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Work and heat at the mesoscale

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Abstract: Understanding the conversion between heat and work by heat engines led to the discoveries of entropy and to the formulation of the Second law of classical macroscopic thermodynamics. At the microscale and mesoscale, quantum coherences are a potential resource for various quantum processes. Quantum coherences can be used to enhance the performance of various devices beyond the limits demanded by classical physics. Recently many models have been established clarifying how coherences affect the speed and irreversibility of thermodynamic processes and raising the question of what experimentally relevant consequences various generalizations of the formalism of classical thermodynamics to the microscopic level may have. Here we study a few of these models in great detail. Specifically, we discuss fluctuations of coherence-enhanced heat currents, propose a model of a heat engine that does work while being in a steady state, and derive a condition on the rate of decoherence that specifies, when coherence-enhanced currents provide a significant advantage over the case without any coherence. Then we discuss coherence-inducing heat bath from the quantum thermodynamics point of view. We show, that coherences generated in this way provide an advantage in the extraction of work. We point out, that there is a need to modify the Second law of thermodynamics for this system. Our results provide new useful physical insights into the active research on the role of coherence in quantum thermodynamics and quantum optics.

Keywords: work, heat, quantum coherence, heat engine, two-level system, entropy production, quantum advantage, open systems, weak coupling, Lindblad master equation

Název práce: Teplo a práce v mesoskopických systémech

Autor: Bc. Šimon Pajger

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Abstrakt: Pochopení přeměny tepla a práce v tepelních strojích vedlo k objevu entropie a k formulaci druhého zákona klasické makroskopické termodynamiky. V mikroskopické a mesoskopické škále jsou kvantové koherence potenciálním zdrojem pro různé kvantové procesy. Kvantové koherence lze využít ke zvýšení výkonu různých zařízení za hranice klasické fyziky. V poslední době bylo vytvořeno mnoho modelů objasňujících, jak koherence ovlivňují rychlost a nevratnost termodynamických procesů, a vyvolávajících otázku, jaké experimentálně relevantní důsledky mohou mít různá zobecnění formalismu klasické termodynamiky na mikroskopickou úroveň. Zde se podrobně zabýváme několika z těchto modelů. Konkrétně se zabýváme fluktuacemi tepelných proudů zesílených koherencí, navrhujeme model tepelného stroje, který vykonává práci, zatímco je v ustáleném stavu, a taky odvozujeme podmínku na rychlost dekoherence, která určuje, kdy proudy zesílené koherencí poskytují významnou výhodu oproti případu bez jakékoli koherence. Dále se zabýváme tepelnou lázní indukující koherenci, z hlediska kvantové termodynamiky. Ukazujeme, že takto generované koherence poskytují výhodu při získávání práce. Poukazujeme na to, že pro tento systém je třeba upravit druhý termodynamický zákon. Naše výsledky poskytují nové užitečné fyzikální poznatky pro aktivní výzkum role koherence v kvantové termodynamice a kvantové optice.

Klíčová slova: práce, teplo, kvantová koherence, tepelný stroj, dvouhladinový systém, produkce entropie, kvantová výhoda, otevřené systémy, slabá vazba, Lindbladova řídíci rovnice

Contents

Introduction

The reason for many of the phenomena that are unique to quantum mechanics is quantum coherence (superposition). That is the fact, that quantum systems may be in different states at the same time. Therefore the goal of many researchers is to use this feature to discover new quantum phenomena, that would provide a quantum advantage in various tasks [1–6].

The theory of quantum coherence is a very wide research field. In our work, we focus on its applications that concern quantum thermodynamics [2, 7–12]. In this area of research, one of the central questions is the effect of quantum coherences on the performance of heat engines, and there is still no clear consensus on the answer [2, 7, 8, 13]. Authors of a recent work [14] have approached this problem by separating the effects of the coherences between the states with the same energy and the coherences between the states with different energy. Authors in [14] presented a model that uses quantum coherences to enhance heat and particle currents beyond the limits of classical physics. We will call this effect coherence-enhanced currents. We will further explore this model, bringing useful physical insight, and calculating fluctuations of the coherence-enhanced current. We will also generalize the model to propose a new heat engine, that utilizes coherence-enhanced particle current to increase the chemical potential of particles, while itself being in a non-equilibrium steady state.

Every realistic system is open to unavoidable interaction with the environment, and this interaction induces irreversible processes, typically decoherence and dissipation [15]. Therefore we also discuss the possible effects decoherence can have on coherence-enhanced currents. And although we will show, that coherence-enhanced currents can provide a significant quantum advantage if the decoherence is not too fast, it is apparent that decoherence is a major obstacle for various applications that exploit quantum coherences as a resource. Therefore there is an effort to neutralize these effects of interaction with the environment [16, 17].

Another remarkable model has been introduced in Ref. [18], where it has been shown, that it is possible to engineer an environment in such a way, that spin interacting with it retains some of its coherences with respect to the energy eigenbasis. This holds true even for long-time dynamics [18]. This phenomenon is called coherence trapping. But it has some limitations: for example, it is impossible to use this mechanism to trap coherences if the system has no coherences, to begin with. The authors of [19] removed these limitations by proposing such a system-bath interaction that does not just trap coherences, but instead forms steady-state coherences in a generic two-level system, for every possible initial state. We will analyze the model proposed in [19] from the perspective of quantum thermodynamics. At first, we ask, whether coherences formed in this way can provide a quantum advantage for the extraction of work from the reservoir. Then we examine possible formulations of the second law for such types of models.

1. Coherence-Enhanced Currents

In a recent paper [14], the authors studied the effects of quantum coherences on particle and heat currents. They presented a model in which current was enhanced by quantum coherences.

In classical physics, the smaller the temperature difference between the reservoirs, the smaller the entropy production, but at the same time the smaller the heat current itself, while the mean heat current between two systems with the same temperature is zero. Thus, if we want the heat engine to have some non-zero power, it must exchange heat with the reservoirs while having different temperature, than those reservoirs. This in turn decreases the efficiency, which is why this problem is in finite-time thermodynamics called power-efficiency trade-off, and it concerns also small systems, that do not have well-defined temperatures [20, 21].

The paper [14] argues that due to coherence-enhanced current, it is possible to have a finite heat current even for a temperature difference approaching 0, which can then be used to construct a heat engine with a finite power and efficiency arbitrarily close to the the Carnot efficiency.

In this chapter, we will bring new physical insight into what causes this effect. At the same time, the fluctuations of this current were not discussed in the original paper, and according to [11], there exists also a trade-off between dissipation and fluctuations. Therefore we will investigate, what is the magnitude of the fluctuations of coherence-enhanced currents, and discuss the possible effect that decoherence can have on coherence-enhanced currents.

1.1 Model With Single Heat Bath

The basic model used in the paper is a two-level system that has each of the levels N times degenerated. The system is interacting with a reservoir of inverse temperature β. Thanks to degeneracy, this model is very convenient for us to see different effects of coherences between states with the same energy and states with different energy. One of the things we are going to be interested in is the asymptotic behavior for $N \gg 1$.

The system is initialized in a state where all excited states have occupation probability p_e/N and all ground states have occupation probability $(1-p_\mathrm{e})/N = p_\mathrm{g}/N$, where p_e is thus a probability of the system being in some of the excited states.

We assume that the evolution of the system is given by the Lindblad master equation

$$\partial_t \rho = -i[H, \rho] + D(\rho)\,, \tag{1.1}$$

where we set $\hbar = 1$, and D is dissipator

$$D(\rho) = \sum_\omega \gamma(\omega)[L_\omega \rho L_\omega^\dagger - \frac{1}{2}\{L_\omega^\dagger L_\omega, \rho\}]\,, \tag{1.2}$$

where the coefficients $\gamma(\omega)$ satisfy the local detailed balance relation

$$\frac{\gamma(\omega)}{\gamma(-\omega)} = \exp(\beta\omega) \tag{1.3}$$

and $L_\omega, L_\omega^\dagger$ are the Lindblad operators describing transitions between states with energy difference ω.

Let us break this down mathematically for a better imagination. If the Hamiltonian is

$$H = \left(\begin{array}{ccc|ccc} \omega_0 & 0 & 0 & & & \\ 0 & \ddots & 0 & & \mathbb{0} & \\ 0 & 0 & \omega_0 & & & \\ \hline & & & 0 & 0 & 0 \\ & \mathbb{0} & & 0 & \ddots & 0 \\ & & & 0 & 0 & 0 \end{array}\right), \tag{1.4}$$

where the blocks are $N \times N$ as N is the degeneracy of both the ground and excited state, then the Lindblad operators will be

$$L_{\omega_0} = L_{-\omega_0}^\dagger = \left(\begin{array}{ccc|c} & \mathbb{0} & & \mathbb{0} \\ \hline 1 & \cdots & 1 & \\ \vdots & \ddots & \vdots & \mathbb{0} \\ 1 & \cdots & 1 & \end{array}\right), \tag{1.5}$$

and

$$L_{\omega_0}^\dagger = L_{-\omega_0} = \left(\begin{array}{c|ccc} & 1 & \cdots & 1 \\ \mathbb{0} & \vdots & \ddots & \vdots \\ & 1 & \cdots & 1 \\ \hline \mathbb{0} & & \mathbb{0} & \end{array}\right). \tag{1.6}$$

This defines the model. In the following subsections, we will calculate how much heat will flow (and with what fluctuations) between the two-level system and a reservoir, and also how much entropy will be produced in the process.

1.1.1 Heat Current

Without Coherences

To study the behavior of the system in a case when the initial state is without coherences, we choose the density matrix by evenly distributing the probabilities among the states with the same energy, i.e.

$$\rho_{\mathrm{nc}}(0) = \left(\begin{array}{ccc|ccc} \frac{p_\mathrm{e}}{N} & 0 & 0 & & & \\ 0 & \ddots & 0 & & \mathbb{0} & \\ 0 & 0 & \frac{p_\mathrm{e}}{N} & & & \\ \hline & & & \frac{p_\mathrm{g}}{N} & 0 & 0 \\ & \mathbb{0} & & 0 & \ddots & 0 \\ & & & 0 & 0 & \frac{p_\mathrm{g}}{N} \end{array}\right), \tag{1.7}$$

then the first term of (1.1) is zero and the time evolution is given just by the dissipator $D(\rho)$ (1.2). For Hamiltonian (1.4) the sum in (1.2) goes over two possible energy differences ω namely $\omega = \omega_0$ describes the transitions from the excited level to the ground level and $\omega = -\omega_0$ the transitions from the ground level to the excited level. For each of the values of ω, we have two terms. For example, for $\omega = -\omega_0$ there will be one term

$$\gamma(-\omega_0)L_{-\omega_0}\rho_{\mathrm{nc}}(0)L^\dagger_{-\omega_0} = \gamma(-\omega_0)\left(\begin{array}{ccc|c} p_{\mathrm{g}} & \cdots & p_{\mathrm{g}} & \\ \vdots & \ddots & \vdots & \mathbb{0} \\ p_{\mathrm{g}} & \cdots & p_{\mathrm{g}} & \\ \hline & \mathbb{0} & & \mathbb{0} \end{array}\right), \tag{1.8}$$

where we just substituted from (1.5), (1.6), (1.7), and the second term

$$-\gamma(-\omega_0)\frac{1}{2}\{L^\dagger_{-\omega_0}L_{-\omega_0}, \rho_{\mathrm{nc}}(0)\} = \gamma(-\omega_0)\left(\begin{array}{c|ccc} \mathbb{0} & & \mathbb{0} & \\ \hline & -p_{\mathrm{g}} & \cdots & -p_{\mathrm{g}} \\ \mathbb{0} & \vdots & \ddots & \vdots \\ & -p_{\mathrm{g}} & \cdots & -p_{\mathrm{g}} \end{array}\right). \tag{1.9}$$

