»Research Internship«
Heat and work in a two-level system through quantum master equations

Scientific Report

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Abstract

The aim of this internship is to learn the formalism of master equations for open quantum systems. This shall be used as the basis for examine the statistical differences between quantum jumps in the classical sense and rabi-oscillations. Therefore, a system with two energy states is considered, which is coupled to one or two thermal baths. With this, the dynamic processes of equilibration and heat transport shall be explored. In the next step, an external energy source in the form of a laser is added, to describe work and heat.

Contents

1 Introduction

Quantum thermodynamics is an upcoming field in physics, where, in contrast to the classical thermodynamics theory, systems of a very small size are considered. The key idea is, that for nanoscopic systems there are different laws, than for the macroscopic scale. Therefore, quantum effects, such as quantization of the single energy levels or Rabi oscillations play an important role in quantum thermodynamics. The foundation stone is laid by more established topics, such as information theory, statistical physics or the many-body theory. **[1]**.

Physical processes that are of interest are for example the relaxation of a qubit and the outgoing heat that origins from this process, or the thermalisation between subsystems with different temperatures as well as the corresponding heat flow between the different parts. What can also be examined, is the power and the efficiency of quantum engines, such as heat engines, or refrigerators.
It is of central technological importance, to produce smaller machines, that work also on the nanoscale and therefore, theoretical understanding of the working mechanisms in that size are essential **[1]**.

Determining the behaviour of a system that consists of two thermal baths, helps also to make assumptions for bigger systems, that consist of more thermal baths, or even in systems, which are for example compound to a long chain. **[2]**.
This can be used for examining the heat transport over many subsystems or over many single qubits. Even other influences to the qubit can be identified, like electric current or a laser that points on the qubit.

Theoretical tools to describe this kind of systems, are the quantum master equation and the density-matrix-formalism (for more detail, see Sec. (2)). The aim of this internship is to determine influences between the qubit and some other subsystems with this tool. The situations, that are part of interest, are the interaction from a single qubit with its surroundings only, with one or two thermal baths or with a laser (and in the last section with all together). Some physical properties like the expectation value of the energy, heat flow, power, von Neumann entropy, and entropy production can be calculated with the help of the solution of the quantum master equation. These properties help to verify the validity of the 1^{st} and 2^{nd} law of thermodynamics.

Also, quantum master equations can be the basement to determine the differences between the perspective of the different concepts of quantum jumps on one hand and Rabi oscillations on the other hand.

2 Theory

The main concept of this project is, to examine different open quantum systems with the mathematical concept of quantum master equations. A quantum master equation in general describes the time evolution of the density matrix, that corresponds to the states of a qubit. Now, these states are under the influence of different external subsystems, such as a laser or a thermal bath. Quantum master equations are used in the field of quantum optics mostly. They describe the non-unitary behaviour, especially the time evolution of open quantum systems, by the help of differential equations. **[4]**
The general form of a quantum master equation, that describes a markovian process, can be written as

$$\partial_t\hat{\rho} = -i[\hat{H},\hat{\rho}] + \sum_k \Big[A_k\hat{\rho}A_k^\dagger - \frac{1}{2}A_k^\dagger A_k\hat{\rho} - \frac{1}{2}\hat{\rho}A_kA_k^\dagger\Big], \tag{1}$$

where the A_k´s are Lindblad operators, which describe the effect on the interaction between a system and the environment on the system´s state. **[1]**
Here shall be mentioned, that the form of a quantum master equation is not unique. It is possible, that other unitary operators describe the same system, but lead to another form of a quantum master equation. **[2]**
A master equation can also be written with the help of the super operator $\mathcal{L}$. This operator describes the influence on the qubit in detail and can be seen separate for each single compartment. With that, the master equation reads i.e.

$$\partial_t\hat{\rho} = -i[\hat{H},\hat{\rho}] + \mathcal{L}_c\hat{\rho} + \mathcal{L}_h\hat{\rho} + \mathcal{L}_{rel}\hat{\rho}, \tag{2}$$

Where c labels the influence of a cold thermal bath, h the influence of a hot thermal bath and rel the general relaxation process, which the qubit undergoes. (This master equation describes the system, that consists of a driven quit, which is coupled with two thermal baths, see Sec. 7).

Which information can be taken out of a quantum master equation?

The main idea for a quantum master equation is to find the general solution for the density matrix $\hat{\rho}(t)$ or the steady-state solution. For the general solution the form of the density matrix which is used in this report is determined with

$$\hat{\rho} := \begin{pmatrix} \rho_{gg} & \rho_{ge} \\ \rho_{eg} & \rho_{ee} \end{pmatrix}, \quad \rho_{ij} = \langle i|\hat{\rho}|j\rangle, \tag{3}$$

Where the g´s label the ground state and the e´s label the excited state, respectively.
The steady-state solution $\hat{\rho}_\infty$ can be found by determining the behaviour of the system after infinite time

$$\lim_{t\to\infty}\hat{\rho}(t) = \hat{\rho}_\infty, \tag{4}$$

or by putting the time derivations of the single density matrix entries zero and then find the solution for the density matrix. With the steady-state solution, the (coherence-free) general solution of the quantum master equation can be rewritten as

$$\hat{\rho}(t) = \rho(0)e^{-\mathcal{K}t} + \rho_{\infty}[1 - e^{-\mathcal{K}t}]. \tag{5}$$

In the next step, there is some information, which can be taken out of the solution, for example the expectation value of the Hamiltonian $\hat{H}$

$$\langle\hat{H}\rangle(t) = Tr\{\hat{H}\hat{\rho}(t)\}, \tag{6}$$

or its time derivative

$$\partial_t\langle\hat{H}\rangle = Tr\{\hat{H}\partial_t\hat{\rho}(t)\}. \tag{7}$$

A base concept of thermodynamics lays in the 1^{st} law of thermodynamics, which gives the relation between the expectation values for work W and heat Q as well as the internal energy U

$$U = \langle Q\rangle + \langle W\rangle. \tag{8}$$

What can also be part of the interest is the von Neumann entropy $S(\hat{\rho})$ and according to that the time derivative of the entropy $\partial_t S(\hat{\rho})$ as well as the entropy production Σ. The von Neumann entropy can be calculated as

$$S(\hat{\rho}) = -k_B \operatorname{Tr}\left\{\hat{\rho}\ln[\hat{\rho}]\right\} \tag{9}$$

which can be rewritten in terms of the probabilities of finding the system in the ground (ρ_{ee}) and excited state (ρ_{gg})

$$S(\hat{\rho}) = -k_B \operatorname{Tr}\left\{\rho_{ee}\ln[\rho_{ee}] + \rho_{gg}\ln[\rho_{gg}]\right\}. \tag{10}$$

The 2^{nd} law of thermodynamics states, that the entropy production Σ is non-negative. It can be calculated as

$$\Sigma = -\frac{J_h}{T_h} - \frac{J_c}{T_c} + \partial_t S(\hat{\rho}); \qquad \Sigma \geqslant 0, \tag{11}$$

where

$$\partial_t S(\hat{\rho}) = -k_B \operatorname{Tr}\left\{\partial_t\hat{\rho}\ln[\hat{\rho}]\right\} = -k_B \operatorname{Tr}\left\{(\partial_t\hat{\rho})\ln[\hat{\rho}] + \hat{\rho}\partial_t\ln[\hat{\rho}]\right\} = -k_B \operatorname{Tr}\left\{(\partial_t\hat{\rho})\cdot[1 + \ln[\hat{\rho}]]\right\}, \tag{12}$$

and J_c as well as J_h are labeling the heat flows from the cold respectively hot bath to the qubit

$$
\begin{aligned}
J_c &= \mathrm{Tr}\left\{\hat{H}\mathcal{L}_c\hat{\rho}_\infty\right\} \\
J_h &= \mathrm{Tr}\left\{\hat{H}\mathcal{L}_h\hat{\rho}_\infty\right\}.
\end{aligned} \tag{13}
$$

Note, that the heat flows can only be calculated with these equations, if the Hamiltonian is time-independent.

