat{\sigma}_z^{(i)} - \frac{1}{2}\Delta_i\hat{\sigma}_x^{(i)}, \tag{2.21}$$

$$\hat{H}_{\text{int}} = \hat{\Sigma}_z \otimes \sum_i \kappa_i\hat{\sigma}_z^{(i)}. \tag{2.22}$$

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 (2.20)-(2.22): exercise! (Identify: $|\downarrow\rangle \leftrightarrow |g\rangle$, $|\uparrow\rangle \leftrightarrow |r\rangle$.

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.
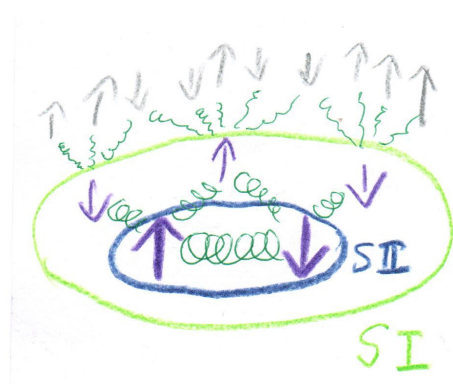
left: In the left figure of many coupled spins (violet and gray), the size of green twiddles indicates the strengths of mutual couplings. In this case it may be not fully clear if we should choose our system as just the two inner spins (S-II), or maybe all violet spins (S-I). This illustrates a certain 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 formalisms 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 initisl classification of the open-system and thus methods to be used for them may differ depending on whether choice I or II is made.