By analogy, for $\omega = \omega_0$ we get in turn the transitions from the excited level to the ground level

$$\begin{aligned} &\gamma(\omega_0)[L_{\omega_0}\rho_{\mathrm{nc}}(0)L^\dagger_{\omega_0} - \frac{1}{2}\{L^\dagger_{\omega_0}L_{\omega_0}, \rho_{\mathrm{nc}}(0)\}] = \\ &= \gamma(\omega_0)\left(\begin{array}{ccc|ccc} -p_{\mathrm{e}} & \cdots & -p_{\mathrm{e}} & & & \\ \vdots & \ddots & \vdots & & \mathbb{0} & \\ -p_{\mathrm{e}} & \cdots & -p_{\mathrm{e}} & & & \\ \hline & & & p_{\mathrm{e}} & \cdots & p_{\mathrm{e}} \\ & \mathbb{0} & & \vdots & \ddots & \vdots \\ & & & p_{\mathrm{e}} & \cdots & p_{\mathrm{e}} \end{array}\right). \end{aligned} \tag{1.10}$$

When we sum those two contributions we get that

$$\partial_t\rho_{\mathrm{nc}}(0) = (\gamma(-\omega_0)p_{\mathrm{g}} - \gamma(\omega_0)p_{\mathrm{e}})\left(\begin{array}{ccc|ccc} 1 & \cdots & 1 & & & \\ \vdots & \ddots & \vdots & & \mathbb{0} & \\ 1 & \cdots & 1 & & & \\ \hline & & & -1 & \cdots & -1 \\ & \mathbb{0} & & \vdots & \ddots & \vdots \\ & & & -1 & \cdots & -1 \end{array}\right), \tag{1.11}$$

where by $\partial_t\rho_{\mathrm{nc}}(0)$ we mean the time derivative of the density matrix $\rho_{\mathrm{nc}}(t)$ in time $t = 0$. The time derivative of the probability of the system being in an excited state is obtained from (1.11) as the trace over the excited block

$$\partial_t p_{\mathrm{e}}(0) = N(\gamma(-\omega_0)p_{\mathrm{g}} - \gamma(\omega_0)p_{\mathrm{e}})\,. \tag{1.12}$$

Interesting choice of p_{e} is

$$p_{\mathrm{e}} = \frac{1}{\left(1 + \frac{1}{N}\right)e^{\beta\omega_0} + 1}\,. \tag{1.13}$$

In the state, with p_{e} chosen according to (1.13), the system will be for large N asymptotically close to equilibrium with the reservoir, and therefore for this choice, less entropy will be produced. Therefore this choice of p_e will be crucial for the efficiency of heat engines to asymptotically approach the Carnot efficiency.

When we substitute (1.13) into (1.12) we get the probability current for this choice of p_e

$$\partial_t p_\mathrm{e}(0) = \gamma(\omega_0)\frac{1}{\left(1+\frac{1}{N}\right)e^{\beta\omega_0}+1}\,. \tag{1.14}$$

We define a heat current J_nc from the reservoir to the system as a time derivative of the mean energy of the system. Then from (1.14), we obtain the heat current from the reservoir to the system

$$J_\mathrm{nc}(0) = \omega_0\partial_t p_\mathrm{e}(0) = \omega_0\gamma(\omega_0)\frac{1}{\left(1+\frac{1}{N}\right)e^{\beta\omega_0}+1}\,. \tag{1.15}$$

We can also write $J_\mathrm{nc}(0) = \omega_0\gamma(\omega_0)p_\mathrm{e}$. But note that this is only true if we choose p_e according to (1.13).

From (1.12) we see that degeneracy would N times increase the magnitude of the current for a fixed probability of the system being in an excited state, but for the choice of p_e according to (1.13) (depending on the degree of degeneracy) the current asymptotically does not depend on degeneracy (we may write $J_\mathrm{nc}(N) = O(1)$).

With Coherences

Now let us choose a density matrix such that the probabilities are evenly distributed among the states with the same energy and all non-diagonal elements in a given block also have this value

$$\rho_\mathrm{c}(0) = \left(\begin{array}{ccc|ccc} \frac{p_\mathrm{e}}{N} & \cdots & \frac{p_\mathrm{e}}{N} & & & \\ \vdots & \ddots & \vdots & & \mathbb{0} & \\ \frac{p_\mathrm{e}}{N} & \cdots & \frac{p_\mathrm{e}}{N} & & & \\ \hline & & & \frac{p_\mathrm{g}}{N} & \cdots & \frac{p_\mathrm{g}}{N} \\ & \mathbb{0} & & \vdots & \ddots & \vdots \\ & & & \frac{p_\mathrm{g}}{N} & \cdots & \frac{p_\mathrm{g}}{N} \end{array}\right), \tag{1.16}$$

i.e. as a mixture of two states

$$|e,+\rangle = (1,\cdots,1|0,\cdots,0)/\sqrt{N}\,, \tag{1.17}$$

$$|g,+\rangle = (0,\cdots,0|1,\cdots,1)/\sqrt{N}\,, \tag{1.18}$$

with weights p_e and p_g, respectively.

There are many valid measures of coherences [22]. Here we use l_1 norm of coherence, similarly, as it was done in [14]. This measure of coherences is defined in [22] as

$$C_{l_1}(\rho) = \sum_{i\neq j}|\rho_{ij}|\,. \tag{1.19}$$

Initial state (1.16) has the l_1 norm of coherence equal to $C_{l_1}(\rho_\mathrm{c}(0)) = N-1$. It is not possible to achieve a higher l_1 norm of coherence if we want the coherences between states with different energies to be zero. We choose the coherences between states with different energies to be zero to isolate the effect of the coherences between the states with the same energies.

Upon plugging (1.16) into (1.1), the first term of (1.1) is zero and the time evolution is given just by the dissipator $D(\rho)$ (1.2). For $\omega = -\omega_0$ we get the transitions from the ground level to the excited level

$$\gamma(-\omega_0)[L_{-\omega_0}\rho_\mathrm{c}(0)L^\dagger_{-\omega_0} - \frac{1}{2}\{L^\dagger_{-\omega_0}L_{-\omega_0}, \rho_\mathrm{c}(0)\}] = \\ = N\gamma(-\omega_0)\left(\begin{array}{ccc|ccc} p_\mathrm{g} & \cdots & p_\mathrm{g} & & & \\ \vdots & \ddots & \vdots & & \mathbb{0} & \\ p_\mathrm{g} & \cdots & p_\mathrm{g} & & & \\ \hline & & & -p_\mathrm{g} & \cdots & -p_\mathrm{g} \\ & \mathbb{0} & & \vdots & \ddots & \vdots \\ & & & -p_\mathrm{g} & \cdots & -p_\mathrm{g} \end{array}\right). \tag{1.20}$$

And for $\omega = \omega_0$ we get the transitions from the excited level to the ground level

$$\gamma(\omega_0)[L_{\omega_0}\rho_\mathrm{c}(0)L^\dagger_{\omega_0} - \frac{1}{2}\{L^\dagger_{\omega_0}L_{\omega_0}, \rho_\mathrm{c}(0)\}] = \\ = N\gamma(\omega_0)\left(\begin{array}{ccc|ccc} -p_\mathrm{e} & \cdots & -p_\mathrm{e} & & & \\ \vdots & \ddots & \vdots & & \mathbb{0} & \\ -p_\mathrm{e} & \cdots & -p_\mathrm{e} & & & \\ \hline & & & p_\mathrm{e} & \cdots & p_\mathrm{e} \\ & \mathbb{0} & & \vdots & \ddots & \vdots \\ & & & p_\mathrm{e} & \cdots & p_\mathrm{e} \end{array}\right). \tag{1.21}$$

When we sum these two contributions we get that

$$\partial_t\rho_\mathrm{c}(0) = N(\gamma(-\omega_0)p_\mathrm{g} - \gamma(\omega_0)p_\mathrm{e})\left(\begin{array}{ccc|ccc} 1 & \cdots & 1 & & & \\ \vdots & \ddots & \vdots & & \mathbb{0} & \\ 1 & \cdots & 1 & & & \\ \hline & & & -1 & \cdots & -1 \\ & \mathbb{0} & & \vdots & \ddots & \vdots \\ & & & -1 & \cdots & -1 \end{array}\right), \tag{1.22}$$

and thus the total change in the probability that the system is excited is N times larger than in the case without coherences. In other words, it is N^2 times larger than in the case where the energy levels are not degenerate (i.e. if the $N = 1$). We have

$$\partial_t p_\mathrm{e}(0) = N^2(\gamma(\omega_0)p_\mathrm{g} - \gamma(-\omega_0)p_\mathrm{e})\,, \tag{1.23}$$

and therefore so does the heat flow from the reservoir to the system

$$J_\mathrm{c}(0) = \omega_0\partial_t p_\mathrm{e}(0)\,. \tag{1.24}$$

This is one of the results of [14]: coherences between states with the same energy enhance heat current between the system and the reservoir. We believe that figure (1.1) brings some new physical intuition into why this happens.

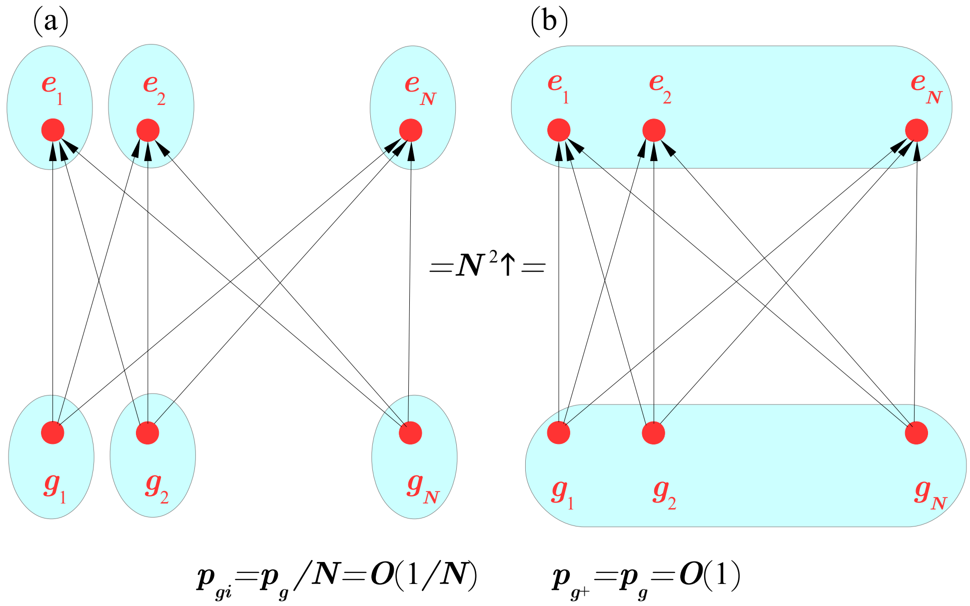

Figure 1.1: There are N^2 channels between the ground and excited states. This is because both of these energy levels are degenerate N times. So this fact does not depend on the chosen initial state. But for the incoherent case (a), each of the states has a probability of occupancy proportional to $1/N$, and hence the current through each of these channels will be $O(1/N)$, and hence (as we see from (1.12)) for a fixed p_e the resulting heat current will be N times larger than if the states were not degenerate. For the coherent case (b) where we chose the initial state as a mixture of states $|e,+\rangle$ and $|g,+\rangle$, the probabilities of occupying these two states are independent of N and in case of this choice of states, the probabilities between them flow through all N^2 channels, and the magnitude of the current through each of these channels is, therefore, independent of N. And hence for a fixed p_e the resulting heat current would be N^2 times larger than if the levels were not degenerate.

If we choose p_{e} according to (1.13) and the states as $|e,+\rangle$ and $|g,+\rangle$ according to (1.17) and (1.18), $J_{\mathrm{c}}(0) = N\omega_0\gamma(\omega_0)p_{\mathrm{e}}$ and hence $J_{\mathrm{c}}(N) = O(N)$.

Also, from (1.22) we can see that there will be no decoherence between the states with the same energy. All elements of each quadrant have the same time derivative. And the density matrix was initially in a state where all elements in the same block had the same value. By combining these two facts we see, that even as these values will change, still all elements in the same block will have the same value as each other.

Choice of Coherent State

We have seen, that coherences between states with the same energy can increase the magnitude of the heat current. In other words, when the initial state contains coherences, the upper bound for the current is higher than in the case when it can not contain coherences, these bounds can be found in [14].