In the case of a laser acting on a system, a time-dependent electromagnetic field couples to the system and the power P quantizes such energy change.This introduced time-dependence can be eliminated by moving from the stationary frame to a rotating one. Therefore, the solution for $\hat{\rho}$ and the Hamiltonian $\hat{H}$ have also to be changed into the new base,

$$
\hat{\rho}_r = \hat{U}\hat{\rho}\hat{U}^\dagger; \qquad H_r = \hat{U}\hat{H}\hat{U}^\dagger - i\hat{H}\partial_t\hat{U}^\dagger, \tag{14}
$$

where $\hat{U}$ is unitary,

$$
\hat{U}\hat{U}^\dagger = \mathbb{1} = \hat{U}^\dagger\hat{U}. \tag{15}
$$

For more detail in the change of the base, see Sec. 4. Now, the power P can be calculated with $\hat{P} = \partial_t\hat{H}$ as

$$
P = \mathrm{Tr}\{\hat{P}\hat{\rho}\} = \mathrm{Tr}\{\hat{U}\hat{P}\hat{U}^\dagger\hat{U}\hat{\rho}\hat{U}^\dagger\} = \mathrm{Tr}\{\hat{U}\hat{P}\hat{U}^\dagger\hat{\rho}_r\}. \tag{16}
$$

Bose-Einstein-distribution and Gibbs state

The Bose-Einstein-distribution $n(T)$ explains the statistical allocation of an ensemble of bosons at different temperatures. It is used inside a master equation for describing the influence of a thermal bath. The Bose-Einstein-distribution states

$$
n(T) = \frac{1}{\exp\left[\frac{\epsilon}{k_B T}\right] - 1}. \tag{17}
$$

In the following sections, it will be part of interest to determine the temperature limits for the systems, which interact with thermal baths. Therefore, the behaviour for very cold temperatures $T \to 0$ or for very hot temperatures $T \to \infty$ shall get examined. The relations, that can be used for these limits, are

$$
\lim_{T\to 0} n = 0; \qquad \lim_{T\to\infty} n = \infty. \tag{18}
$$

For the next part, the equilibrium behaviour shall get examined more in detail. A

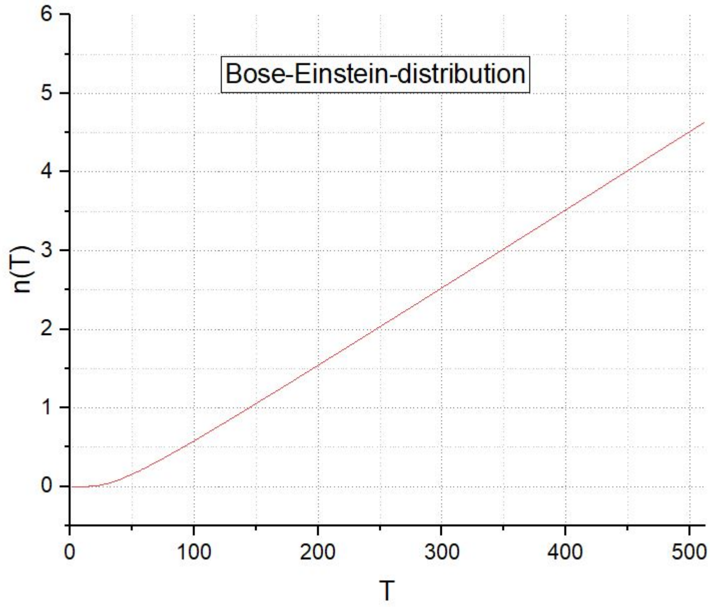

Figure 1: The Bose-Einstein-distribution in dependence of temperature T for $\epsilon = 100$ and for $k_B := 1$.

Gibbs state is a probability distribution, which occurs in equilibrium. Its main feature is, that it remains invariant under a possible further evolution of the system. **[3]**
The Gibbs state is defined by

$$\hat{\rho}_G = \frac{e^{-\beta\hat{H}}}{\mathrm{Tr}\left[e^{-\beta\hat{H}}\right]}, \tag{19}$$

Where the term $\mathrm{Tr}\left[e^{-\beta\hat{H}}\right]$ is also known as the partition function Z and $\beta = \frac{1}{k_B T}$.

In the particular case of thermal bath that interacts with a qubit, the Gibbs state is

$$\hat{\rho}_G = \frac{1}{1+e^{-\beta\epsilon}}\begin{pmatrix} 1 & 0 \\ 0 & e^{-\beta\epsilon} \end{pmatrix} = \begin{pmatrix} 1-n_F & 0 \\ 0 & n_F \end{pmatrix}, \tag{20}$$

Where n_F labels the Fermi-Dirac-distribution

$$n_F(T) = \frac{1}{\exp\left[\frac{\epsilon}{k_B T}\right]+1}. \tag{21}$$

3 Master equation for relaxation 2-level-system

In this section, the process of relaxation for a single qubit without external influences shall be examined.

3.1 General solution for the density matrix and steady-state solution

The master equation, which describes the relaxation process of a two level system, where the two states are the ground state $|g\rangle$ and the excited state $|e\rangle$ reads:

$$\partial_t \hat{\rho} = -i[\hat{H}, \hat{\rho}] + \mathcal{K}\hat{\mathcal{D}}[\hat{\sigma}]\hat{\rho}, \tag{22}$$

with

$$\hat{\mathcal{D}}[\hat{\sigma}]\hat{\rho} = \hat{\sigma}\hat{\rho}\hat{\sigma}^\dagger - \frac{1}{2}\{\hat{\sigma}^\dagger\hat{\sigma}, \hat{\rho}\}. \tag{23}$$

Now, the Hamiltonian $\hat{H}$, the lowering operator $\hat{\sigma}$ and a boundary condition for the density matrix $\hat{\rho}(t=0)$ are given by:

$$\hat{\sigma} = |g\rangle\langle e| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{H} = \epsilon|e\rangle\langle e| = \begin{pmatrix} 0 & 0 \\ 0 & \epsilon \end{pmatrix}, \tag{24}$$

$$\rho(0) = P|e\rangle\langle e| + (1-P)|g\rangle\langle g| + \alpha|e\rangle\langle g| + \alpha^*|g\rangle\langle e| = \begin{pmatrix} 1-P & \alpha^* \\ \alpha & P \end{pmatrix}. \tag{25}$$

Where α captures the coherence between the ground and excited states, such that the variable $\alpha = 0$ for the coherence-free solution. Note also how the general form of the density matrix is determined (see Eq. (3)). Now, inserting Eqs. (24) and (3) into the master equation as well as concerning the boundary condition (Eq. (25)) results in

$$\begin{aligned}
\partial_t \rho = -i&\left[\begin{pmatrix} 0 & 0 \\ 0 & \epsilon \end{pmatrix}\begin{pmatrix} \rho_{gg} & \rho_{ge} \\ \rho_{eg} & \rho_{ee} \end{pmatrix} - \begin{pmatrix} \rho_{gg} & \rho_{ge} \\ \rho_{eg} & \rho_{ee} \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & \epsilon \end{pmatrix}\right] \\
&+ \mathcal{K}\left\{\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \rho_{gg} & \rho_{ge} \\ \rho_{eg} & \rho_{ee} \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\right. \\
&- \frac{1}{2}\left[\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \rho_{gg} & \rho_{ge} \\ \rho_{eg} & \rho_{ee} \end{pmatrix}\right. \\
&+ \left.\left.\begin{pmatrix} \rho_{gg} & \rho_{ge} \\ \rho_{eg} & \rho_{ee} \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\right]\right\}.
\end{aligned} \tag{26}$$

By calculating now the single matrix products, the following form can be received in the end

$$\partial_t \hat{\rho} = -i\epsilon\begin{pmatrix} 0 & -\rho_{ge} \\ \rho_{eg} & 0 \end{pmatrix} + \mathcal{K}\begin{pmatrix} \rho_{ee} & -\frac{1}{2}\rho_{ge} \\ -\frac{1}{2}\rho_{eg} & -\rho_{ee} \end{pmatrix}. \tag{27}$$

This can be written in a system of rate equations:

$$\partial_t \rho_{gg} = \mathcal{K} \rho_{ee}, \tag{28a}$$

$$\partial_t \rho_{ge} = \rho_{ge}(i\epsilon - \frac{1}{2}\mathcal{K}), \tag{28b}$$

$$\partial_t \rho_{eg} = \rho_{eg}(- i\epsilon - \frac{1}{2}\mathcal{K}), \tag{28c}$$

$$\partial_t \rho_{ee} = - \mathcal{K} \rho_{ee} = -\partial_t \rho_{gg}. \tag{28d}$$

By integration, a general solution can be obtained, where the constants are determined by the boundary condition, i.e. for the density matrix at time $t = 0$. With this condition, we find the following general solution,

$$\boxed{\hat{\rho}(t) = \begin{pmatrix} -Pe^{-\mathcal{K}t} + 1 & \alpha^* e^{(i\epsilon - \frac{1}{2}\mathcal{K})t} \\ \alpha e^{(-i\epsilon - \frac{1}{2}\mathcal{K})t} & Pe^{-\mathcal{K}t} \end{pmatrix}.} \tag{29}$$

Eq. (29) *indeed is a valid solution of the master equation* (22)*, because*

- trace condition: $Tr(\hat{\rho}) = -Pe^{-\mathcal{K}t} + 1 + Pe^{-\mathcal{K}t} = 1$
- positivity: the eigenvalues ρ_{ee} and ρ_{gg} are ≥ 0, since $P \in [0; 1]$ (which implies that $\hat{\rho}(t)$ is Hermitian)

The next step is now to examine the steady-state solution of this system. As Eq. (4) from the theory part states, the steady-state can be calculated by taking the limit for the time against infinity for each entry of the density matrix Eq. (29). The steady-state solution for the relaxation process is

$$\hat{\rho}_\infty(t) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{30}$$

This means, that after infinite time, the system is fully proceeded into the ground state with probability 1.

Which information can be taken out of this solution now?

First of all, P describes the probability for the system to be in the state $|e\rangle$ in the beginning, or $(1 - P)$, the probability for the system to be in the state $|g\rangle$ in the beginning. So in fact, the equation describes the relaxation of the system into the ground state. The transition occurs with the rate $\mathcal{K}$, whereby the ground state is approached exponentially. Besides, if coherence is present initially, the off-diagonal terms in the density matrix oscillate and decay over time.

