Lindblad Master equation
and the Quantum Brachistochrone

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Outline

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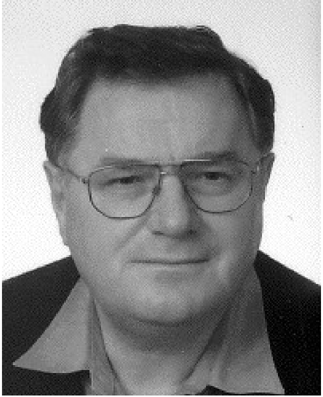
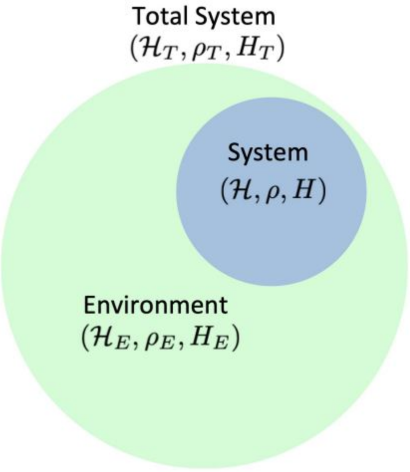
Göran Lindblad †



(1940-2022)

How to extract the system dynamics?



Lev Landau

- Already in 1927 Landau formulated the concept of density matrix for the first time (defined in more formal way by von Neumann the same year)
- Landau derived the kinetic equation for the elements of the density matrix of the radiation field interacting with charged matter (in the dipole approximation)

$$\dot{\rho} = \frac{1}{2}\gamma(2a\rho a^\dagger - \rho a^\dagger a - a^\dagger a\rho). \tag{1}$$

$a, a^\dagger$ - annihilation/creation operators for radiation field, γ - damping constant (> 0).

Lamb equation

- Lamb considered the unnormalized density matrix of a two level atom

$$\dot{\rho} = -i[H, \rho] - \frac{1}{2}(\Gamma\rho - \rho\Gamma), \quad (2)$$

where Γ - diagonal matrix with positive entries corresponding to the decay constants of the states of the atom.

- This equation generates the proper evolution, but is not trace preserving

$$\rho_t = e^{(-iH - \frac{1}{2}\Gamma)t}\rho_0 e^{(iH - \frac{1}{2}\Gamma)t}. \quad (3)$$

Redfield equation

- Redfield derived the following master equation

$$\dot{\rho} = -i[H, \rho] - \sum_{\alpha} [V_\alpha, X_\alpha \rho - \rho X_\alpha^\dagger], \tag{4}$$

  where the operators V_k are defined via the system–bath interaction Hamiltonian in the interaction picture, and X_α depends on the correlation function between the system and the bath.
- Preserves trace, but the positivity of ρ_t is not guaranteed.
- From this equation we can proceed to the final Lindblad Master equation.

Birth of the GKLS equation

- Two independent groups worked on developing a master equation for open quantum systems: Vittorio Gorini, Andrzej Kossakowski and George Sudarshan (GKS), and Göran Lindblad.
- At the end of 1974 Lindblad participated in the Symposium on Mathematical Physics, organized in Torun by Roman Ingarden — Kossakowski's PhD supervisor. Ingarden mentioned that he has seen similar results.
- A month after that Gorini visited Lindblad to compare their results to find they are in fact vastly similar.

GKS group

Figure: From left to right: Roman Ingarden, Andrzej Kossakowski, George Sudarshan and Vittorio Gorini.

Preliminary Problem

Consider the evolution of an isolated two-level system described by the Hamiltonian

$$H = E_0 |0\rangle \langle 0| + E_1 |1\rangle \langle 1| . \tag{5}$$

Since the states $|0\rangle$ and $|1\rangle$ are eigenstates of the Hamiltonian, if at $t = 0$ the system is at the excited state $|\psi(0)\rangle = |1\rangle$, after a time t the state would become

$$|\psi(t)\rangle = e^{-iHt} |1\rangle = e^{-iE_1 t} |1\rangle , \tag{6}$$

gaining only phase during the evolution, without changing its physical properties.