But we would like to point out, that coherences may not always increase this current, on the contrary – they can also decrease it. We choose the initial state to be a mixture of two states

$$|e, alter.\rangle = (1,-1,1,-1,\cdots|0,\cdots,0)/\sqrt{N}\,, \tag{1.25}$$

$$|g, alter.\rangle = (0,\cdots,0|1,-1,1,-1,\cdots)/\sqrt{N}\,, \tag{1.26}$$

with weights p_{e} and p_{g} respectively. The density matrix of this state $\rho_{\mathrm{c,alter.}}$ would be block-diagonal, with p_{e}/N and $-p_{\mathrm{e}}/N$ (resp. p_{g}/N and $-p_{\mathrm{g}}/N$) alternating in blocks as squares on the chessboard (with always positive values on the diagonal). By substituting $\rho_{\mathrm{c,alter.}}$ into (1.19) we get, that it has l_1 norm of coherence $C_{l_1}(\rho_{\mathrm{c,alter.}}(0)) = N-1$, which is same as the state ρ_{c} (1.16).

In state $\rho_{\mathrm{c,alter.}}$, however, for N even, after substituting in (1.1) and following a procedure analogous to the one in subsection 1.1.1, we get that $\partial_t\rho_{\mathrm{c,alter.}} = 0$, so also $J_{\mathrm{c,alter.}}(0) = 0$. Thus we see that although allowing the coherences between the states with the same energy increases the upper bound for the heat current, the heat current may not increase if we just add coherences to a state that had no coherences. The heat current may as well decrease as a result of adding coherences into a state.

1.1.2 Entropy Production

In classical thermodynamics, when there is heat current J from a reservoir with inverse temperature β_{h} to a reservoir with inverse temperature β_{c}, the entropy production is

$$\partial_t S = J(\beta_{\mathrm{c}} - \beta_{\mathrm{h}})\,. \tag{1.27}$$

In our case, the heat is not flowing into the reservoir, but into the system, which has no defined temperature. But let us imagine that this system is “part of” a reservoir and is therefore in thermal equilibrium with the reservoir. From this, we can calculate what temperature such a reservoir would have to have, let us call it β_{EF}. We choose p_{e} according to (1.13) and set it to be equal to the probability of the system being in an excited state, if it would be in thermal equilibrium with a reservoir with inverse temperature $\beta_{\rm EF}$

$$p_{\rm e} = \frac{1}{\left(1+\frac{1}{N}\right)e^{\beta\omega_0}+1} = \frac{1}{e^{\beta_{\rm EF}\omega_0}+1}\,, \tag{1.28}$$

from that, we can express $\beta_{\rm EF}$ as

$$\ln\left(1+\frac{1}{N}\right)+\beta\omega_0 = \beta_{\rm EF}\omega_0\,, \tag{1.29}$$

from which we can express the ratio between the heat transferred and the entropy produced, by substituting into (1.27)

$$\frac{\partial_t S}{J} = \beta_{\rm EF}-\beta = \frac{1}{\omega_0}\ln\left(1+\frac{1}{N}\right)\,. \tag{1.30}$$

This is indeed the correct ratio which was derived in [14], where instead of using the trick with effective temperature the authors calculated the change in the entropy of the two-level system from the von Neumann entropy. Our derivation aimed to demonstrate, that coherences between states with the same energy do not affect this ratio. It is the feature of this model, that if coherences only occur between states with the same energy (i.e., the density matrix is in energy basis block-diagonal), there is no decoherence. Conversely, if there are any coherences between states with different energies, these coherences will decay over time. Then the ratio (1.30) will no longer hold, as the decoherence will contribute to the entropy production. Therefore, one of the conclusions of the paper [14] is that coherences between states with different energies degrade the efficiency of heat engines.

We can calculate the entropy production, in the case without coherences, by combining (1.15) and (1.30) as $\partial_t S_{\rm nc}(0) = \gamma(\omega_0)p_{\rm e}\ln\left(1+\frac{1}{N}\right) = O(1/N)$ and in the case with coherences by combining (1.24) and (1.30) as $\partial_t S_{\rm c}(0) = \gamma(\omega_0)p_{\rm e}N\ln\left(1+\frac{1}{N}\right) = O(1)$. That is, the initial probability of the system being in an excited state (1.13) is chosen such that if we use the initial state (1.16), the entropy production asymptotically does not depend on the degeneracy N, while the magnitude of the current grows linearly with N. So it is possible to use quantum coherence to enhance current in such a way, that does not increase irreversibility.

1.1.3 Current Fluctuations

To determine the current fluctuations, we use the energy transfer generating function according to [23] $G(\lambda,t) = \mathrm{Tr}(\rho(\lambda,t))$, where $\rho(\lambda,t)$ is a dressed density matrix whose time evolution is given by

$$D(\rho) = \sum_\omega \gamma(\omega)[e^{-\lambda\omega}L_\omega\rho(\lambda,t)L_\omega^\dagger - \frac{1}{2}\{L_\omega^\dagger L_\omega,\rho(\lambda,t)\}]\,. \tag{1.31}$$

After substituting initial state (1.16), we get a time derivative analogous to (1.22)

$$\partial_t \rho(\lambda, t) = N(\gamma(-\omega_0)e^{\lambda\omega_0}p_\mathrm{g} - \gamma(\omega_0)p_\mathrm{e}) \left(\begin{array}{ccc|ccc} 1 & \cdots & 1 & & & \\ \vdots & \ddots & \vdots & & \mathbb{0} & \\ 1 & \cdots & 1 & & & \\ \hline & & & -e^{-\lambda\omega_0} & \cdots & -e^{-\lambda\omega_0} \\ & \mathbb{0} & & \vdots & \ddots & \vdots \\ & & & -e^{-\lambda\omega_0} & \cdots & -e^{-\lambda\omega_0} \end{array}\right), \tag{1.32}$$

from which we get $\partial_t G(\lambda, t) = \mathrm{Tr}(\partial_t \rho(\lambda, t)) = N^2(\gamma(-\omega_0)e^{\lambda\omega_0}p_\mathrm{g} - \gamma(\omega_0)p_\mathrm{e})(1 - e^{-\lambda\omega_0})$, which is formally the same as a non-degenerate two-level system with rates

$$k_+ = N^2\gamma(-\omega_0)\,, \tag{1.33}$$

$$k_- = N^2\gamma(\omega_0)\,. \tag{1.34}$$

Thus we can use counting statistics similar to [24]. The matrix that describes the evolution will be

$$U(\lambda) = \begin{pmatrix} -k_- & k_+e^{\lambda\omega_0} \\ k_-e^{-\lambda\omega_0} & -k_+ \end{pmatrix}. \tag{1.35}$$

Now we need to solve the dynamic equation for this matrix, namely, we solve the differential equation $\partial_t \vec{p}(t, \lambda) = U(\lambda)\vec{p}(t, \lambda)$, for the initial state $\vec{p_0} = (p_\mathrm{e}, p_\mathrm{g})$. The solution is

$$\vec{p}(t, \lambda) = \frac{1}{k_- + k_+} \begin{pmatrix} p_\mathrm{e}\left(k_-e^{-t(k_-+k_+)} + k_+\right) + p_\mathrm{g}e^{\lambda\omega_0}k_+\left(1 - e^{-t(k_-+k_+)}\right) \\ p_\mathrm{e}e^{-\lambda\omega_0}k_-\left(1 - e^{-t(k_-+k_+)}\right) + p_\mathrm{g}\left(k_- + k_+e^{-t(k_-+k_+)}\right) \end{pmatrix}, \tag{1.36}$$

from which the generating function is $G(t, \lambda) = p_1(t, \lambda) + p_2(t, \lambda)$

$$G(t, \lambda) = \frac{1}{k_- + k_+}\left[\left(1 - e^{-t(k_-+k_+)}\right)\left(p_\mathrm{e}e^{-\lambda\omega_0}k_- + p_\mathrm{g}e^{\lambda\omega_0}k_+\right) + C\right], \tag{1.37}$$

where we have denoted as $C = p_\mathrm{e}\left(k_-e^{-t(k_-+k_+)} + k_+\right) + p_\mathrm{g}\left(k_- + k_+e^{-t(k_-+k_+)}\right)$ the terms that do not depend on λ.

Note that for the fixed p_e, the degeneracy N is present in the $G(t, \lambda)$ only trough rates $k_\pm$. And if we were to substitute for those rates from (1.33) and (1.34), all of those N would cancel out except the ones in the exponent of $e^{-t(k_-+k_+)}$. From this, we can anticipate, that by increasing the N we will just speed up the whole process.

Consequently, the mean heat transferred in time t will be the first derivative of the generating function $Q(t) = C_1(t, \lambda)|_{\lambda=0} = \partial_\lambda G(t, \lambda)|_{\lambda=0}$ and from it we get the heat current as $J(t) = \partial_t Q(t)$. Because as we will discuss, in the cycle this system only needs to be connected to the reservoirs for very short times, namely asymptotically $\tau = O(1/N^2)$, we are only interested in the limit $t \to 0$.

The heat transferred is

$$\begin{aligned} Q(t) &= C_1(t, \lambda)|_{\lambda=0} = \partial_\lambda G(t, \lambda)|_{\lambda=0} \\ &= \frac{1}{k_- + k_+}\left(1 - e^{-t(k_-+k_+)}\right)(-\omega_0 p_\mathrm{e} k_- + \omega_0 p_\mathrm{g} k_+)\,, \end{aligned} \tag{1.38}$$

then the current for short times

$$J(0) = \partial_t Q(t)|_{t=0} = \omega_0(p_\mathrm{g}k_+ - p_\mathrm{e}k_-)\,, \tag{1.39}$$

which, when substituted for $k_\pm$ from (1.33) and (1.34) and $p_{\mathrm{g,e}}$ according to (1.13), gives the current $J_\mathrm{c}(0) = N\omega_0\gamma(\omega_0)p_\mathrm{e}$, which fits with the result from (1.24). We can also check, that if we substitute for $k_\pm$ values corresponding to the case without coherences (namely $k_+ = N\gamma(-\omega_0)\,, k_- = N\gamma(\omega_0)$) we get the current for case without coherences (1.15).

Now we derive the fluctuations of the heat current as the second cumulant of the generating function $\langle\sigma^2_{Q_c}(t)\rangle = C_2(t,\lambda)|_{\lambda=0} = \partial^2_\lambda G(t,\lambda)|_{\lambda=0}$

$$\begin{aligned}\langle\sigma^2_{Q_c}(t)\rangle &= C_2(t,\lambda)|_{\lambda=0} = \partial_\lambda C_1(t,\lambda)|_{\lambda=0}\\ &= \frac{1}{k_- + k_+}\left(1 - e^{-t(k_- + k_+)}\right)\left(\omega_0^2 p_\mathrm{e}k_- + \omega_0^2 p_\mathrm{g}k_+\right)\,,\end{aligned} \tag{1.40}$$

which has a derivative at time 0

$$\partial_t\langle\sigma^2_{Q_c}(t)\rangle|_{t=0} = \omega_0^2(p_\mathrm{g}k_+ + p_\mathrm{e}k_-)\,, \tag{1.41}$$

which, when substituted for $k_\pm$ from (1.33) and (1.34) and $p_{\mathrm{g,e}}$ according to (1.13), gives

$$\partial_t\langle\sigma^2_{Q_c}(t)\rangle|_{t=0} = \omega_0^2 N^2\gamma(\omega_0)\frac{2 + \frac{1}{N}}{\left(1 + \frac{1}{N}\right)e^{\beta\omega_0} + 1} \approx 2\omega_0^2 N^2\gamma(\omega_0)p_\mathrm{e}\,. \tag{1.42}$$

In this subsection, we derived the fluctuations of heat current between a heat reservoir and the two-level system. The general result is in (1.41), and for coherence-enhanced heat current with the choice of p_e as (1.13) we got (1.42). We can therefore for this case write $\partial_t\langle\sigma^2_{Q_c}(t)\rangle|_{t=0} = O(N^2)$.