Now, the general solution can be written in another form, when the constants are determined as $\alpha = 0$ and with that, of course also $\alpha^* = 0$. The coherence-free general solution can be written with the help of the steady-state by the use of Eq. (5), which reads in this particular case

$$\hat{\rho}(t) = \begin{pmatrix} 1-P & 0 \\ 0 & P \end{pmatrix} e^{-\mathcal{K}t} + \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} [1 - e^{-\mathcal{K}t}]. \tag{31}$$

3.2 Energy considerations

The expectation value for the energy of the system can be calculated as with Eq. (6) as

$$\langle \hat{H} \rangle(t) = Tr\left\{ \begin{pmatrix} 0 & 0 \\ 0 & \epsilon \end{pmatrix} \begin{pmatrix} -Pe^{-\mathcal{K}t} + 1 & 0 \\ 0 & Pe^{-\mathcal{K}t} \end{pmatrix} \right\} = \epsilon P e^{-\mathcal{K}t} \tag{32}$$

The time derivative of the expectation value of the Hamiltonian stands in general for the exchange of energy between the qubit and the environment. In this case, energy can only leave the system. Physically, this situation corresponds to a qubit which interacts with a thermal bath at temperature $T = 0$. The time derivative of the expectation value of the Hamiltonian can be calculated with Eq. (7) as

$$\partial_t \langle \hat{H} \rangle = \epsilon \dot{\rho}_{ee} = -\epsilon \mathcal{K} P e^{-\mathcal{K}t} = -\mathcal{K} \langle \hat{H} \rangle(t). \tag{33}$$

Interpretation of the results

The solution for the energy-expectation value has at the beginning the value ϵP. It declines with time, because of the relaxation process which proceeds with the transition rate $\mathcal{K}$, until the system has released all of its initial energy ϵ in form of the heat current to the environment. The transition process declines with time.

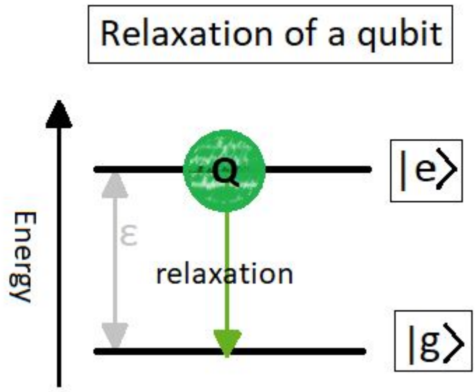

Figure 2: Construction of the system, relaxation process, energy levels, energy difference ϵ between the ground state $|g\rangle$ and the excited state $|e\rangle$

4 Master equation for interaction between laser and 2-level-system

In this section, the mechanisms of a driven-dissipative system shall get examined. Therefore, a laser gets placed next to the qubit, such that the external power leads to an energy growth in the qubit.

4.1 Rotating base versus stationary base

For this kind of calculation, the concept of base transformation gets used, since the problem in a fixed base would have to deal with a time-dependent Hamiltonian $\hat{H}(t)$, whereas the Hamiltonian, that can be used in the rotating frame, is constant. For the following base transformation, the unitary operator $\hat{U}$ gets used. For this system, it can be determined as

$$\hat{U} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\epsilon t} \end{pmatrix}. \tag{34}$$

Now, the original, time-dependent Hamiltonian $\hat{H}(t)$ can be calculated with the use of Eq. (14). It reads

$$\hat{H}(t) = \epsilon|e\rangle\langle e| + f(\hat{\sigma}^\dagger \cdot e^{-i\epsilon t} + \hat{\sigma} \cdot e^{i\epsilon t}) = \begin{pmatrix} 0 & fe^{i\epsilon t} \\ fe^{-i\epsilon t} & \epsilon \end{pmatrix}. \tag{35}$$

The base transformation for the density matrix leads to

$$\hat{\rho}_r = \hat{U}\hat{\rho}\hat{U}^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\epsilon t} \end{pmatrix} \begin{pmatrix} \rho_{gg} & \rho_{ge} \\ \rho_{eg} & \rho_{ee} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\epsilon t} \end{pmatrix} = \begin{pmatrix} \rho_{gg} & \rho_{ge} \cdot e^{-i\epsilon t} \\ \rho_{eg} \cdot e^{i\epsilon t} & \rho_{ee} \end{pmatrix}. \tag{36}$$

If this gets used for the time-dependent Hamiltonian $\hat{H}(t)$, the time dependence can be eliminated and the result is the time-independent Hamiltonian $\hat{H}$, that can be used for calculations in the rotating frame

$$\hat{H} = f\Big(|e\rangle\langle g| + |g\rangle\langle e|\Big) = \begin{pmatrix} 0 & f \\ f & 0 \end{pmatrix}. \tag{37}$$

Now, the time derivative of the density matrix can be determined with the help of the base transformation as

$$\begin{aligned} \partial_t\hat{\rho}_r &= \hat{U}(\partial_t\hat{\rho})\hat{U}^\dagger + (\partial_t\hat{U})\hat{\rho}\hat{U}^\dagger + \hat{U}\hat{\rho}(\partial_t\hat{U}^\dagger) \\ &= \hat{U}(\partial_t\hat{\rho})\hat{U}^\dagger + (\partial_t\hat{U})\hat{U}^\dagger\hat{U}\hat{\rho}\hat{U}^\dagger + \hat{U}\hat{\rho}\hat{U}^\dagger\hat{U}(\partial_t\hat{U}^\dagger). \end{aligned} \tag{38}$$

With the relation

$$\partial_t\hat{U}\hat{U}^\dagger = 0 \rightarrow (\partial_t\hat{U})\hat{U}^\dagger = -\hat{U}(\partial_t\hat{U}^\dagger), \tag{39}$$

it can be shown that

$$\partial_t\hat{\rho}_r = \hat{U}(\partial_t\hat{\rho})\hat{U}^\dagger - \hat{U}(\partial_t\hat{U}^\dagger)\hat{\rho}_r + \hat{\rho}_r\hat{U}(\partial_t\hat{U}^\dagger). \tag{40}$$

Inserting now the general form of the master equation (which is given in the rotating frame),

$$\partial_t \hat{\rho} = -i[\hat{H}, \hat{\rho}] + \hat{\mathcal{L}}\hat{\rho}, \tag{41}$$

into the expression, leads to

$$\partial_t \hat{\rho}_r = -i\hat{U}\hat{H}\hat{\rho}\hat{U}^\dagger + i\hat{U}\hat{\rho}\hat{H}\hat{U}^\dagger + \hat{U}\hat{\mathcal{L}}\hat{\rho}\hat{U}^\dagger + \hat{U}\hat{\rho}(\partial_t \hat{U}^\dagger). \tag{42}$$

If now the base transformation is performed into the lab frame for the whole equation, whereby the Hamiltonian $\hat{H}$ has to be changed into the rotating-frame Hamiltonian $\hat{H}(t) = \hat{H}_r$ (see Eq. (14)), the expression gets

$$\partial_t \hat{\rho}_r = -i\hat{H}_r\hat{\rho} + i\hat{\rho}\hat{H}_r + \hat{\mathcal{L}}\hat{\rho} = -i[\hat{H}_r, \hat{\rho}] + \hat{\mathcal{L}}\hat{\rho}, \tag{43}$$

as the master equation in the lab frame.

4.2 Steady-state solution

Now, for calculating the different properties, like the power of the system, or the heat flow, the master equation in the rotating frame is used. By inserting the super operator $\hat{\mathcal{L}}$, it reads

$$\partial_t \hat{\rho} = -i[\hat{H}, \hat{\rho}] + \mathcal{K}\hat{\mathcal{D}}[\hat{\sigma}]\hat{\rho}. \tag{44}$$

The master equation is equal to the master equation for the 2-level-system (see Eq. (22)), as can be seen. Also, the lowering operator $\hat{\sigma}$ (Eq. (24)) and the initial condition $\hat{\rho}(t = 0)$ (Eq. (25))are the same as before. But, since the energy situation is a different, there is also a different Hamiltonian $\hat{H}$ (see Eq. (37)). With that, the master equation can also be written as

$$\hat{\rho} = -if \begin{pmatrix} \rho_{eg} - \rho_{ge} & \rho_{ee} - \rho_{gg} \\ \rho_{gg} - \rho_{ee} & \rho_{ge} - \rho_{eg} \end{pmatrix} + \mathcal{K} \begin{pmatrix} \rho_{ee} & -\frac{1}{2}\rho_{ge} \\ -\frac{1}{2}\rho_{eg} & -\rho_{ee} \end{pmatrix}. \tag{45}$$

The steady-state solution for the laser system can now be found by solving the following equation system

$$0 = -if[\rho_{eg} - \rho_{ge}] + \mathcal{K}\rho_{ee}, \tag{46a}$$

$$0 = -if[\rho_{ee} - \rho_{gg}] - \frac{1}{2}\mathcal{K}\rho_{ge}, \tag{46b}$$

$$0 = -if[\rho_{gg} - \rho_{ee}] - \frac{1}{2}\mathcal{K}\rho_{eg}, \tag{46c}$$

$$0 = -if[\rho_{ge} - \rho_{eg}] - \mathcal{K}\rho_{ee}, \tag{46d}$$

Where the solution is

$$\boxed{\hat{\rho}_\infty = \frac{1}{4f^2 + \frac{1}{2}\mathcal{K}^2} \cdot \begin{pmatrix} 2f^2 + \frac{1}{2}\mathcal{K}^2 & if\mathcal{K} \\ -if\mathcal{K} & 2f^2 \end{pmatrix}.} \tag{47}$$

In the next step, the power of the driven-dissipative system, as well as the heat flow can be determined.