Problem

If an excited state does not change, why do atoms decay?

The Fock-Liouville space

The goal is to construct a Hilbert space of density operators. Thanks to that we can effectively convert the density matrices into vectors ($\rho \rightarrow |\rho\rangle$), e.g.

$$|\rho\rangle = \begin{pmatrix}\rho_{00} & \rho_{01} & \rho_{10} & \rho_{11}\end{pmatrix}^T . \tag{7}$$

The scalar product is usually defined as $\langle\phi|\rho\rangle = Tr[\phi^\dagger \rho]$. We also define the *Liouvillian superoperator* $\tilde{\mathcal{L}}$, which can then be expressed in a matrix form. Thanks to that, the evolution equation can be written is a concise way

$$\frac{d\,|\rho\rangle}{dt} = \tilde{\mathcal{L}}\,|\rho\rangle . \tag{8}$$

Positivity of maps

To find a map that would describe the evolution of the density operator $\rho \in \rho(\mathcal{H})$, we impose certain conditions:

- We are looking for a map $\mathcal{V}$ such that $\mathcal{V} : \rho(\mathcal{H}) \to \rho(\mathcal{H})$,
- that is trace preserving $Tr[\mathcal{V}A] = Tr[A]$, $\forall A \in \mathcal{O}(\mathcal{H})$,
- and is completely positive.

Definition 1

A map $\mathcal{V}$ is positive iff $\forall A \in B(\mathcal{H})$ s.t. $A \geq 0 \Rightarrow \mathcal{V}A \geq 0$.

Definition 2

A map $\mathcal{V}$ is completely positive iff $\forall n \in$, $\mathcal{V} \otimes \mathbb{1}_n$ is positive.

Hamiltonian separation

The evolution of the total system is given by the von Neumann equation

$$\dot{\rho_T}(t) = -i[H_T, \rho_T(t)]. \tag{9}$$

To separate the effect of the total hamiltonian in the system and the environment we divide it in the form

$$H_T = H \otimes \mathbb{1}_E + \mathbb{1} \otimes H_E + \alpha H_I, \tag{10}$$

with $H \in \mathcal{H}$, $H_E \in \mathcal{H}_E$, and $H_I \in \mathcal{H}_T$, and α being the measure of the strength of the system-environment interaction. H_I can be further decomposed into

$$H_I = \sum_i S_i \otimes E_i, \tag{11}$$

where $S_i \in B(\mathcal{H})$, and $E_i \in B(\mathcal{H}_E)$.

Interaction Picture

In the interaction picture, the density matrices evolve due to the interaction Hamiltonian, while operators evolve with the system and environment Hamiltonian. Time evolution of operators $O \in B(\mathcal{H}_T)$ is then described by

$$\hat{O}(t) = e^{i(H+H_E)t} O e^{-i(H+H_E)t}, \tag{12}$$

whereas the time evolution of the total density matrix in given by

$$\frac{d\hat{\rho}_T(t)}{dt} = -i\alpha \left[\hat{H}_I(t), \hat{\rho}_T(t) \right], \tag{13}$$

which after simple integration gives us

$$\hat{\rho}_T(t) = \hat{\rho}_T(0) - i\alpha \int_0^t ds \left[\hat{H}_I(s), \hat{\rho}_T(t) \right]. \tag{14}$$

Interaction Picture cont.

To avoid integrating the density matrix in all previous times we can insert the integrated expression into the evolution equation, obtaining

$$\frac{d\hat{\rho}_T(t)}{dt} = -i\alpha\left[\hat{H}_I(t), \hat{\rho}_T(0)\right] - \alpha^2\int_0^t ds\left[\hat{H}_I(t), \left[\hat{H}_I(s), \hat{\rho}_T(s)\right]\right], \quad (15)$$

and applying this method one more time we get

$$\frac{d\hat{\rho}_T(t)}{dt} = -i\alpha\left[\hat{H}_I(t), \hat{\rho}_T(0)\right] - \alpha^2\int_0^t ds\left[\hat{H}_I(t), \left[\hat{H}_I(s), \hat{\rho}_T(0)\right]\right] + \mathcal{O}(\alpha^3). \quad (16)$$

Small coupling approximation

Now we perform our first approximation, by assuming small interaction strength α and omitting the terms of order $\mathcal{O}(\alpha^3)$ and higher.