1.2 Cyclic Heat Engine

So far we calculated, that in case of coherence-enhanced heat current between the heat reservoir and two-level system, with the choice of p_e as (1.13) the heat current will be $J_\mathrm{c}(0) = N\omega_0\gamma(\omega_0)p_\mathrm{e} = O(N)$ and its fluctuations will be $\partial_t\langle\sigma^2_{Q_c}(t)\rangle|_{t=0} = 2\omega_0^2 N^2\gamma(\omega_0)p_\mathrm{e} = O(N^2)$. This raises an interesting question: would not the work done by a heat engine using these coherences, and this choice of p_e be negligible with respect to its own fluctuations? We will answer this question in this section.

Let us first clarify in what cycle can heat engine that is consisting of a two-level system operate. To construct a working heat engine we need a two-level system and a way to change the energy gap between these levels, we also need two heat reservoirs i.e., a hot reservoir with inverse temperature β_h and a cold reservoir with inverse temperature $\beta_\mathrm{c} > \beta_\mathrm{h}$ and a way to connect and disconnect these reservoirs with the two-level system, so the two-level system is in each point of the cycle connected to at most one heat reservoir.

We have to address one more aspect: so far we only used coherences to enhance the heat current from the hot reservoir to the system, but we need to enhance the current from the system to the cold reservoir. To do this, we just have to set the

p_e of the initial state to be $p_\mathrm{e} > 1/(e^{\beta\omega}+1)$, where ω is the energy gap between the levels and β is the inverse temperature of reservoir system is interacting with.

As we have already mentioned, if we want to achieve efficiency close to the the Carnot efficiency, we have to choose initial states to be close to equilibrium with a reservoir the system will interact with because in such cases dissipation is low. Namely at the beginning of the heating step we choose p_e according to (1.13) and at the beginning of the cooling step we choose it so

$$p_\mathrm{e} = \frac{1}{\left(1-\frac{1}{N}\right)e^{\beta_\mathrm{c}\omega}+1}\,. \tag{1.43}$$

If we substitute this probability to (1.23) we see, that we get coherence-enhanced heat current of the same form, as if we choose p_e according to (1.13), except in this case, heat flows from the system to the reservoir.

Then the cycle may then look like this

1. We use the coherence-enhanced heat current to get heat current from the hot reservoir into the system. Thus, at the beginning of this step, $p_{e1} = 1/((1+1/N)\,e^{\beta_h\omega_1}+1)$ must hold.
2. We reduce the energy gap to ω_2, thus in average we are getting work. This change is adiabatic and therefore does not change the populations of states and takes a negligibly short time.
3. We use the coherence-enhanced heat current to get heat current out of the system and into the cold reservoir. Thus, at the beginning of this step, $p_{e2} = 1/((1-1/N)\,e^{\beta_c\omega_2}+1)$ must hold.
4. We increase the energy gap back to ω_1, we need to apply some work to do this, but this work is on average lower than the work we got in step 2. This change happens also adiabatically.

We would like to point out, that work is not a quantum observable. If we wanted to have a well-defined quantum work, we would have to, for example, perform two measurements [25]. But performing any measurement would destroy the state that is necessary for the engine to work as intended. Because even if we measure into a base containing states $|e,+\rangle$ and $|g,+\rangle$ and thus measurement would not change the l_1 norm of coherence, we would still be unable to set p_e according to desired initial conditions at the beginning of steps 1. and 3. Therefore, we will not perform any measurements and instead define mean work done during one cycle from energy conservation, as it is done in [21]. In other words, mean work done during one cycle is equal to heat extracted from the hot reservoir during one cycle, minus heat dumped into the cold reservoir during one cycle. From now on we will use the word "work" in this looser way.

Then the ratio of the heat transferred in step 1 and the heat transferred in step 3 is going to be $1-\eta$, where by η we denoted the efficiency of the engine. With growing N this value will approach the Carnot efficiency $\eta_\mathrm{C} = 1-\frac{\beta_\mathrm{h}}{\beta_\mathrm{c}}$ as $\eta = \eta_\mathrm{C} - O(1/N)$ [14], this is direct consequence of choices (1.13) and (1.43). Inverse temperatures $\beta_\mathrm{h}, \beta_\mathrm{c}$ are arbitrary, therefore the ratio of transferred energies is in general sufficiently different than 1 so we can say, that work performed over one cycle is in the same order as transferred heat, and therefore also fluctuations of work are in the same order as fluctuations of transferred heat.

Steps 2 and 4 take arbitrarily short times, therefore the time of one cycle is in the same order as the duration of steps 1 and 3. We have checked the assertions from the Supplemental Material of [14] and can confirm that as the degeneracy N increases, the time per cycle decreases as $\tau = O(1/N^2)$, while the mean work decreases only as $\bar{W} = O(1/N)$. The previous section shows that the work variance of one cycle will be $\sigma_W^2 \sim \partial_t \langle \sigma_Q^2(t) \rangle|_{t=0}\tau = O(1)$ so that for large N there will indeed be $\bar{W} \ll \sigma_W$ for one cycle. But the main advantage of using this cycle is, that the duration of it is short and therefore we can repeat the cycle many times during some fixed time interval, therefore we are mainly interested in how the work and its fluctuation behave from this perspective. And for some fixed "unit time", the total work will be $W_t = \bar{W}/\tau = O(N)$ and its deviation $\sigma_{W_t} = \sqrt{\sigma_W^2/\tau} = O(N)$. The good news is, that the time, that it takes work to catch up with its fluctuations, does not asymptotically increase with N.

That is, regardless of N the work will be equal to its deviation somewhere around "unit time", and then it will grow faster than the deviation. That means that answer to the question we raised at the beginning of this section is, that the work done by a heat engine using coherence-enhanced heat current is not negligible with respect to its own fluctuations, and therefore this mechanism gives heat engines using it an advantage.

1.3 Nonequilibrium Steady State Heat Engine

When we connect our two-level system to two reservoirs simultaneously, it can mediate a heat or particle current between them, and again we can use quantum coherences to enhance this current. This was discussed in [14], what was not discussed is, that if those reservoirs differ in both temperature and chemical potential, we can construct an engine that will do work and yet be in a stationary state.

Let us have two reservoirs of particles with inverse temperature and chemical potential $\beta_{\mathrm{R}}, \mu_{\mathrm{R}}$ and $\beta_{\mathrm{L}}, \mu_{\mathrm{L}}$ respectively. Both of these reservoirs interact with our system, where a transition from the ground level to the excited level means that the particle moves from the reservoir to the two-level system, and transition from the excited level to the ground level means that it moves from the system to the reservoir.

Now the dissipator D has to sum not only over energy differences but also over both reservoirs, the system is interacting with. We rewrite it in the following manner

$$D(\rho) = \sum_{s,A} \Gamma_{s,A}(\omega_0, \mu_A)[L_{s\omega_0}\rho L_{s\omega_0}^\dagger - \frac{1}{2}\{L_{s\omega_0}^\dagger L_{s\omega_0}, \rho\}] , \tag{1.44}$$

where by s we index the sign: $s = +1$ represents transitions from the excited level to the ground level and $s = -1$ transitions from the ground level to the excited level, and A we index reservoirs, so it can equal either R or L. The coefficients Γ

must satisfy the detailed balance relation conditions

$$\frac{\Gamma_{-,\mathrm{R}}}{\Gamma_{+,\mathrm{R}}} = \exp(\beta_\mathrm{R}(\omega_0 - \mu_\mathrm{R}))\,, \tag{1.45}$$

$$\frac{\Gamma_{-,\mathrm{L}}}{\Gamma_{+,\mathrm{L}}} = \exp(\beta_\mathrm{L}(\omega_0 - \mu_\mathrm{L}))\,. \tag{1.46}$$

If we initialize the two-level system in a coherent state (1.16), then we can by analogy to (1.22), get the total rate of particles moving from the reservoir R to the system as $k_{+,\mathrm{R}} = N^2\Gamma_{+,\mathrm{R}}(\omega_0, \mu_\mathrm{R})$ and from the system to the reservoir $k_{-,\mathrm{R}} = N^2\Gamma_{-,\mathrm{R}}(\omega_0, \mu_\mathrm{R})$. Similarly the rates for the reservoir L will be $k_{+,\mathrm{L}} = N^2\Gamma_{+,\mathrm{L}}(\omega_0, \mu_\mathrm{L}), k_{-,\mathrm{L}} = N^2\Gamma_{-,\mathrm{L}}(\omega_0, \mu_\mathrm{L})$.

We in turn want to choose a state close to equilibrium, hence (by analogy with (1.13) and (1.43))

$$p_\mathrm{e} = \frac{1}{\left(1 + \frac{1}{N}\right) e^{\beta_\mathrm{R}(\omega_0 - \mu_\mathrm{R})} + 1} = \frac{1}{\left(1 - \frac{1}{N}\right) e^{\beta_\mathrm{L}(\omega_0 - \mu_\mathrm{L})} + 1}\,, \tag{1.47}$$

this gives us the condition

$$\beta_\mathrm{R}(\omega_0 - \mu_\mathrm{R}) - \beta_\mathrm{L}(\omega_0 - \mu_\mathrm{L}) = \ln \frac{1 - \frac{1}{N}}{1 + \frac{1}{N}}\,. \tag{1.48}$$

For such conditions, particles on average flow from reservoir R to reservoir L. If only the R reservoir was connected, the change in p_e would be (by analogy with (1.23))

$$\begin{aligned}\partial_t p_\mathrm{e}(0) &= N^2(\Gamma_{+,\mathrm{R}}(\omega_0, \mu_\mathrm{R}) p_\mathrm{g} - \Gamma_{-,\mathrm{R}}(\omega_0, \mu_\mathrm{L}) p_\mathrm{e}) \\ &= N\Gamma_{-,\mathrm{R}}(\omega_0, \mu_\mathrm{R}) \frac{1}{\left(1 + \frac{1}{N}\right) e^{\beta_\mathrm{R}(\omega_0 - \mu_\mathrm{R})} + 1}\,,\end{aligned} \tag{1.49}$$

which is therefore the mean number of particles leaving the reservoir R per unit time. By analogy, if only the reservoir L was connected, the change in p_e would be

$$\begin{aligned}\partial_t p_\mathrm{e}(0) &= N^2(\Gamma_{+,\mathrm{L}}(\omega_0, \mu_\mathrm{L}) p_\mathrm{g} - \Gamma_{-,\mathrm{L}}(\omega_0, \mu_\mathrm{L}) p_\mathrm{e}) \\ &= -N\Gamma_{-,\mathrm{L}}(\omega_0, \mu_\mathrm{L}) \frac{1}{\left(1 - \frac{1}{N}\right) e^{\beta_\mathrm{L}(\omega_0 - \mu_\mathrm{L})} + 1}\,,\end{aligned} \tag{1.50}$$

which in turn is, in absolute value, the mean number of particles added to the reservoir L per unit time.