4.3 Power and heat flow

The power for the laser system can be calculated with Eq. (16) (see Theory part), as

$$\begin{aligned} P &= \mathrm{Tr}\left\{ \begin{pmatrix} 1 & 0 \\ 0 & e^{i\epsilon t} \end{pmatrix} \begin{pmatrix} 0 & i\epsilon f e^{i\epsilon t} \\ -i\epsilon f e^{-i\epsilon t} & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\epsilon t} \end{pmatrix} \frac{1}{4f^2 + \frac{1}{2}\mathcal{K}^2} \cdot \begin{pmatrix} 2f^2 + \frac{1}{2}\mathcal{K}^2 & if\mathcal{K} \\ -if\mathcal{K} & 2f^2 \end{pmatrix} \right\} \\ &= \frac{2f^2\epsilon\mathcal{K}}{4f^2 + \frac{1}{2}\mathcal{K}^2} \end{aligned} \tag{48}$$

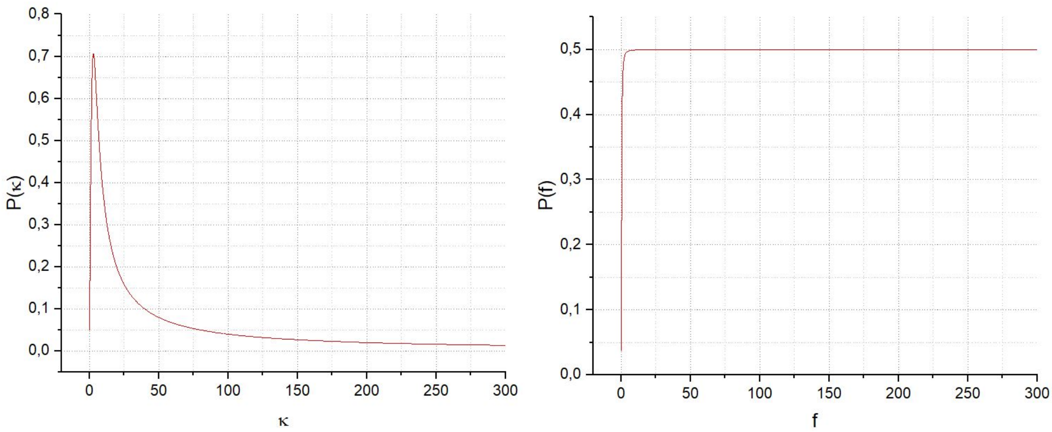

Figure 3: Power of the laser system. On the left side in dependence of the rate $\mathcal{K}$, where the parameters are determined as $f = 1$ and $\epsilon = 1$ and on the right side the plot shows the power in dependence of the energy f, where the parameters are determined as $\mathcal{K} = 1$ and $\epsilon = 1$.

Now, the heat flow for the laser system can be calculated as

$$J_h = \mathrm{Tr}\left\{\epsilon|e\rangle\langle e|\hat{\mathcal{L}}_h\hat{\rho}\right\} = \frac{\epsilon\mathcal{K}_h[\frac{1}{2}n_h\mathcal{K}^2 - 2f^2]}{4f^2 + \frac{1}{2}\mathcal{K}^2}. \tag{49}$$

So, for the situation of the laser, there are two counteracting heat flows, the one for the relaxation process, which leaves the qubit and the one from the laser influence, which comes into the system. The whole process is also described in the following picture, which shows the setup of the laser system.

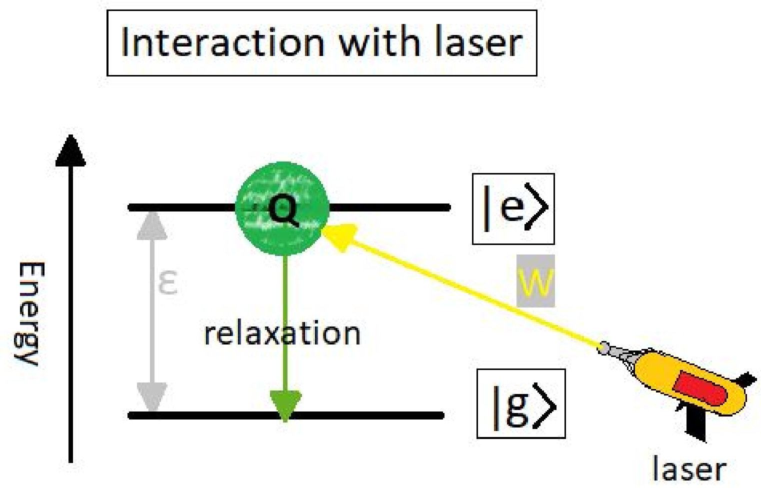

Figure 4: Construction of the system, which consists of a qubit and a laser, working mechanisms, change in energy, Work W is done by the laser.

5 Master equation for interaction between thermal bath and 2-level-system

5.1 General solution and steady-state solution

The aim in this section is, to examine the heat transition between a thermal bath and a 2-level system, and in correlation to this, the relaxation process of the system. So in fact, the process is an equilibration process between the two sub-systems (2-level-system and the thermal bath).
The master equation reads the following

$$\partial_t \hat{\rho} = -i[\hat{H}, \hat{\rho}] + \mathcal{K}(n+1)\hat{\mathcal{D}}[\hat{\sigma}]\hat{\rho} + \mathcal{K}n\hat{\mathcal{D}}[\hat{\sigma}^\dagger]\hat{\rho}. \tag{50}$$

Some of the heat considerations can already be taken out of the master equation: The second term labels the heat that goes out of the qubit, while the third term labels the incoming heat. This point will be considered in more detail in Sec. 5.2.
In the master equation the same Hamiltonian $\hat{H}$, the same lowering operator $\hat{\sigma}$, given in Eq. (24) as well as the same initial condition $\hat{\rho}(t=0)$ (see Eq. (25)) as in section 4 was used. Note also that n refers to the Bose-Einstein-distribution (see Eq. (17))
Fully written, the master equation reads

$$\begin{aligned}\partial_t \hat{\rho} = -i(\hat{H}\hat{\rho} - \hat{\rho}\hat{H}) + \mathcal{K}(n+1)\Big(\hat{\sigma}\hat{\rho}\hat{\sigma}^\dagger - \frac{1}{2}(\hat{\sigma}^\dagger\hat{\sigma}\hat{\rho} + \hat{\rho}\hat{\sigma}^\dagger\hat{\sigma})\Big) \\ + \mathcal{K}n\Big(\hat{\sigma}^\dagger\hat{\rho}\hat{\sigma} - \frac{1}{2}(\hat{\sigma}\hat{\sigma}^\dagger\hat{\rho} + \hat{\rho}\hat{\sigma}\hat{\sigma}^\dagger)\Big)\end{aligned} \tag{51}$$

From this master equation, the following rate equations can be received

$$\partial_t \rho_{gg} = \rho_{ee}\mathcal{K}(n+1) - \rho_{gg}\mathcal{K}n, \tag{52a}$$

$$\partial_t \rho_{ee} = -\rho_{ee}\mathcal{K}(n+1) + \rho_{gg}\mathcal{K}n = -\partial_t \rho_{gg}, \tag{52b}$$

$$\partial_t \rho_{ge} = \rho_{ge}\Big[i\epsilon - \mathcal{K}n - \frac{1}{2}\mathcal{K}\Big], \tag{52c}$$

$$\partial_t \rho_{eg} = \rho_{eg}\Big[-i\epsilon - \mathcal{K}n - \frac{1}{2}\mathcal{K}\Big]. \tag{52d}$$

From Eqs. (52) (c and d) follows straight with an exponential ansatz

$$\rho_{ge} = \alpha^* \cdot exp[(i\epsilon - \mathcal{K}n - \frac{1}{2}\mathcal{K})t], \tag{53}$$

$$\rho_{eg} = \alpha \cdot exp[(-i\epsilon - \mathcal{K}n - \frac{1}{2}\mathcal{K})t] = \rho_{ge}^*, \tag{54}$$

where the initial condition from Eq. (25) was used. $\rho_{gg} + \rho_{ee} = 1$ results in

$$\partial_t \rho_{ee} = -\rho_{ee}\mathcal{K}(2n+1) + \mathcal{K}n, \tag{55}$$

Where the solution of this equation is

$$\rho_{ee} = \frac{n - a \cdot \exp[(-\mathcal{K}t(2n+1)]}{2n+1}. \tag{56}$$

The integration constant a is determined by the initial condition (25) as $a = -P(2n+1) + n$. Also, by using the Fermi-Dirac-distribution,

$$n_F = \frac{1}{1 + \exp\left[\frac{\epsilon}{k_B T}\right]} \tag{57}$$

And the trace-relation $\rho_{gg} + \rho_{ee} = 1$, the general solution for the case of a 2-level-system which interacts with a thermal bath is

$$\boxed{\hat{\rho}(t) = \begin{pmatrix} -n_F + (n_F - P) \cdot \exp[-\mathcal{K}t(2n+1)] + 1 & \alpha^* \cdot \exp\left[(i\epsilon - \mathcal{K}(n + \frac{1}{2}))t\right] \\ \alpha \cdot \exp\left[(-i\epsilon - \mathcal{K}(n + \frac{1}{2}))t\right] & n_F + (P - n_F) \cdot \exp[-\mathcal{K}t(2n+1)] \end{pmatrix}.} \tag{58}$$