Extracting the system dynamics

$$\frac{d\hat{\rho}(t)}{dt} = Tr_E\left[\frac{d\hat{\rho}_T(t)}{dt}\right]$$
$$= -i\alpha Tr_E\left[\hat{H}_I(t), \hat{\rho}_T(0)\right] - \alpha^2 \int_0^t ds Tr_E\left[\hat{H}_I(t), \left[\hat{H}_I(s), \hat{\rho}_T(0)\right]\right] \tag{17}$$

Assumption 1

We will consider the case where at $t = 0$, the system and the environment have a separable state in the form

$$\rho_T(0) = \rho(0) \otimes \rho_E(0). \tag{18}$$

This is equivalent to stating that there are no correlations between the system and the environment (or they are very short lived).

Extracting the system dynamics cont.

Applying the assumption and remembering the interaction Hamiltonian decomposition $H_I = \sum_i S_i \otimes E_i$ we can consider the first term in our system's density matrix evolution

$$Tr_E\left[\hat{H}_I, \hat{\rho}_T(0)\right] = \sum_i \Big(\hat{S}_i(t)\hat{\rho}(0)\, Tr_E\left[\hat{E}_i(t)\hat{\rho}_E(0)\right] - \hat{\rho}(0)\hat{S}_i(t)\, Tr_E\left[\hat{\rho}_E(0)\hat{E}_i(t)\right]\Big), \tag{19}$$

where we have used the definition of a partial trace. Now we can observe that $Tr_E[\hat{E}_i(t)\hat{\rho}_E(0)] = \langle E_i \rangle$ and since we can always move the energy spectrum without affecting the dynamics so that

$$\langle E_i \rangle = 0, \tag{20}$$

and the whole term vanishes.

Removing the leftover ρ_T dependence

So far we have arrived at an expression

$$\dot{\hat{\rho}}(t) = -\alpha^2 \int_0^t ds Tr_E \left[\hat{H}_I(t), \left[\hat{H}_I(s), \hat{\rho}_T(t)\right]\right], \tag{21}$$

which is problematic as it depends on the total system state.

(Strong) Assumption 2

We will assume, that due to the small coupling, correlation between the system and the environment are much smaller than the typical system timescale, and the environment state is stationary (thermal)

$$\hat{\rho}_T(t) = \hat{\rho}(t) \otimes \hat{\rho}_E(0). \tag{22}$$

The Redfield equation

By applying our assumption and chaning the integral slightly by taking its limit $t \to \infty$ (which doesn't change the outcome of the integration significantly), and changing the variable to $s \to s - t$, we obtain the *Redfield equation*

$$\dot{\hat{\rho}}(t) = -\alpha^2 \int_0^\infty ds Tr_E \left[\hat{H}_I(t), \left[\hat{H}_I(s-t), \hat{\rho}(t) \otimes \hat{\rho}_E(0)\right]\right]. \tag{23}$$

However, it is well studied, that this equation does not warrant the positivity of the map, so we still have some work to do. Due to the existence of similar terms in our expression we will make use of the spectrum of superoperator

$$\tilde{H}A \equiv [H, A], \forall A \in B(\mathcal{H}). \tag{24}$$

Ensuring complete positivity

The eigenvectors of the H superoperator for a complete basis of $B(\mathcal{H})$, so we can expand the system-environment operators in the basis

$$S_i = \sum_{\omega} S_i(\omega), \tag{25}$$

where the operators $S_i(\omega)$ fulfill

$$[H, S_i(\omega)] = -\omega S_i(\omega), \quad [H, S_i^\dagger(\omega)] = \omega S_i^\dagger(\omega) \tag{26}$$