If we want our two-level system to be in a stationary state, these two values must be equal in absolute value (i.e. the number of particles leaving the reservoir R must be the same as the number of particles entering the reservoir L, otherwise the probability of particle occupying the two-level system will change, which makes sense), after a comparison with (1.47) this gives us a condition $\Gamma_{-,\mathrm{R}}(\omega_0, \mu_\mathrm{R}) = \Gamma_{-,\mathrm{L}}(\omega_0, \mu_\mathrm{L})$. For brevity, let us denote

$$\Gamma_{-,\mathrm{R}}(\omega_0, \mu_\mathrm{R}) = \Gamma_{-,\mathrm{L}}(\omega_0, \mu_\mathrm{L}) = \Gamma\,. \tag{1.51}$$

For such choice of the state and properties of the reservoirs and the system, we get a stationary particle current

$$J^n_{\mathrm{R}\to\mathrm{L}} = \partial_t n_\mathrm{L} = -\partial_t n_\mathrm{R} = N\Gamma p_\mathrm{e}\,. \tag{1.52}$$

Then we identify the work done by this engine with the increase in the chemical potential of the particles. The power of the engine will be

$$P = J^n_{\mathrm{R}\to\mathrm{L}}(\mu_\mathrm{L} - \mu_\mathrm{R}) = N\Gamma p_\mathrm{e}(\mu_\mathrm{L} - \mu_\mathrm{R})\,. \tag{1.53}$$

Where the difference in chemical potentials of the reservoirs is given by the condition (1.48). For $N \gg 1$ we can neglect the right-hand side and we are left with

$$\mu_\mathrm{L} - \mu_\mathrm{R} = (\omega_0 - \mu_\mathrm{L})\left(\frac{\beta_\mathrm{L}}{\beta_\mathrm{R}} - 1\right) + O\left(\frac{1}{N}\right)\,. \tag{1.54}$$

Suppose $\omega_0 - \mu_\mathrm{L} > 0$, then $\mu_\mathrm{L} - \mu_\mathrm{R} > 0$ if and only if $\beta_\mathrm{L} > \beta_\mathrm{R}$, and hence that is also a condition for the work done by this heat engine to be positive. This makes sense since the energy flows out of the reservoir R, which thus plays the role of a heater, i.e. it must be at a higher temperature than the cooler L in order for positive work to be done. At the same time, if we define the heat supplied by reservoir R as the energy that the particles get when they move from the reservoir to the system, i.e.

$$\partial_t Q_\mathrm{in} = J^n_{\mathrm{R}\to\mathrm{L}}(\omega_0 - \mu_\mathrm{R})\,, \tag{1.55}$$

we get that the efficiency of such an engine is

$$\begin{aligned} \eta &= \frac{W}{Q_\mathrm{in}} = \frac{P}{\partial_t Q_\mathrm{in}} = \frac{\mu_\mathrm{L} - \mu_\mathrm{R}}{\omega_0 - \mu_\mathrm{R}} = \frac{(\omega_0 - \mu_\mathrm{L})\left(\frac{\beta_\mathrm{L}}{\beta_\mathrm{R}} - 1\right)}{\frac{\beta_\mathrm{L}}{\beta_\mathrm{R}}(\omega_0 - \mu_\mathrm{L})} + O\left(\frac{1}{N}\right) \\ \eta &= 1 - \frac{\beta_\mathrm{R}}{\beta_\mathrm{L}} + O\left(\frac{1}{N}\right)\,, \end{aligned} \tag{1.56}$$

where in the penultimate step we just substituted from (1.48) and (1.54).

We see that, similarly as in the section 1.2, as N increases the efficiency of the engine approaches the Carnot efficiency as $\eta = \eta_\mathrm{C} + O(1/N)$ (where $O(1/N)$ is negative), while the power increases as $P = O(N)$.

The advantage of this engine over the one described in section 1.2 is that even though it is out of equilibrium, it is in a stationary state, i.e., it does not itself evolve in time, it only mediates the particle flow between the reservoirs. In contrast, for the cycle described in section 1.2 to benefit from this coherence-enhanced current, the times it is connected to the reservoirs must asymptotically decrease as $\tau = O(1/N^2)$ and we also need such a way to change the energy gap ω, that allows us to extract work. The details, limitations, and costs of such quantum driving were addressed in [26]. We have shown, that it is possible to use coherence-enhanced particle current to extract work without the need for any driving.

1.4 Effect of Decoherence

In order to discuss the effect of decoherence on the coherence-enhanced current we will again generalize the model. We can assume, that even though our differential equations for density matrix (such as (1.22)) do not suggest decoherence, some decoherence might still take place. We may model this for example by multiplying all non-diagonal elements of the density matrix by $\exp(-ft)$, where f is some constant, that characterizes the rate of decoherence.

In other words, according to this model, if we connect our two-level degenerate system to two reservoirs of particles, with all parameters of reservoirs, system, and coupling being the same as in the section 1.3, then unlike in that section, the density matrix would not be constant but instead would evolve as

$$\rho_{\mathrm{c,f}}(t) = \left(\begin{array}{cccc|cccc} \frac{p_\mathrm{e}}{N} & e^{-ft}\frac{p_\mathrm{e}}{N} & \cdots & e^{-ft}\frac{p_\mathrm{e}}{N} & & & & \\ e^{-ft}\frac{p_\mathrm{e}}{N} & \ddots & \ddots & \vdots & & & & \\ \vdots & \ddots & \ddots & e^{-ft}\frac{p_\mathrm{e}}{N} & & \multicolumn{2}{c}{\mathbb{0}} & \\ e^{-ft}\frac{p_\mathrm{e}}{N} & \cdots & e^{-ft}\frac{p_\mathrm{e}}{N} & \frac{p_\mathrm{e}}{N} & & & & \\ \hline & & & & \frac{p_\mathrm{g}}{N} & e^{-ft}\frac{p_\mathrm{g}}{N} & \cdots & e^{-ft}\frac{p_\mathrm{g}}{N} \\ & \multicolumn{2}{c}{\mathbb{0}} & & e^{-ft}\frac{p_\mathrm{g}}{N} & \ddots & \ddots & \vdots \\ & & & & \vdots & \ddots & \ddots & e^{-ft}\frac{p_\mathrm{g}}{N} \\ & & & & e^{-ft}\frac{p_\mathrm{g}}{N} & \cdots & e^{-ft}\frac{p_\mathrm{g}}{N} & \frac{p_\mathrm{g}}{N} \end{array}\right), \tag{1.57}$$

if we wanted to get the same time evolution directly from the Lindblad master equation (1.1), we would just need to add into a dissipator (1.2) Lindblad operators, that would describe transitions between the states with the same energy.

In this case, in rates $k_\pm$ there will be a change $N^2 \to N(1+(N-1)\exp(-ft))$, resulting in the particle current to change from (1.52) to $J^n_{\mathrm{R}\,\to\,\mathrm{L}}(t) = (1+(N-1)\exp(-ft))\Gamma p_\mathrm{e}$. For $t \gg 1/f$ we get current for the incoherent case.

To say, in which cases would coherence-enhanced current make a significant contribution, we will compute both work and its fluctuations in a general time interval $t \in (0, \tau)$, and require work to be greater than its own fluctuations.

Work grows over time as

$$\partial_t W(t) = P(t) = J^n_{\mathrm{R}\,\to\,\mathrm{L}}(t)(\mu_\mathrm{R}-\mu_\mathrm{L}) = (1+(N-1)\exp -ft)\Gamma p_\mathrm{e}(\mu_\mathrm{R}-\mu_\mathrm{L})\,. \tag{1.58}$$

By integrating this relation from time 0 to τ we get

$$\begin{aligned} W(\tau) &= \int_0^\tau \mathrm{d}t(1+(N-1)e^{-ft})\Gamma p_\mathrm{e}(\mu_\mathrm{R}-\mu_\mathrm{L}) \\ &= \left(\tau + (N-1)\frac{1-e^{-f\tau}}{f}\right)\Gamma p_\mathrm{e}(\mu_\mathrm{R}-\mu_\mathrm{L})\,. \end{aligned} \tag{1.59}$$

In both reservoirs, the mean square deviation of the number of particles will grow as $\partial_t\langle\sigma_n^2\rangle = 2p_\mathrm{e}\Gamma N(1+(N-1)e^{-ft})$. Then

$$\partial_t\langle\sigma_W^2(t)\rangle = 2p_\mathrm{e}\Gamma N(1+(N-1)e^{-ft})(\mu_\mathrm{R}^2+\mu_\mathrm{L}^2)\,. \tag{1.60}$$

By integration we get

$$\begin{aligned} \langle\sigma_W^2(\tau)\rangle &= \int_0^\tau \mathrm{d}t 2(1+(N-1)e^{-ft})N\Gamma p_\mathrm{e}(\mu_\mathrm{R}-\mu_\mathrm{L})^2 \\ &= 2\left(\tau + (N-1)\frac{1-e^{-f\tau}}{f}\right)N\Gamma p_\mathrm{e}(\mu_\mathrm{R}-\mu_\mathrm{L})^2\,. \end{aligned} \tag{1.61}$$

In both (1.59) and (1.61) we can see a term that is proportional to τ and does not depend on f, we can therefore identify this term with incoherent contribution (and indeed, we can trace the origin of this term back to the diagonal elements of $\rho_{\mathrm{c,f}}(t)$). Then the other term in both (1.59) and (1.61) proportional to $(N-1)(1-e^{-f\tau})/f$ is the contribution of the coherence-enhanced current. We, therefore, denote these contributions as W_{coh} and $\langle \sigma^2_{W_{\mathrm{coh}}} \rangle$ respectively. Then

$$\begin{aligned} W_{\mathrm{coh}}(\tau) &= (N-1)\frac{1-e^{-f\tau}}{f}\Gamma p_{\mathrm{e}}(\mu_{\mathrm{R}}-\mu_{\mathrm{L}}) \\ \langle \sigma^2_{W_{\mathrm{coh}}}(\tau) \rangle &= 2(N-1)\frac{1-e^{-f\tau}}{f} N\Gamma p_{\mathrm{e}}(\mu_{\mathrm{R}}-\mu_{\mathrm{L}})^2 \,. \end{aligned} \tag{1.62}$$

Then, for the coherences to make a significant contribution, we require $W_{\mathrm{coh}}(\tau) > \sqrt{\langle \sigma^2_{W_{\mathrm{coh}}}(\tau) \rangle}$. After performing limit $N \gg 1$ we are left with

$$\begin{aligned} \left(1-e^{-f\tau}\right)\frac{\Gamma}{f}p_{\mathrm{e}}(\mu_{\mathrm{R}}-\mu_{\mathrm{L}}) &> \sqrt{2\left(1-e^{-f\tau}\right)\frac{\Gamma}{f}p_{\mathrm{e}}(\mu_{\mathrm{R}}-\mu_{\mathrm{L}})^2 + O\left(\frac{1}{N}\right)} \\ \left(1-e^{-f\tau}\right)\frac{\Gamma}{f}p_{\mathrm{e}} &> 2 + O\left(\frac{1}{N}\right) \,. \end{aligned} \tag{1.63}$$

There is still a dependence on the duration of the time interval τ. We can either say, that if coherences are to make any important contribution, they must do so on the time scale $1/f$, and set $\tau = 1/f$, or if we know the actual time, the process will take we may set τ to be equal that time. In either case, we get some condition on the coefficient of decoherence f, that does not depend on N explicitly.

So we see, that whether the contribution of coherence-enhanced current is significant in the case when coherences gradually decrease, depends on how fast the decoherence is. We derived the condition, that specifies with how fast decoherence do coherences have enough time, to make a significant contribution. This is only a rough estimate, made for the specific model with some assumptions, but it might work as a rule of thumb even in different situations.

1.5 Summary

In [14] authors proposed a way, how quantum coherences may enhance a current. In this chapter, we studied this enhancement via three different models and we hope, that we brought a new physical intuition into what causes this effect. One of our models expands on models from the article showing, that coherence-enhanced particle current can be used to construct an engine, that does work while being in a nonequilibrium steady state.

One of the possible usages of this enhancement is, that it makes it possible to choose an initial state to be close to equilibrium, and thus reduce entropy production, while maintaining the magnitude of the current. Authors of [14] propose a limit in which as the degree of degeneracy N increases, the efficiency of the heat engine, that is using this enhancement, approaches the Carnot efficiency, while the power of the engine increases. This is possible because the transition rates in the two-level system scale with N as $k_{\pm} = O(N^2)$.

With degeneracy alone, the rates scale only as $k_{\pm} = O(N)$. Analogously in classical heat engine heat current is proportional to its size [20], in other words, if we use N identical heat engines, the resulting heat current during heating and cooling (and therefore also resulting power) will be N times greater. Thus, an interesting result from the paper [14] is that coherences between states with the same energy can increase the rates by factor $O(N^2)$, which is $O(N)$ times more than degeneracy alone, thus increasing the heat current between the system and the reservoir, thus improving the performance of heat engines. This improvement does not have a classical counterpart. Or in other words, a heat engine that utilizes coherence-enhanced currents can exceed the power-efficiency trade-off relations for classical engines [20, 21].