By determining the steady-state solution, the general solution for the case without coherence can again be rewritten by using the Eq. (5).
The steady-state solution for the system with a thermal bath states

$$\hat{\rho}_\infty = \begin{pmatrix} \frac{1}{\exp\left[\frac{-\epsilon}{k_B T}\right]+1} & 0 \\ 0 & \frac{1}{1+\exp\left[\frac{\epsilon}{k_B T}\right]} \end{pmatrix} = \begin{bmatrix} 1 - n_F & 0 \\ 0 & n_F \end{bmatrix}. \tag{59}$$

Putting now the steady-state solution in the expression (5) gives

$$\hat{\rho}(t) = \begin{pmatrix} 1 - P & 0 \\ 0 & P \end{pmatrix} e^{-\mathcal{K}(2n+1)t} + \begin{pmatrix} 1 - n_F & 0 \\ 0 & n_F \end{pmatrix} \cdot \left[1 - e^{-\mathcal{K}(2n+1)t}\right]. \tag{60}$$

5.2 Energy considerations

Equivalent to Sec. 4, the expectation value of the system´s energy can be calculated by taking the trace over the Hamiltonian $\hat{H}$ times the solution for the density matrix $\hat{\rho}(t)$ (see Eq. (6)).

$$\langle \hat{H} \rangle(t) = tr[\hat{H}\hat{\rho}] = \epsilon \cdot \rho_{ee} = \epsilon \cdot \{n_F + (P - n_F) \cdot \exp[-\mathcal{K}t(2n+1)]\}. \tag{61}$$

In the next step, the time derivative of this expectation value shall be calculated, which will lead to a result, that is equal to the heat flow J from the thermal bath to the 2-level-system,

$$\begin{aligned} J \equiv \partial_t \langle \hat{H} \rangle(t) = \epsilon \cdot \partial_t \rho_{ee} &= -\epsilon \mathcal{K}(2n+1)(P - n_F)\exp[-\mathcal{K}t(2n+1)] \\ &= \{\epsilon(1-P)\mathcal{K}n - P\epsilon\mathcal{K}(n+1)\} \cdot \exp[(-\mathcal{K}t(2n+1)]. \end{aligned} \tag{62}$$

5.3 Conclusion (so far)

The equilibration process consists in a part with outgoing heat and a part with incoming heat. These two flows can be identified in Eq.(50). There, the rates are $\mathcal{K}n$ and $\mathcal{K}(n+1)$ which give together the rate for the equilibration process. In the heat current J (see Eq. (62)) appear two counteracting terms: $-P\epsilon\mathcal{K}(n+1)$ describes the outgoing heat, while the incoming heat is described by the term $\epsilon(1-P)\mathcal{K}n$.
The two terms act against each other, until the two level system has reached the same temperature, as the thermal bath. The process slows down more and more, since the rate appears with a negative sign in the exponential function. In the end, when the steady-state is reached, the system is in a classical mixture out of $|e\rangle$ and $|g\rangle$, where the ratio between these two state probabilities is described by the Fermi-Dirac-statistics (57). The term n_F corresponds to the state $|e\rangle$ and $1 - n_F$ corresponds to the state $|g\rangle$, respectively.

5.4 Temperature limits

In this section the behaviour of the system for very hot or very cold temperatures shall be considered.
With the relation $\lim_{T\to 0} n = 0$ from the introduction (see Eq. (18)), the following solution for the cold-limit-density-matrix can be obtained by putting $n = 0$ in Eq. (58)

$$\hat{\rho}(t)_{T\to 0} = \begin{pmatrix} -P\exp[-\mathcal{K}t] + 1 & \alpha^* \cdot \exp\Big[(i\epsilon - \frac{1}{2}\mathcal{K})t\Big] \\ \alpha \cdot \exp\Big[(-i\epsilon - \frac{1}{2}\mathcal{K})t\Big] & P\exp\{-\mathcal{K}t\} \end{pmatrix}. \tag{63}$$

As can be seen, this solution is the same as for the 2-level-system that interacts with a thermal bath with temperature $T = 0$ (compare Eq. (29)).

Now, for the case of the hot temperature limit, $T \to \infty$, the approximation $\lim_{T\to\infty} n = \infty$ can be used for the Bose-Einstein-distribution. Putting this into the general solution gives

$$\hat{\rho}(t)_{T\to\infty} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}, \tag{64}$$

Which fits with the equipartition of energy-principle. It states, that the different energy levels of a system are equally occupied at high temperatures.
Note also that, as expected, the Gibbs state (see Introduction) is equal to the steady-state of this system (see Eq. (64)).

5.5 Von Neumann entropy

For the system with one thermal bath, the von Neumann-entropy $S(\hat{\rho})$ can be calculated with the use of Eqs. (9) and (10) as

$$S(\hat{\rho}) = -k_B\Big\{\Big(- n_F + (n_F - P)\cdot \exp[-\mathcal{K}t(2n+1)] + 1\Big)\cdot \ln\Big[- n_F + (n_F - P)\cdot \exp[-\mathcal{K}t(2n+1)] + 1\Big] + \Big(n_F + (P - n_F)\cdot \exp[-\mathcal{K}t(2n+1)]\Big)\cdot \ln\Big[n_F + (P - n_F)\cdot \exp[-\mathcal{K}t(2n+1)]\Big]\Big\}. \tag{65}$$

In the next step, the entropy production Σ, can be calculated for this system with

$$\Sigma = -\frac{J}{T} + \partial_t S, \tag{66}$$

where $\partial_t S$ is given by

$$\partial_t S = -k_B Tr\{\partial_t \hat{\rho} \ln[\hat{\rho}]\}. \tag{67}$$

By calculating $\partial_t S$ first, one can receive the following interim result

$$\partial_t S = -k_B\Big\{ - \mathcal{K}(2n+1)(n_F - P)\cdot e^{-\mathcal{K}t(2n+1)}\cdot \ln\Big(\frac{1}{n_F + (P - n_F)e^{-\mathcal{K}t(2n+1)}} - 1\Big)\Big\}. \tag{68}$$

With these results, the entropy production can be calculated as

$$\begin{aligned}\Sigma = &\frac{\mathcal{K}\epsilon}{T}(2n+1)(P - n_F)\exp[-\mathcal{K}t(2n+1)] \\ &+ k_B\Big\{\mathcal{K}(2n+1)(n_F - P)\cdot e^{-\mathcal{K}t(2n+1)}\cdot \ln\Big(\frac{1}{n_F + (P - n_F)e^{-\mathcal{K}t(2n+1)}} - 1\Big)\Big\}.\end{aligned} \tag{69}$$

By using Eq. (52) b one receives

$$\Sigma = k_B\mathcal{K}(2n+1)\Big[n_F(1-\rho_{ee}) - \rho_{ee}(1-n_F)\Big]\Big\{ \ln[n_F(1-\rho_{ee}] - \ln[\rho_{ee}(1-n_F)]\Big\} \geqslant 0. \tag{70}$$

This inequation is true, since it has the same form as the following inequation, which is in general true

$$(k - g)(\ln[k] - \ln[g]) \geqslant 0. \tag{71}$$

Note also, that there is no entropy production in the steady-state, because the time derivation of the entropy has to be equal to 0, as well as the heat flow, since the time derivation of the steady-state density matrix is also 0 for each entry and appears in both equations. (see Eq. (7) and (67))

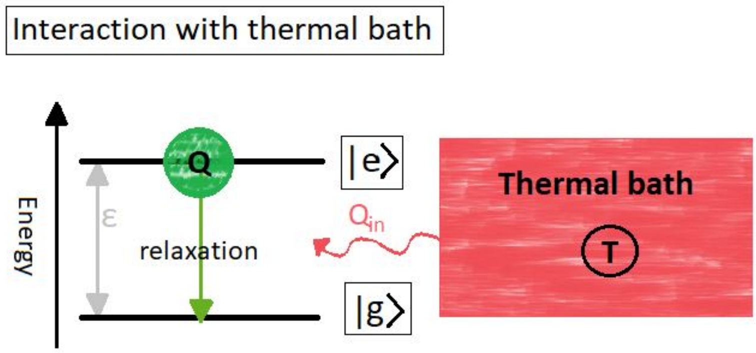

Figure 5: Construction of the system, which consists of a thermal bath and the qubit, working mechanisms, change in energy, heat Q enters the qubit.

6 Master equation for interaction between 2 thermal baths and 2-level-system

6.1 General solution and steady-state solution

In this section, the aim is to examine the interaction between two thermal baths at different temperatures, T_c and T_h and a two level system. From everyday experience, one would suppose, that the heat flows from the hot system to the cold system. Because the qubit is located between the two baths, some of the energy in form of heat has to be absorbed by the qubit. If there would be thermal systems of finite size, then, of course, after some time, the equilibration process is done and all three subsystems have the same final temperature. But in this case, the thermal baths are described as large reservoirs, which can not change their temperature.