To apply the decomposition we will change back to the Schrödinger picture for the S_i operators $\hat{S}_k = e^{iHt} S_k e^{-iHt}$, arriving to

$$\hat{H}_i(t) = \sum_{k,\omega} e^{-i\omega t} S_k(\omega) \otimes \hat{E}_k(t) = \sum_{k,\omega} e^{i\omega t} S_k^\dagger(\omega) \otimes \hat{E}_k^\dagger(t). \tag{27}$$

Applying the decomposition

After applying the decomposition and a lot of non-trivial algebra we obtain

$$\dot{\hat{\rho}}(t) = \sum_{\omega,\omega',k,l} \Big(e^{i(\omega'-\omega)t} \Gamma_{kl}(\omega) \left[S_l(\omega)\hat{\rho}(t), S_k^\dagger(\omega') \right] + e^{i(\omega-\omega')t} \Gamma_{lk}^*(\omega') \left[S_l(\omega), \hat{\rho}(t) S_k^\dagger(\omega') \right] \Big), \tag{28}$$

where the effect of the environment has been absorbed into the Γ factors

$$\Gamma_{kl}(\omega) \equiv \int_0^\infty ds e^{i\omega s} Tr_E \left[\hat{E}_k^\dagger(t) \hat{E}_l(t-s) \rho_E(0) \right]. \tag{29}$$

Applying the decomposition cont.

By investigating the time dependence of our expression, we can conclude that the terms with $|\omega - \omega'| >> \alpha^2$ will oscillate much faster that the typical timescale of the system evolution, and they will average out in the integration process.

Rotating wave approximation

In the low coupling regime $\alpha \to 0$ we can consider that only the resonant terms $\omega = \omega'$ contribute to the dynamics.

This leaves us with the expression

$$\dot{\hat{\rho}}(t) = \sum_{\omega,k,l} \left(\Gamma_{kl}(\omega) \left[S_l(\omega)\hat{\rho}(t), S_k^\dagger(\omega) \right] + \Gamma_{lk}^* \left[S_l(\omega), \hat{\rho}(t) S_k^\dagger(\omega) \right] \right). \quad (30)$$

Splitting the expression

To return to more friendly form of the expression we divide it into a Hermitian, and non-Hermitian parts and come back to Schrödinger picture

$$\dot{\rho}(t) = i[H + H_{Ls}, \rho(t)] + \sum_{\omega,k,l} \gamma_{kl}(\omega) \left(S_l \rho(t) S_k^\dagger - \frac{1}{2}\{S_k^\dagger S_k, \rho(t)\} \right) \quad (31)$$

Lamb shift Hamiltonian

The role of the term H_{Ls} is to renormalize the system energy levels due to the interaction with the environment.

This expression is the first version of the Markovian Master Equation, but is not in the Lindblad form yet.

The Lindblad Master Equation

By diagonalizing the interaction part of our expression we obtain our desired result.

Lindblad master equation

$$\dot{\rho}(t) \equiv \tilde{\mathcal{L}}\rho(t)$$
$$= -i[H + H_{Ls}, \rho(t)] + \sum_{i,\omega} \left(L_i(\omega)\rho(t)L_i^\dagger(\omega) - \frac{1}{2}\left\{ L_i^\dagger(\omega)L_i(\omega), \rho(t) \right\} \right) \tag{32}$$

In the simplest case, there will be only one relevant frequency ω and the equation will be further simplified.

A master equation for a two-level system

The answer to the atom decay problem is that the emission happens due to the interaction with the surrounding vacuum state. The complete system is then the atom and the vacuum, and the evolution of the reduced density matrix of the atom is given by

$$\frac{d}{dt}\rho(t) = -i[H,\rho] + \Gamma\left(\sigma^-\rho\sigma^+ - \frac{1}{2}\{\sigma^+\sigma^-,\rho\}\right), \tag{33}$$

where σ^-, σ^+ are the Pauli ladder operators.