However to create and maintain coherences is not for free, so we see, that claim from [21], that "the power-efficiency dilemma relates to computational complexity" still holds, as both quantum heat engines and quantum computers benefit from coherences between a large number of states. More about quantum coherence as a resource can be found in [1, 2, 9]. To use this quantum advantage in practice, we need to find a system with a suitable Hamiltonian, or somehow modify this approach to some existing system. According to [10] "...it is not straightforward to find a physical counterpart of their model. For a better interpretation of the quantum phenomena, it is preferable to seek another concrete model that provides the quantum enhancement with a physically realizable setting." So far no one has managed to use this model to construct a working engine but as a general framework, it is very useful, because it shows different effects of coherences between states with the same energy and coherences between states with different energy.

The paper [14] did not mention the fluctuations of this coherence-enhanced current, so we calculated them in our work. The main goal of our analysis was to show, that the work done by a heat engine that uses these coherences can be higher than these fluctuations. We have shown, that it takes a certain time for this to happen, but that time does not asymptotically depend on N.

Article [14] does not consider any decoherence between states with the same energy. So we explored the behavior of coherence-enhanced current if such decoherence took place. The main result of that section is, that we derived a condition that estimates how fast can decoherence be, so coherence-enhanced current still gives a significant advantage.

2. Coherence-Inducing Heat Bath

Let us now turn our attention to coherence generation. Namely, we shall discuss a model introduced in [19], in which the authors write about a system whose stationary state has non-zero coherences. The system converges to this stationary state even if it had no coherences, to begin with. Perhaps most interestingly, this happens just thanks to the interaction with a bosonic reservoir. In particular, the main model in this paper is spin in a magnetic field interacting with such a reservoir. The Hamiltonian of the full system is

$$H = H_{\mathrm{S}} + H_{\mathrm{R}} + H_{\mathrm{I}} = \frac{\omega_0}{2}\sigma_z \otimes \mathbb{1} + \mathbb{1} \otimes \sum_k \omega_k^R b_k^\dagger b_k + (f_1\sigma_z + f_2\sigma_x) \otimes B_{\mathrm{R}}\,, \quad (2.1)$$

where ω_0 is the energy gap between the ground and excited state of the spin, $b_k, b_k^\dagger$ are bosonic annihilation and creation operators, ω_k^R are energies of different modes of the reservoir, f_1, f_2 are coupling constants and $B_{\mathrm{R}} = \sum_k g_k(b_k + b_k^\dagger)$.

The density matrix of the spin can be decomposed using the Bloch vector $\vec{v} = (v_1, v_2, v_3)$

$$\rho(\vec{v}) = \frac{1}{2}\begin{pmatrix} 1 + v_3 & v_1 - iv_2 \\ v_1 + iv_2 & 1 - v_3 \end{pmatrix}. \quad (2.2)$$

Thus, the component of the Bloch vector in the magnetic field direction (which is the z-direction) v_3 describes the probabilities of the spin being in ground or excited state, and the remaining two components describe the coherences. The coherences are zero if and only if $v_1 = v_2 = 0$.

In Supplementary Material of [19] the Bloch equations for the time evolution of this vector were derived as

$$\partial_t \vec{v}(t) = M(t)\vec{v}(t) + \vec{b}(t) \quad (2.3)$$

where

$$M(t) = \begin{pmatrix} -f_1^2\gamma_1(t) & -\omega_0 & f_1 f_2 \gamma_1^c(t) \\ \omega_0 + f_2^2\gamma_1^s(t) & -f_1^2\gamma_1(t) - f_2^2\gamma_1^c(t) & f_1 f_2 \gamma_1^s(t) \\ f_1 f_2 \gamma_1(t) & 0 & -f_2^2\gamma_1^c(t) \end{pmatrix} \quad (2.4)$$

and

$$\vec{b}(t) = \begin{pmatrix} f_1 f_2 \gamma_2^s(t) \\ f_1 f_2(\gamma_2(t) - \gamma_2^c(t)) \\ -f_2^2\gamma_2^s(t) \end{pmatrix}. \quad (2.5)$$

Formulas for coefficients γ can be found in that supplement.

So we have specified the model from [19] and wrote its equations of motion. In the rest of this chapter, we will explore the properties of this model in a framework of quantum thermodynamics. At first, we will focus on extraction of work and then we will discuss entropy and the Second law of thermodynamics.

2.1 Fast Work Extraction with One Heat Bath

Let us see how the spin behaves very shortly after connecting to the reservoir. We denote a short time Δt. Then in the previous relations the $\gamma_{1,2}^s(\Delta t) \sim \sin(\omega_0 \Delta t)$, i.e., $\gamma_{1,2}^{s}(\Delta t) \approx 0$. Similarly in the $\gamma_{1,2}^{c}(\Delta t) \sim \cos(\omega_0 \Delta t)$ we can consider the cosine to be approximately equal to 1 for small Δt. So then

$$\gamma_{1,2}^{c}(\Delta t) \approx \gamma_{1,2}(\Delta t) = \int_0^{\Delta t} \mathrm{d}\tau 2D_{1,2}(\tau) \approx 2D_{1,2}(0)\Delta t \tag{2.6}$$

where D_2 is, in turn, proportional to the sine, so it goes to zero for short times. There is a cosine in D_1, that will go to 1. It remains

$$D_1(0) = 2\int_0^{\infty} \mathrm{d}\omega \lambda \frac{\omega^s}{\Omega^{s-1}} \exp\left(-\frac{\omega}{\Omega}\right) \coth\left(\frac{\omega}{2T}\right) , \tag{2.7}$$

where Ω is the cutoff frequency, s is the Ohmicity parameter, T is the temperature of the reservoir and we set $k_{\mathrm{B}} = 1$.

We see that $\vec{b}(0) = 0$ and

$$M(\Delta t) = \begin{pmatrix} -f_1^2 2D_1(0)\Delta t & -\omega_0 & f_1 f_2 2D_1(0)\Delta t \\ \omega_0 & -(f_1^2 + f_2^2)2D_1(0)\Delta t & 0 \\ f_1 f_2 2D_1(0)\Delta t & 0 & -f_2^2 2D_1(0)\Delta t \end{pmatrix} . \tag{2.8}$$

Note that we have made the approximation to the second order, i.e., we have assumed that

$$\begin{aligned} \int_0^{\Delta t} \mathrm{d}\tau 2D_1(\tau)\sin(\omega_0\tau) \sim D_1(0)\omega_0\Delta t^2 &\ll 1/\Delta t \\ \omega_0 D_1(0)\Delta t^3 &\ll 1 , \end{aligned} \tag{2.9}$$

but we do not neglect $D_1(0)\Delta t^2$, so there are linear terms left in the matrix M.

The mean energy of the spin itself is given by

$$\langle H_{\mathrm{S}} \rangle = \mathrm{Tr}(H_{\mathrm{S}}\rho) = \mathrm{Tr}\left(\frac{\omega_0}{2}\sigma_z \frac{1}{2}(1 + v \cdot \sigma)\right) = \frac{\omega_0}{4}\mathrm{Tr}(\sigma_z v_3 \sigma_z) = \frac{\omega_0}{2} v_3 , \tag{2.10}$$

this gives the mean work done by the spin when the energy gap ω changes suddenly (jump-like change) from ω_0 to ω_1, as

$$W = -\Delta\langle H_{\mathrm{S}} \rangle = \langle H_{\mathrm{S}0} \rangle - \langle H_{\mathrm{S}1} \rangle = \frac{\omega_0}{2} v_3 - \frac{\omega_1}{2} v_3 = -\frac{\Delta\omega}{2} v_3 . \tag{2.11}$$

This is only the mean work deduced from energy conservation. In particular, when we change the energy gap of the spin, its energy changes, and if the change of the energy gap is sudden, the state of the reservoir does not change. Therefore the energy of the reservoir does not change as well. That means, that the energy of the spin-reservoir system changes by the same value, by which the energy of the spin changes. Therefore we call this change in the spin-reservoir energy the work done by the spin (or the work done on the spin, depending on the sign of the energy).

Let us now use the above model to compare extraction of the work in cases when $f_1 = 0 , f_2 \neq 0$ and when $f_1 \neq 0 , f_2 \neq 0$. We do not discuss cases when $f_2 = 0$ in the same way, because in these cases we see from (2.4) and (2.5), that $\dot{v}_3 = 0$. Therefore there will be no energy exchange between the spin and the reservoir, so we can not use this case to extract work from the reservoir.

We will assume that the initial state of the spin is given by thermalization. Where under thermalization, we understand long-time ($t \to \infty$) interaction of the spin with the given reservoir.

We can formulate our task in the following way: We start with a spin, that was coupled to the reservoir for a time $t \to \infty$. We disconnect the spin from the reservoir, and we ask how much work we can extract from the reservoir if we connect this spin to the same reservoir again, but only for a short period of time.

In the case with $f_1 = 0$ the initial state of the spin will be incoherent and also no coherences will be created during the work extraction. On the contrary, in the case with $f_1 \neq 0$, initial state will contain coherences, giving us an opportunity to see the role coherences can play in the extraction of work.

2.1.1 Without Coherences

If $f_1 = 0$, and and the initial state has no coherences, the evolution of v_3 is given by the differential equation

$$\partial_t v_3 = -f_2^2 2D_1(0) t v_3 \,. \tag{2.12}$$

The solution to this equation is $v_3(t) = v_3(0)\exp(-f_2^2 D_1(0)t^2)$ (so again we see that the approximation was to second order). We denote

$$f_2^2 D_1(0) = c > 0 \tag{2.13}$$

for brevity. We are left with $v_3(t) = v_3(0)\exp(-ct^2)$. Thus, the resulting work is

$$\begin{aligned} W = \sum_{i=0}^{\infty} W_i &= \sum_{i=0}^{\infty} -\frac{\omega_{i+1} - \omega_i}{2} v_3(0)\exp(-ct_i^2) \\ &= v_3(0)\frac{\omega_0}{2} + v_3(0)\sum_{j=1}^{\infty} \frac{\omega_j}{2}(\exp(-ct_j^2) - \exp(-ct_{j-1}^2))\,, \end{aligned} \tag{2.14}$$

where t_i is the time of the change of the energy gap from ω_i to ω_{i+1}. Let us have $\omega_0 > 0$, then because we assume that the initial state is a result of thermalization, we get that [19]

$$v_3(0) = -\tanh(\omega_0/(2T)) < 0\,. \tag{2.15}$$

Thus, the first term on the right-hand side of Eq. (2.14) is negative. If $\omega_j > 0$, we see that the given term of the sum is positive. We formally rewrite the parenthesis in the sum

$$(\exp(-ct_j^2) - \exp(-ct_{j-1}^2)) = [\exp(-ct^2)]_{t_{j-1}}^{t_j} = \int_{t_{j-1}}^{t_j} -2ct\exp(-ct^2)\mathrm{d}t\,. \tag{2.16}$$

We can then define a piecewise-constant function $\omega(t)$ value of which is equal to the energy gap at time t, formally $\omega(t) = \omega_j$ if $t \in (t_{j-1}, t_j)$. We use the fact that the boundary points of integrals occur in successive terms of the sum, once as a lower and once as an upper bound, to express each term of the sum as integral. Then we use the fact that the integral is additive over intervals, to rewrite the sum of integrals as a single integral. Finally, we set $t_0 = 0$, and if there is no change in energy gap at time $t = 0$, we can formally take $\omega_1 = \omega_0$

$$\begin{aligned} W &= v_3(0)\frac{\omega_0}{2} + v_3(0)\sum_{j=1}^{\infty}\frac{\omega_j}{2}(\exp(-ct_j^2) - \exp(-ct_{j-1}^2)) \\ &= v_3(0)\frac{\omega_0}{2} - v_3(0)\sum_{j=1}^{\infty}\int_{t_{j-1}}^{t_j}\omega(t)ct\exp(-ct^2)\mathrm{d}t \\ &= v_3(0)\frac{\omega_0}{2} - cv_3(0)\int_0^{\infty}\omega(t)t\exp(-ct^2)\mathrm{d}t\,. \end{aligned} \tag{2.17}$$

Since $t\exp(-ct^2)$ is positive for $t > 0$, the integral will have the largest value if $\omega(t)$ is maximal. Because the prefactor $-cv_3(0) > 0$, the work is maximal if the integral is maximal. Therefore, the condition for maximizing work is, that $\omega(t)$ is maximal.