The master equation is very similar to the case of one thermal bath. Here, the index c labels the cold bath and the index h the hotter one.

$$\partial_t \hat{\rho}(t) = -i[\hat{H}, \hat{\rho}] + \sum_{\alpha=c,h} \mathcal{K}_\alpha \Big[(n_\alpha + 1)\hat{\mathcal{D}}[\hat{\sigma}] + n_\alpha \hat{D}[\hat{\sigma}^\dagger]\Big]\hat{\rho}, \tag{72}$$

with

$$n_\alpha = \frac{1}{\exp\left[\frac{\epsilon}{k_B T_\alpha}\right] - 1}. \tag{73}$$

This leads equivalent to the situation with one thermal bath to the following rate equations:

$$\partial_t \rho_{gg} = \rho_{ee} \square - \rho_{gg} \triangle, \tag{74a}$$

$$\partial_t \rho_{ge} = \rho_{ge} \Big[i\epsilon - \frac{1}{2}\square - \frac{1}{2} \triangle \Big], \tag{74b}$$

$$\partial_t \rho_{eg} = \rho_{eg} \Big[-i\epsilon - \frac{1}{2}\square - \frac{1}{2} \triangle \Big], \tag{74c}$$

$$\partial_t \rho_{ee} = -\rho_{ee} \square + \rho_{gg} \triangle \,. \tag{74d}$$

With the substituted variables $\square$ and $\triangle$:

$$\begin{aligned} \square &:= \mathcal{K}_c[n_c + 1] + \mathcal{K}_h[n_h + 1] \\ \triangle &:= \mathcal{K}_h n_h + \mathcal{K}_c n_c. \end{aligned} \tag{75}$$

The solutions for ρ_{eg} and ρ_{ge} follow immediately, by using an exponential ansatz and by considering the initial condition (25)

$$\begin{aligned} \rho_{eg} &= \alpha \cdot \exp\Big[(-i\epsilon - \frac{1}{2}\square - \frac{1}{2}\triangle)t\Big], \\ \rho_{ge} &= \alpha^* \cdot \exp\Big[(i\epsilon - \frac{1}{2}\square - \frac{1}{2}\triangle)t\Big]. \end{aligned} \tag{76}$$

By the usage of the trace preservation $\rho_{ee} + \rho_{gg} = 1$, terms for ρ_{gg} and ρ_{ee} can be obtained,

$$\begin{aligned} \rho_{gg} &= \frac{\square + a\exp[(-\square - \triangle)t]}{\square + \triangle}, \\ \rho_{ee} &= \frac{\triangle - a\exp[(-\square - \triangle)t]}{\square + \triangle}. \end{aligned} \tag{77}$$

Because of the initial condition, the constant a can be determined as
$a = -P(\square + \triangle) + \triangle$. Therefore, the general solution of the 2 thermal baths density matrix is

$$\boxed{\hat{\rho}(t) = \begin{pmatrix} \exp[(-\square - \triangle)t] \cdot \{-P + \frac{\triangle}{\square+\triangle}\} + \frac{\square}{\square+\triangle} & \alpha^* \cdot \exp\Big[(i\epsilon - \frac{1}{2}\square - \frac{1}{2}\triangle)t\Big] \\ \alpha \cdot \exp\Big[(-i\epsilon - \frac{1}{2}\square - \frac{1}{2}\triangle)t\Big] & \exp[(-\square - \triangle)t] \cdot \{P - \frac{\triangle}{\square+\triangle}\} + \frac{\triangle}{\square+\triangle} \end{pmatrix}}. \tag{78}$$

From this general solution one can receive the steady-state solution, where the coherence disappears,

$$\hat{\rho}_\infty = \begin{pmatrix} \frac{\square}{\square+\triangle} & 0 \\ 0 & \frac{\triangle}{\square+\triangle} \end{pmatrix}. \tag{79}$$

The steady-state case, now, can be used in the general solution form again (see. Eq. (5))

$$\hat{\rho}(t) = \begin{pmatrix} 1-P & 0 \\ 0 & P \end{pmatrix} e^{-(\triangle+\square)t} + \begin{pmatrix} \frac{\square}{\square+\triangle} & 0 \\ 0 & \frac{\triangle}{\square+\triangle} \end{pmatrix}. \tag{80}$$

6.2 Energy considerations, heat flow and temperature limits

Determining now the expectation value of the Hamiltonian with Eq. (6) gives

$$\langle \hat{H} \rangle(t) = \epsilon \Big[\exp[(-\triangle - \square)t] \Big\{ P - \frac{\triangle}{\triangle + \square} \Big\} + \frac{\triangle}{\square + \triangle} \Big]. \tag{81}$$

If now the time derivative of this expectation value gets determined (see Eq. (7), the solution is the same as the sum of the heat flows from the hot and the cold bath

$$\epsilon \cdot \Big\{ [P(-\triangle - \square) + \triangle] \exp[(-\triangle - \square)t] \Big\} := J_c + J_h. \tag{82}$$

In contrast to the case with one thermal bath, there exists a heat flow even in the steady-state. This can be separated into the heat flow J_h from the hot bath to the qubit and J_c as the heat flow from the qubit to the cold bath. The relation $J_h = -J_c$ can be used for these two part-flows. Also, the heat flow J_c in the steady-state can be calculated with Eq. (13), where $\mathcal{L}_c$ labels the super-operator for the cold thermal bath term in the master equation. This can be taken out of the rate equations Eqs. (74) (a-d).

With the formula for the heat flow J_c, the two heat flows can be determined as

$$\begin{aligned} J_c &= \frac{\epsilon \mathcal{K}_c \mathcal{K}_h [n_c - n_h]}{\mathcal{K}_c(2n_c + 1) + \mathcal{K}_h(2n_h + 1)}, \\ J_h &= \frac{\epsilon \mathcal{K}_c \mathcal{K}_h [n_h - n_c]}{\mathcal{K}_c(2n_c + 1) + \mathcal{K}_h(2n_h + 1)}. \end{aligned} \tag{83}$$

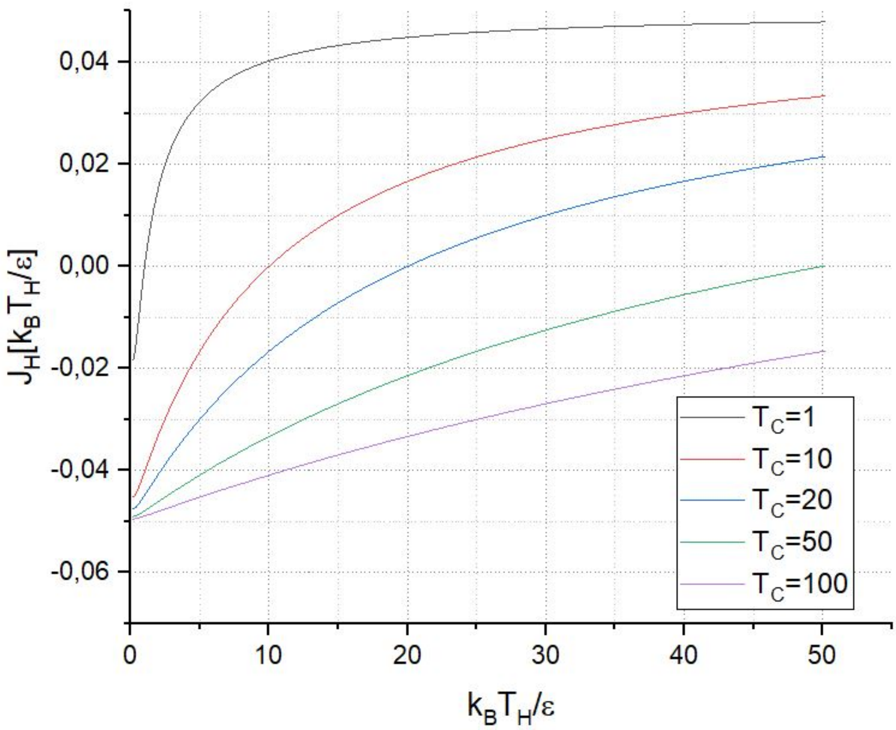

Figure 6: Heat flow J_h in dependence of relation between the hot temperature T_h and the energy ϵ for different cold temperature baths.

For the thermal limits, the relations $\lim_{T_c \to 0} n = 0$ and $\lim_{T_h \to \infty} n = \infty$ from the introduction give the following result for the density matrix

$$\hat{\rho}(t) = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}. \tag{84}$$

Physically, it is the same situation as the interaction of the qubit with a thermal bath at temperature $T_c = 0$ (ref. (64)) and the hot limit for one thermal bath. Also, the solution for the density matrix labels the equipartition of energy, since the probabilities for being in the ground state ρ_{gg} and the probability for being in the excited state ρ_{ee} are equal.

Now, the situation, where the two temperatures of the thermal baths have hardly a difference, can also be examined. Therefore, $T_c \approx T_h$ and $n_h \approx n_c$. For the substituted variables $\square$ and $\triangle$ it applies

$$\begin{aligned} \square &= (\mathcal{K}_c + \mathcal{K}_h)[n+1] = \mathcal{K}(n+1), \\ \triangle &= (\mathcal{K}_c + \mathcal{K}_h)n = \mathcal{K}n, \end{aligned} \tag{85}$$

Where $\mathcal{K}_c + \mathcal{K}_h = \mathcal{K}$ was used.
Putting this into the generall solution for the density matrix, leads to

$$\hat{\rho}(t) = \begin{pmatrix} -n_F + (n_F - P) \cdot \exp[-\mathcal{K}t(2n+1)] + 1 & \alpha^* \cdot \exp\Big[(i\epsilon - \mathcal{K}(n + \frac{1}{2}))t\Big] \\ \alpha \cdot \exp\Big[(-i\epsilon - \mathcal{K}(n + \frac{1}{2}))t\Big] & n_F + (P - n_F) \cdot \exp[-\mathcal{K}t(2n+1)] \end{pmatrix}. \tag{86}$$

Which is exactly the same as Eq. (58).