Comment

The evolution is given by the usual term $-i[H,\rho]$ and the term of interaction that is similar to the one proposed by Landau, mediated by the coupling coefficient Γ.

Time evolution of the two-level system

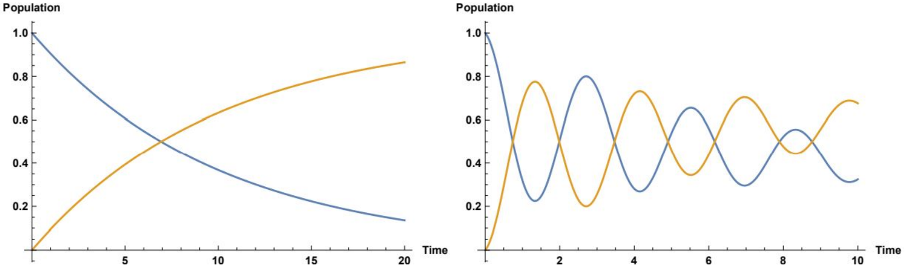


Figure: Blue line represents ρ_{11}, and the orange one ρ_{00}.
The left panel describes evolution with decay and no coherence between states $\rho_{01} = \rho_{10} = 0$, and the right one presents the dynamics with both coherent driving and decay.

Classical Brachistochrone problem

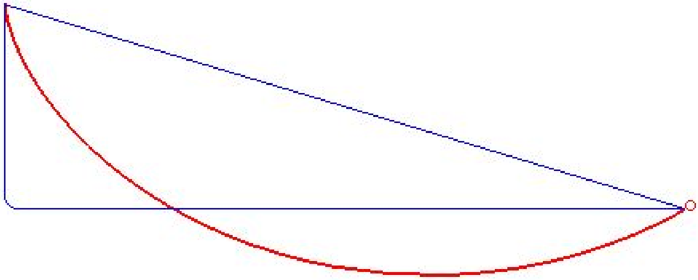


Figure: Different paths between the upper and the lower point.

The cycloid

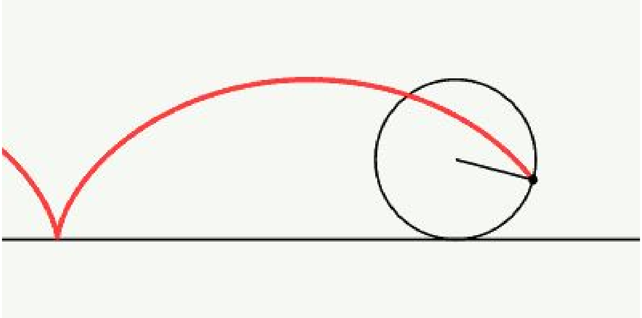


Figure: Construction of the cycloid

Quantum Brachistochrone problem for pure states

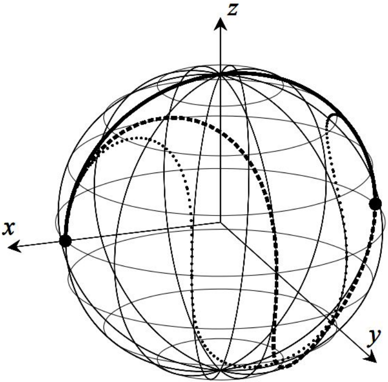


Figure: Time optimal curves of evolution on the Bloch sphere.

Quantum Brachistochrone problem for mixed states

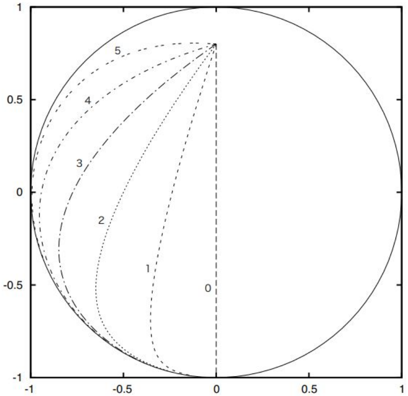


Figure: Time optimal curves of evolution on the XY crossection of the Bloch sphere.

Thank you for your attention!

References:

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