For example, if we have the constraint $|\omega(t)| \leq \omega_{\max}$, the greatest work by the system will be done, if we immediately change ω to $\omega_{\max}$ and then do not change it again. Formally, if $\omega(t) = \omega_{\max}$. We can also calculate how much work we have lost if we chose a suboptimal procedure

$$W_{\mathrm{opt}} - W = -cv_3(0)\int_0^{\infty}(\omega_{\max} - \omega(t))t\exp(-ct^2)\mathrm{d}t\,. \tag{2.18}$$

We can also note that if $\omega_0 = \omega_{\max}$, it is not worth changing the energy gap at all, and hence $W_{\mathrm{opt}} = 0$. More generally,

$$W_{\mathrm{opt}} = v_3(0)(\omega_0 - \omega_{\max})/2\,. \tag{2.19}$$

Finally, we remind that the time evolution (2.12) assumes a short-time limit i.e., there is only some limited time (in the order of less than $(\omega_{\max}D_{1,2}(0))^{\frac{-1}{3}}$) while the system behaves according to (2.12). W_{opt} represents an upper bound on the work that can be extracted from the spin in this limit.

2.1.2 With Coherences

If both f_1 and f_2 are non-zero, the differential equations for the coherences in the short time limit are

$$\partial_t v_1 = -f_1^2 2D_1 t v_1 - \omega v_2 + f_1 f_2 2D_1 t v_3 \tag{2.20}$$

$$\partial_t v_2 = \omega v_1 - (f_1^2 + f_2^2)2D_1 t v_2\,. \tag{2.21}$$

For the short-time limit, it is natural to assume that $|\omega| \gg |(f_1^2 + f_2^2)2D_1 t| > |2ct|$ whereby all terms up to two drop out and we get a simple system of linear differential equations for the evolution of the coherences in time. So far we have assumed that $t^3\omega D_1(0) \ll 1$, therefore now we have two scales compared to which the time must be small, one increasing with ω and the other decreasing. Let us now focus on the combination of these conditions, which we will write down

$$\omega D t^3 \ll 1; \frac{Dt}{\omega} \ll 1\,, \tag{2.22}$$

we modify the first one to make the left-hand side of the second condition appear

$$\frac{Dt}{\omega}(\omega t)^2 \ll 1\,, \tag{2.23}$$

and we see that ωt is not necessarily small, it just can not be too big.

With these approximations, we get a simple system of linear equations for the evolution of the coherences

$$\partial_t v_1 = -\omega v_2 \,, \tag{2.24}$$

$$\partial_t v_2 = \omega v_1 \,, \tag{2.25}$$

that has a solution $v_1(t) = \cos(\omega t) v_1(0) - \sin(\omega t) v_2(0); v_2(t) = \sin(\omega t) v_1(0) + \cos(\omega t) v_2(0)$. If we assume, that the initial state is a result of thermalization, then from [19] that $v_2(0) = 0$. We denote $f_1 f_2 D_1 v_1(0) = cb$, then

$$b = \frac{f_1}{f_2} v_1(0) \,, \tag{2.26}$$

and the differential equation for v_3 will be

$$\partial_t v_3 = f_1 f_2 2 D_1 t \cos(\omega t + \phi) v_1(0) - f_2^2 2 D_1 t v_3 = 2tc(b \cos(\omega t + \phi) - v_3) \,, \tag{2.27}$$

where $\phi = 0$ if $v_2(0) = 0$, but this generalization is handy when we vary ω. Then $\phi_j = \sum_{i=1}^{j} \omega_i (t_i - t_{i-1})$ is the phase at time t_j. For the time $t \in (t_j, t_{j+1})$ we can write this equation as

$$\partial_t v_3 = 2tc(b \cos(\omega_{j+1}(t - t_j) + \phi_j) - v_3) \,. \tag{2.28}$$

We see that at time $t = 0$ the right-hand side will be positive i.e., v_3 will be increasing. So, as in the case without coherences, it will be optimal to immediately change ω to $\omega_{\max}$, doing the same work W_{opt} as in the case without coherences. But the difference is that if $f_1 \neq 0$, v_3 may stop increasing after some time and start decreasing, still during the short-time limit. At that time it is worth doing the work and in the local maximum $v_{3_{\max}}$ decrease ω to ω', to in turn in the local minimum $v_{3_{min}}$ increase ω back to $\omega_{\max}$, thus we will (in addition to W_{opt}) extract the work of

$$W_{\text{c}} = \frac{1}{2}(\omega_{\max} - \omega')(v_{3_{\max}} - v_{3_{min}}) > 0 \,. \tag{2.29}$$

It is impossible to obtain similar work in the case without coherences, since there (in the short-time limit) v_3 is monotone.

We remind that equations (2.28) were derived for the case $|\omega| \gg |2ct|, |\omega c t^3| \ll 1$, therefore it is not possible to repeat similar jumps indefinitely, on the contrary, typically one can manage on the order of units of jumps back and forth. Also, one cannot choose ω' too low, since this limits the time the approximation holds. However, since the smaller the ω', the more work we get from the jump, it seems to be most worthwhile to choose ω' as the smallest possible at which a jump can still be made.

The main result of this section is, that the coherences between the states with different energy provide an advantage in the fast work extraction from one heat bath.

2.2 Examining the Model within the Framework of the Second Law of Thermodynamics

If we look again at subsection 2.1.1, we see that we could build an engine working as follows:

1. we let spin thermalize ($v_1(0) = v_2(0) = 0; v_3(0) = -\tanh\left(\frac{\omega_1}{2T}\right)$)

2. we increase ω by $\Delta\omega$ to get $W_{\text{out}} = -\Delta\omega v_3(0)$

3. turn on the interaction with the reservoir for some sufficiently short time τ (the condition is $\partial_t v_3(t) > 0$ for $t < \tau$)

4. reduce ω to its original value, to do this we have to do the work $W_{\text{in}} = \Delta\omega v_3(\tau)$. But $|W_{\text{in}}| < |W_{\text{out}}|$, because v_3 has decreased in absolute value since step 2, so we have obtained a net positive work during one cycle

5. we let the spin thermalize again

We have gained positive work during the cycle, and at the end of the cycle, our heat engine (spin) is in the same state as at the beginning. In other words, here we have a cyclic heat engine interacting with a single reservoir i.e., a perpetual motion machine of the second kind, or in other words an engine forbidden by the Kelvin–Planck statement of the Second law of thermodynamics.

In this section, we will investigate this supposed conflict of the model from [19] with the Second law of thermodynamics and try to explain what happens.

One possible explanation might be, that because for this heat engine to work, the interaction must be turned on only for a sufficiently short time τ, it might be that there is an approximation in the description used, which does not describe short time scales accurately enough. But in paper [19] authors claim, that Bloch equations were derived with only the assumption of weak coupling between spin and reservoir and without secular or Born-Markov approximation, so they describe both the short-time and long-time limit well. We will come back to this claim later.

Another explanation might be that for quantum heat engines, it is possible to overcome the Carnot efficiency without reducing the entropy, as shown by [2]. The principle is that decoherence increases entropy. If the reservoir is initially in a coherent state, it is possible to use these coherences as a quantum source of work. This is in principle very similar to the Szilard Engine [27], it too can work with an efficiency $\eta = 1$ if we do not require memory erasing (i.e. if we do not require periodicity). But in our case, the reservoir starts in a thermal equilibrium state (which is without any coherences), so we can not use this explanation.

Next, we will examine the role that interaction Hamiltonian H_{I} from (2.1) plays. Specifically, we ask how changing the coupling constants f_1, f_2 affects the behavior of the system from the perspective of the production of entropy.

2.2.1 The Role of Interaction in the Investigated Phenomenon: Mathematical Derivation

In this subsection, we will calculate the time derivatives of the entropy of the whole closed system, at first in the case with coupling constant $f_2 = 0$ and then in the case with coupling constant $f_1 = 0$. But before we do that, we have to define, what we mean by "the entropy of the whole closed system".

We decompose the closed system as the spin and the reservoir. To derive the equations of motion, the weak coupling, which means, the assumption that there is no correlation between the spin and the reservoir, was used [15]. Thus the entropy of the whole system is a sum of the entropy of the spin and the entropy of the reservoir. And lastly, we are not interested in absolute entropy, only in its derivatives. As the equation of motion is written in terms of the Bloch vector, we should calculate derivatives of entropy with respect to the components of the Bloch vector.

We start with the spin. We can write its density matrix given by the Bloch vector

$$\rho(\vec{v}) = \frac{1}{2} \begin{pmatrix} 1 + v_3 & v_1 - iv_2 \\ v_1 + iv_2 & 1 - v_3 \end{pmatrix}, \tag{2.30}$$

and then define the entropy of the spin as a Von Neumann entropy of such a density matrix. It can be obtained from its eigenvalues, which are $\lambda_\pm = (1 \pm |\vec{v}|)/2$. Thus

$$S_\text{S}(\vec{v}) = -\frac{1 + ||\vec{v}|}{2} \ln \frac{1 + ||\vec{v}|}{2} - \frac{1 - |\vec{v}|}{2} \ln \frac{1 - |\vec{v}|}{2}, \tag{2.31}$$

and the derivatives of it with respect to the components of the Bloch vector are

$$\nabla S_\text{S}(\vec{v}) = \frac{\vec{v}}{|\vec{v}|} \ln \frac{1 - |\vec{v}|}{1 + |\vec{v}|}. \tag{2.32}$$

The reservoir starts in the state of thermal equilibrium and stays in thermal equilibrium, therefore the change in the entropy of the reservoir is given only by the change in its energy. Because the spin-reservoir system is closed, we can use conservation of energy to get that the change of energy of the reservoir is equal to minus the change of energy of the spin. As we have already discussed, the mean energy of the spin is $\langle H_\text{S} \rangle = \frac{\omega}{2} v_3$. Therefore if we keep the energy gap ω constant, the energy of the reservoir will change as $\mathrm{d}Q_\text{R} = -\omega/2 \mathrm{d}v_3$. Then the derivative of the entropy of the reservoir with respect to the components of the Bloch vector is

$$\nabla S_\text{R}(\vec{v}) = -\frac{\omega}{2T} e_3, \tag{2.33}$$

where e_3 is a unit vector in the space of the Bloch sphere, pointing in the z-direction.

To sum up, we derived, that derivatives of "the entropy of the whole closed system" with respect to the components of the Bloch vector are

$$\nabla S(\vec{v}) = \frac{\vec{v}}{|\vec{v}|} \ln \frac{1 - |\vec{v}|}{1 + |\vec{v}|} - \frac{\omega}{2T} e_3. \tag{2.34}$$

We can verify that at the point $\vec{v_T} = \left(0, 0, -\tanh\left(\frac{\omega}{2T}\right)\right)$ the $\nabla S(\vec{v_T}) = \vec{0}$ and the Hessian matrix is negatively definite, thus it is a state with maximum entropy according to our definition.

Consequently, the total time derivative of entropy will be given by

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \nabla S(\vec{v}) \cdot \partial_t \vec{v} \,, \tag{2.35}$$

where the time derivative of $\vec{v}$ is obtained from (2.3).