6.3 Heat, work, entropy growth and the laws of thermodynamics

A basis concept in thermodynamics consists of the laws of thermodynamics. These were mentioned in the theory part already and here, they shall get proofed for the system of 2 thermal baths and a qubit. As the 1$^{\text{st}}$ law of thermodynamics states,

$$U = \langle Q \rangle + \langle W \rangle. \tag{87}$$

For this system, $\langle W \rangle = 0$, because $\partial_t \hat{H} = 0$, such that the internal energy (as well as the expectation value of the heat), can be determined as

$$U = \langle Q \rangle = \epsilon \Bigg[\exp[(-\triangle - \square)t] \Big\{ P - \frac{\triangle}{\triangle + \square} \Big\} + \frac{\triangle}{\square + \triangle} \Bigg] \equiv \langle \hat{H} \rangle. \tag{88}$$

The aim now, is to proof the 2$^{\text{nd}}$ law of thermodynamics. Therefore, the entropy growth Σ (in the steady-state) can be calculated equivalent to Eq. (66). $\partial_t S = 0$, because $\partial_t \hat{\rho} = 0$ in the steady-state. Because of that, the entropy growth is determined as

$$\begin{aligned} \Sigma &= -\frac{J_c}{T_c} - \frac{J_h}{T_h} = \frac{J_h(T_h - T_c)}{T_c T_h} \\ &= \frac{\epsilon \mathcal{K}_c \mathcal{K}_h [n_h - n_c](T_h - T_c)}{\mathcal{K}_c[2n_c + 1] + \mathcal{K}_h[2n_h + 1] T_c T_h} \geqslant 0. \end{aligned} \tag{89}$$

The inequality $\Sigma \geqslant 0$, which is equal to the 2$^{\text{nd}}$ law of thermodynamics, is true, because all variables are determined as positive and because $n_h \geqslant n_c$ as well as $T_h \geqslant T_c$, since T_c is defined as the colder temperature and T_h as the hotter one.

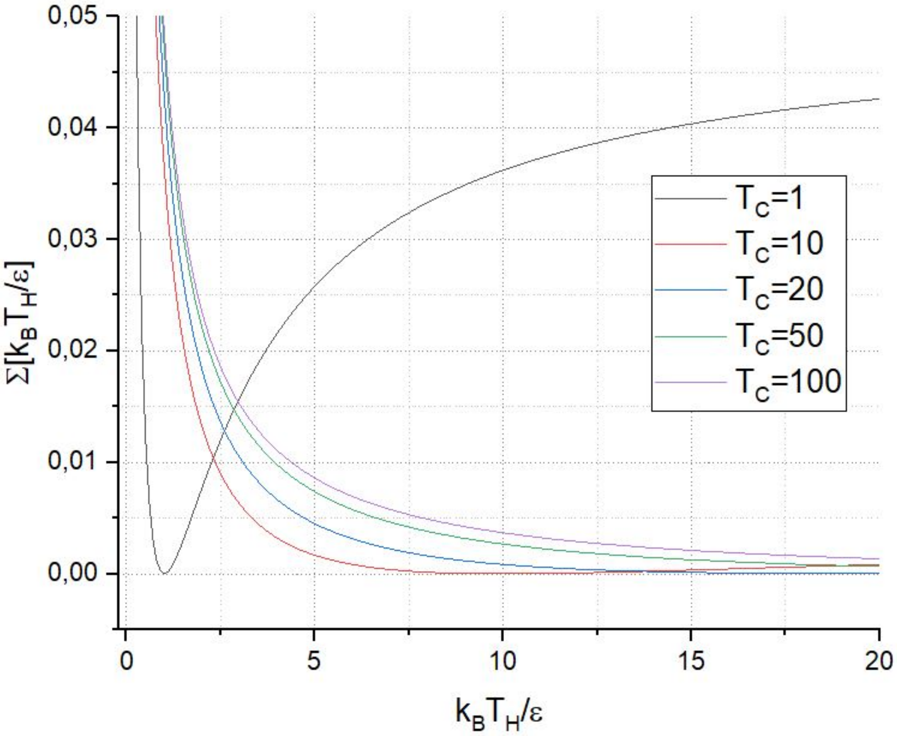

Figure 7: Entropy production Σ in steady-state for a system that consists of 2 thermal baths for the same temperatures T_c as in the plot for the heat flow in dependence of the hot temperature T_h in relation to the energy ϵ

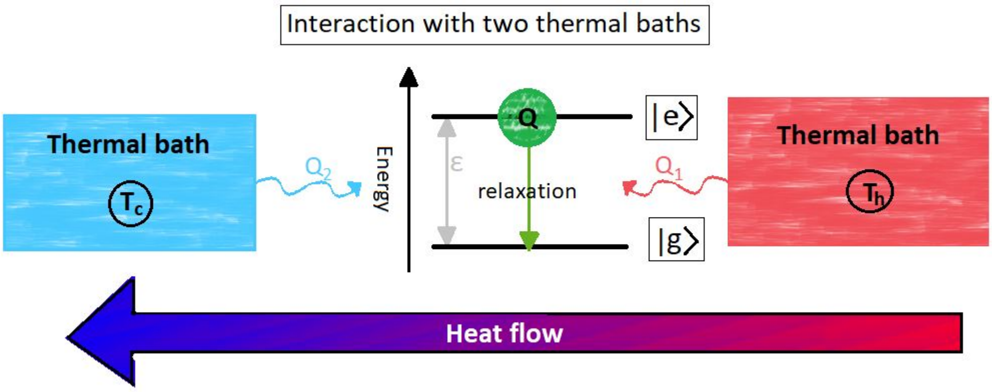

Figure 8: Construction of the system, which consists of two thermal baths and the qubit, working mechanisms, change in energy, heat Q_1 from the hot bath and heat Q_2 from the cold bath; heat flow.

7 Driven qubit coupled with two thermal baths

In the last section, a system is combined from two thermal baths and a laser, which all together influence the qubit.

7.1 Steady-state solution

Since there acts a laser on the qubit, the quantum master equation would have to deal with a time-dependent Hamiltonian, which is the same as in section 4 (see Eq. (35)).
Thats why, again a base transformation into a rotating base has to be done. This leads to a time independent Hamiltonian, which is again the same as in section 4 (see Eq. (37)). The whole calculation is done in the rotating frame.

The master equation for this system reads

$$\partial_t \hat{\rho} = -i[\hat{H}, \hat{\rho}] + \sum_{\alpha=c,h} \mathcal{K}_\alpha (n_\alpha + 1) \hat{\mathcal{D}}[\hat{\sigma}]\hat{\rho} + \mathcal{K}_\alpha n_\alpha \hat{\mathcal{D}}[\hat{\sigma}^\dagger]\hat{\rho}, \tag{90}$$

which is the same as the master equation for the situation with two thermal baths (without the laser; see Eq. (72)).
The master equation can be rewritten as a system of rate equations

$$\begin{aligned}
\partial_t \rho_{gg} &= -\rho_{gg}(\mathcal{K}_h n_h + \mathcal{K}_c n_c) + \rho_{ee}[\mathcal{K}_c(n_c + 1) + \mathcal{K}_h(n_h + 1)] - if[\rho_{eg} - \rho_{ge}], && \text{(91a)}\\
\partial_t \rho_{ge} &= -\rho_{ge}\left\{\mathcal{K}_c\left(n_c + \frac{1}{2}\right) + \mathcal{K}_h\left(n_h + \frac{1}{2}\right)\right\} - if[\rho_{ee} - \rho_{gg}], && \text{(91b)}\\
\partial_t \rho_{eg} &= -\rho_{eg}\left\{\mathcal{K}_c\left(n_c + \frac{1}{2}\right) + \mathcal{K}_h\left(n_h + \frac{1}{2}\right)\right\} - if[\rho_{gg} - \rho_{ee}], && \text{(91c)}\\
\partial_t \rho_{ee} &= \rho_{gg}(\mathcal{K}_h n_h + \mathcal{K}_c n_c) - \rho_{ee}[\mathcal{K}_c(n_c + 1) + \mathcal{K}_h(n_h + 1)] - if[\rho_{ge} - \rho_{eg}]. && \text{(91d)}
\end{aligned}$$

Now, these rate equations can be solved for the steady-state by putting all time derivative terms equal to zero. This steady-state solutions for the driven qubit, which is coupled with two thermal baths, reads

$$\boxed{\hat{\rho}_\infty = \begin{pmatrix} \frac{\star\heartsuit}{8f^2+4(\heartsuit)^2} + \frac{1}{2} & \frac{if\star}{4f^2+2(\heartsuit)^2} \\ \frac{-if\star}{4f^2+2(\heartsuit)^2} & \frac{-\star\heartsuit}{8f^2+4(\heartsuit)^2} + \frac{1}{2} \end{pmatrix},} \tag{92}$$

with the substituted variables are determined as

$$\begin{aligned}
\heartsuit &= \mathcal{K}_c\left(n_c + \frac{1}{2}\right) + \mathcal{K}_h\left(n_h + \frac{1}{2}\right),\\
\star &= \mathcal{K}_c + \mathcal{K}_h.
\end{aligned} \tag{93}$$

7.2 Power and heat flow

Now, the power of the driven system shall get examined. Therefore, Eq. (16) leads to

$$\begin{aligned} P &= \mathrm{Tr}\left\{ \begin{pmatrix} 0 & i\epsilon f \\ -i\epsilon f & 0 \end{pmatrix} \begin{pmatrix} \frac{\star\heartsuit}{8f^2+4(\heartsuit)^2} + \frac{1}{2} & \frac{if\star}{4f^2+2(\heartsuit)^2}, \\ \frac{-if\star}{4f^2+2(\heartsuit)^2} & \frac{-\star\heartsuit}{8f^2+4(\heartsuit)^2} + \frac{1}{2} \end{pmatrix} \right\} \\ &= \frac{2\epsilon f^2 \star}{4f^2 + 2(\heartsuit)^2}, \end{aligned} \tag{94}$$

where the first matrix is calculated as the product of $\hat{U}\hat{P}\hat{U}^\dagger$ and the substituted variables (93) were used. The power depends on the rates $\mathcal{K}_c$ and $\mathcal{K}_h$ through Eq. (93), with which the heat transition between the two thermal baths and the qubit proceeds, also from the energy differences ϵ between the two states of the qubit and f between the states of the laser. It leads to growth in the internal energy of the qubit until the steady state is reached, then there is no growth or decline anymore. Therefore the entropy production is non-negative for all times.

In the next step, the heat flow, which comes from the two thermal baths, shall be determined. Equivalent to the calculation of the heat flow for the system with just the laser and the qubit (see Eq. (49)), the heat flow for this system can be calculated as

$$\begin{aligned} J_h &= \mathrm{Tr}\left\{\epsilon|e\rangle\langle e|\hat{\mathcal{L}}_h\hat{\rho}\right\} \\ &= \frac{-\epsilon\mathcal{K}_h \star \heartsuit(2n_h+1)}{8f^2+4(\heartsuit)^2} + \frac{1}{2}\epsilon\mathcal{K}_h, \end{aligned} \tag{95}$$

and equivalent to that, the heat flow from the cold bath

$$J_c = \frac{-\epsilon\mathcal{K}_c \star \heartsuit(2n_c+1)}{8f^2+4(\heartsuit)^2} + \frac{1}{2}\epsilon\mathcal{K}_c. \tag{96}$$

In this situation, the two heat flows J_c and J_h do not just have the same magnitude with a different sign, since the presence of the laser changes the heat flow for the qubit.

7.3 Entropy, entropy production and 2nd law of thermodynamics

Now, the 2nd law of thermodynamics shall get verified, by calculating the entropy growth and by showing, that it is non-negative. First, the entropy is calculated by using the formula for the von Neumann entropy (see Eq. (57)) and the populations from Eq. (92) as

$$\begin{aligned} S(\hat{\rho}) = -k_B&\left\{\left(\frac{\star\heartsuit}{8f^2+4(\heartsuit)^2} + \frac{1}{2}\right)\cdot\ln\left[\frac{\star\heartsuit}{8f^2+4(\heartsuit)^2} + \frac{1}{2}\right]\right. \\ &\left.+\left(\frac{-\star\heartsuit}{8f^2+4(\heartsuit)^2} + \frac{1}{2}\right)\cdot\ln\left[\frac{-\star\heartsuit}{8f^2+4(\heartsuit)^2} + \frac{1}{2}\right]\right\}. \end{aligned} \tag{97}$$

Now, the time derivative of the von Neumann entropy is equal to zero, because it gets calculated with the time derivative of the density matrix and therefore, the steady-state density matrix is used. (see Eq. (92))
This result can be used for determining the entropy production Σ as

$$\begin{aligned}\Sigma &= -\frac{J_h}{T_h} - \frac{J_c}{T_c} \geqslant 0 \\ &= \frac{\epsilon\mathcal{K}_h \star \heartsuit(2n_h+1)}{T_h[8f^2+4(\heartsuit)^2]} - \frac{1}{2}\frac{\epsilon\mathcal{K}_h}{T_h} + \frac{\epsilon\mathcal{K}_c \star \heartsuit(2n_c+1)}{T_c[8f^2+4(\heartsuit)^2]} - \frac{1}{2}\frac{\epsilon\mathcal{K}_c}{T_c}.\end{aligned} \tag{98}$$

The inequation $\Sigma \geqslant 0$ from the first line of Eq. (98) expresses the 2^{nd} law of thermodynamics. It is true, because

$$\begin{aligned}&\frac{\epsilon\mathcal{K}_i \star \heartsuit(2n_i+1)}{T_i[8f^2+4(\heartsuit)^2]} \geqslant \frac{1}{2}\frac{\epsilon\mathcal{K}_i}{T_i}, \\ \Leftrightarrow\ &\frac{\star\heartsuit(2n_i+1)}{4f^2+2(\heartsuit)^2} \geqslant 1,\end{aligned} \tag{99}$$

where $i \in [c, h]$. Now, since all elements are determined as positive, this is always true.

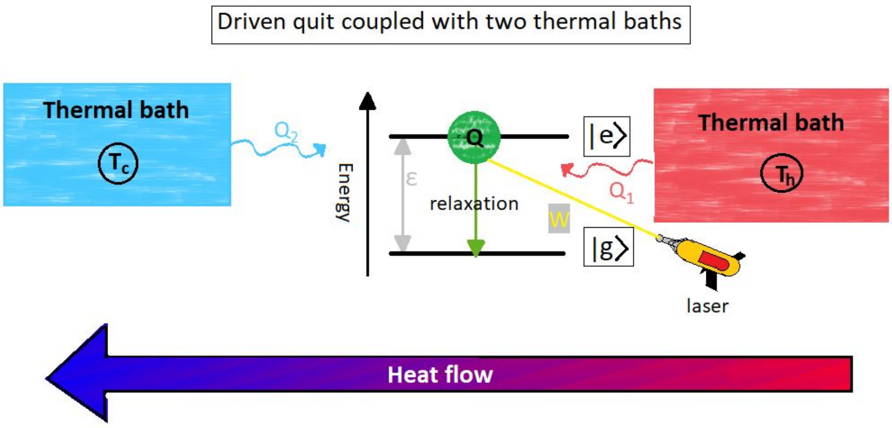

Figure 9: Construction of the system, which consists of two thermal baths, a laser and the qubit, working mechanisms, change in energy and heat flow.

8 Results

In the examples, that were discussed in the previous sections, some fundamental systems were described and from that, physical properties like power and heat flow, or like the von Neumann entropy could be determined. Also, the 1st and 2nd law of thermodynamics were proven for some of the systems.
The density matrices of the single processes looked very different at the end of the interactions, since the influence of a thermal bath changes the mixture of the system in another way, than the laser system does. The qubit ends up in a not well-defined state for all systems except of the relaxation process itself, as can be seen in the sketches at the end of the sections. The only thing, that can be well defined for the other systems, is the probability for the qubit to be in the excited state $|e\rangle$ or in the ground state $|g\rangle$. The actual state of the qubit can be determined separate, by a measurement.

In general, the theory fits well with the expectations from practical experiences, i.e. that for the system with one thermal bath after the system has equilibrated with the qubit, there is no heat flow anymore. Or, in contrast to this system, that for the system with two thermal baths, there is a heat flow, even in the steady-state, because the two reservoirs are so big, that they aren't able to equilibrate with each other.
For the single systems, properties like the heat, that gets released from the qubit, or transported by it, and the power, that has to be expended by the laser, were calculated. With calculations like these, the single magnitudes can be found for heat engines or refrigerators, which are the most important applications in quantum thermodynamics.

9 Outlook

In this report, only a few basic aspects of quantum thermodynamics were considered, also the examined systems were combined from just a few elements. The whole quantum thermodynamics field is rapidly evolving and there is still much research, that can be done in it. The focus, in general, lies on the different aspects of quantum mechanics and thermodynamics as well as the question on how they can be combined. What is also interesting in practical usage, is, how quantum engines, like Carnot engines (with spins as the working fluid), Otto engines or Diesel engines (that operate with a particle in a box as the working fluid), can be designed and how their efficiency can be improved. Also possible are refrigerators. For those machines, the heat flow is reversed. **[1]**

Therefore, other systems are possible, too, i.e. a system that is combined out of two qubits and two thermal baths, where the two qubits interact with the thermal baths, but also with each other. In this example, entanglement is also an important mechanism **[1]**.

There are some more effects in quantum thermodynamics, that can be examined. These are, for example, fluctuations, or the principle, that energy can be taken out of coherence **[1]**. Until this point, the effects are known, but it is also possible to examine some new aspects.

One of these aspects would be the different point of few, when effects from the first quantization are considered, than when effects of the second quantization are considered. According to that, effects of entanglement can be considered, which also can be used for gaining energy. The differences in the two quantization levels are dealing among others with classical jumps (first quantization) and Rabi oscillations on the other hand (second quantization). I.e., this has a big effect on electrical current.

For these effects, which the different point of few has, there is still research necessary.

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