If we set $f_2 = 0$ in (2.4) (i.e. we turn off coupling of the reservoir with the projection of the spin to the x-direction) we get

$$M(t)|_{f_2=0} = \begin{pmatrix} -f_1^2\gamma_1(t) & -\omega_0 & 0 \\ \omega_0 & -f_1^2\gamma_1(t) & 0 \\ 0 & 0 & 0 \end{pmatrix} \,, \tag{2.36}$$

and $\vec{b}(t) = 0$. (Note that there is a typo here in [19]: the $f_2^2\gamma_1^s(t)$ has been changed to $f_1^2\gamma_1^s(t)$ in the M_{21} element.) Then

$$\partial_t \vec{v}(t)|_{f_2=0} = \begin{pmatrix} -f_1^2\gamma_1(t)v_1(t) - \omega_0 v_2(t) \\ \omega_0 v_1(t) - f_1^2\gamma_1(t)v_2(t) \\ 0 \end{pmatrix} \,. \tag{2.37}$$

This, when substitued to (2.35) gives

$$\frac{\mathrm{d}S(t)}{\mathrm{d}t}|_{f_2=0} = \frac{1}{2|\vec{v}|} \ln \frac{1+|\vec{v}|}{1-|\vec{v}|}(v_1(t)^2 + v_2(t)^2) f_1^2 \gamma_1(t) \,. \tag{2.38}$$

The only one of the factors in this product that is not non-negative trivially is $\gamma_1(t) = 2\int_0^t \mathrm{d}\tau D_1(\tau)$, where

$$D_1(\tau) = 2\int_0^\infty \mathrm{d}\omega \cos(\omega\tau) \coth\left(\frac{\omega}{2T}\right) \lambda \frac{\omega^s}{\Omega^{s-1}} e^{-\frac{\omega}{\Omega}} \,. \tag{2.39}$$

There is an error in the paper [19], since the result given for $D_1(\tau)$ does not fit in 0, for example. According to the paper [19], $D_1(0) = 2\lambda T\Omega(-T/\Omega)^s[\psi^{(s)}(T/\Omega) + \psi^{(s)}(1+T/\Omega)]$, But when we set $\tau = 0$ in (2.39), we get that the $D_1(0) = s\Gamma(s)[2(T/\Omega)^{s+1}\zeta(s+1, T/\Omega) - 1]$, where ζ is the Hurwitz Zeta function. By substituting in some values we can verify that these expressions do not equal. In figure (2.1) we explain why the expression from the paper does not give accurate results at least in some cases. It is reasonable to assume that also for times other than 0, this formula for D_1 does not give accurate results. Although we have not been able to compute the integral generally, we do not need a specific value of D_1, it is enough to show the non-negativity of the function $\gamma_1(t)$. We substitute D_1 as an integral, make the substitution $x = \omega/\Omega$ and swap the integrals

$$\begin{aligned} \gamma_1(t) &= 4\lambda\Omega^2 \int_0^\infty \mathrm{d}x \coth\left(x\frac{\Omega}{2T}\right) x^s e^{-x} \int_0^t \mathrm{d}\tau \cos(x\Omega\tau) \\ &= 4\lambda\Omega \int_0^\infty \mathrm{d}x \coth\left(x\frac{\Omega}{2T}\right) x^{s-1} e^{-x} \sin(x\Omega t) = 4\lambda\Omega \int_0^\infty \mathrm{d}x F(x) \sin(x\Omega t) \,. \end{aligned} \tag{2.40}$$

Since the parameter $s \leq 1$, $F(x)$ is the product of three functions that are non-increasing and positive on the interval, and hence $F(x)$ itself is non-increasing and positive. Thus, if we chop the x-axis into individual periods of the sine

$$\gamma_1(t) = \lambda\Omega \sum_{i=0}^\infty \int_{i\frac{2\pi}{\Omega t}}^{(i+1)\frac{2\pi}{\Omega t}} \mathrm{d}x F(x) \sin(x\Omega t) \,, \tag{2.41}$$

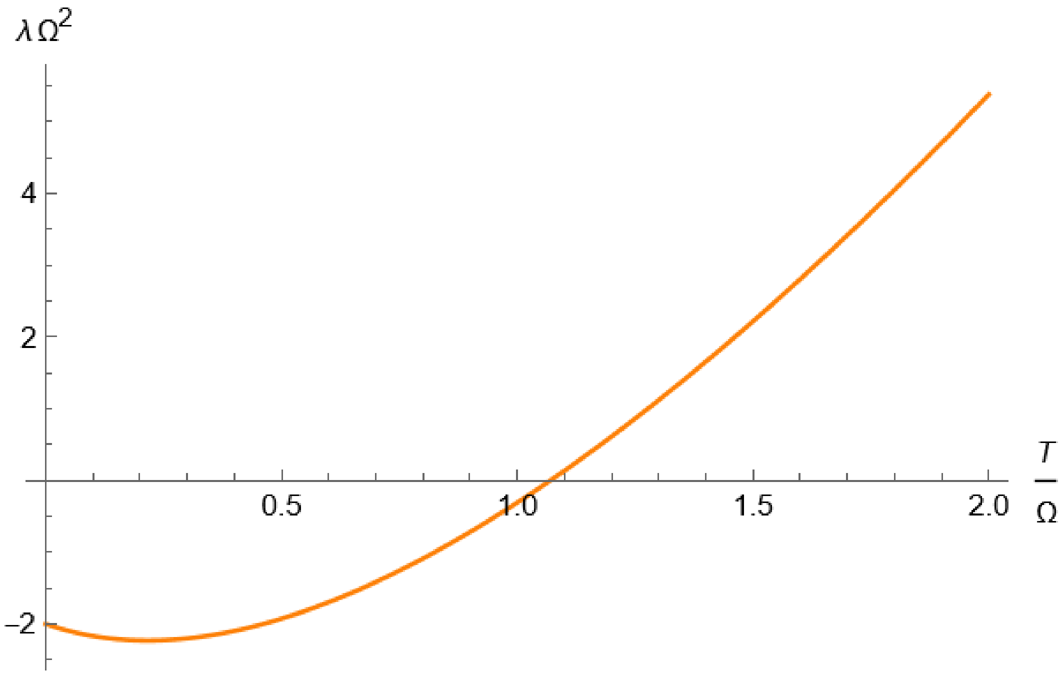

Figure 2.1: $2\lambda T\Omega(-T/\Omega)^s[\psi^{(s)}(T/\Omega)+\psi^{(s)}(1+T/\Omega)]$ for $s=0$. If $D_1(0)$ were given by this relation, then for some combination of values it would be negative, which in $t=0$ cannot happen, because then there would be a positive value on the diagonal of M. Then if the initial state had a component of the Bloch vector in the x or y direction equal to 1, this component would immediately grow over 1, which does not make physical sense. Therefore we know that this formula given in [19] does not give accurate results, at least in $t=0$. For higher times we can no longer use this argument, D_1 can be negative, just its integral $\gamma(\tau)$ turns out to be positive. But even if there were a time $\tau>0$ such that $\gamma(\tau)<0$, nothing guarantees that any component of the Bloch vector could be high enough at that time to exceed 1 as a result of that. Therefore we have to derive that $\gamma(\tau)>0$ differently.

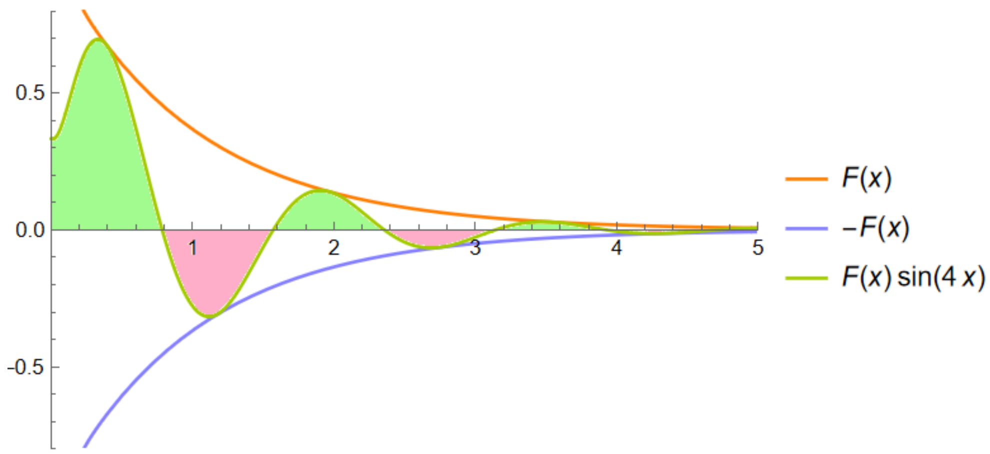

Figure 2.2: Figure representing formula (2.41) for values $\Omega t=4$, $\Omega/(2T)=12$ and $s=1$. We can see from the figure that the green areas are always larger than the following red areas, so the resulting integral will be positive

each term of the sum will be non-negative since the contribution in the positive part of the period of the sine will be larger in absolute value than the one in the negative part, we express this statement graphically in (2.2).

Thus $\gamma_1(t) \geq 0$. When we plug this information into (2.38), we see that assuming $f_2 = 0$, the time derivative of the entropy is non-negative. Thus it is clear that coupling of the reservoir with the projection of the spin to the z-direction is by itself behaving as one would expect.

But on the contrary, if we put $f_1 = 0$ and $f_2 \neq 0$ in (2.4) (i.e. we turn off coupling with the z-direction, but turn coupling with the x-direction back on), we get

$$M(t)|_{f_1=0} = \begin{pmatrix} 0 & -\omega_0 & 0 \\ \omega_0 + f_2^2\gamma_1^s(t) & -f_2^2\gamma_1^c(t) & 0 \\ 0 & 0 & -f_2^2\gamma_1^c(t) \end{pmatrix}, \tag{2.42}$$

and $b(t)|_{f_1=0} = -e_3 f_2^2 \gamma_2^s$. Then

$$\partial_t \vec{v}(t)|_{f_1=0} = \begin{pmatrix} -\omega_0 v_2(t) \\ \omega_0 v_1(t) + f_2^2\gamma_1^s(t)v_1(t) - f_2^2\gamma_1^c(t)v_2(t) \\ -f_2^2\gamma_1^c(t)v_3(t) - f_2^2\gamma_2^s(t) \end{pmatrix}. \tag{2.43}$$

This, when plugged into (2.35) gives

$$\begin{aligned} \frac{\mathrm{d}S(t)}{\mathrm{d}t}|_{f_1=0} &= \frac{\omega}{2T} f_2^2(\gamma_1^c v_3(t) + \gamma_2^s) + \\ &+ \frac{1}{2|\vec{v}|}\ln\frac{1+|\vec{v}|}{1-|\vec{v}|} f_2^2\left[(v_2(t)^2 + v_3(t)^2)\gamma_1^c(t) - v_1(t)v_2(t)\gamma_1^s(t) + v_3(t)\gamma_2^s(t)\right]. \end{aligned} \tag{2.44}$$

Now, we will show, that the first term of the (2.44) can be negative. The parenthesis $(\gamma_1^c(t)v_3(t) + \gamma_2^s(t))$ can be negative for small times since for small times $\gamma_1^c(t) = O(t)$ while $\gamma_2^s(t) = O(t^2)$. So there will be a time τ such that $\gamma_1^c(\tau) \gg \gamma_2^s(\tau)$, during that time it suffices that $v_3(\tau)$ is negative and also has some non-negligible size (namely at least $|v_3(\tau)| > |\gamma_2^s(\tau)/\gamma_1^c(\tau)|(\ll 1)$) and $(\gamma_1^c(\tau)v_3(\tau) + \gamma_2^s(\tau)) < 0$ holds.

Since the second term of (2.44) does not depend on ω, in case, that the first bracket of (2.44) is negative, there exists an ω for which $\mathrm{d}S(t)/\mathrm{d}t|_{f_1=0} < 0$. Thus, we see that the interaction of the reservoir with the projection of the spin in the x-direction is itself responsible for the decrease in entropy, as we defined it. Note, that the "perpetual motion machine of the second kind" we outlined at the beginning of this section also needs $f_2 \neq 0$, but no condition on f_1. Also, note that coherences are not necessary. We needed a condition, that $v_3 < 0$ but no assumptions concerning v_1, v_2.

In fact, there is no need to calculate the whole evolution, if we just plug in the state, that has the maximum entropy according to our definition ($\vec{v_T}$) into (2.3) we see that while for the case with $f_2 = 0$, we get $\partial_t \vec{v_T} = 0$, for $f_2 \neq 0$ this is generally not the case, i.e., there may be a decrease in entropy (or rather in what we defined as entropy). This is even a necessary property of systems that converge to a state with steady-state coherences from any initial state (for this, not only $f_2 \neq 0$ but also $f_1 \neq 0$ is needed in this model). If we start from a state $\vec{v_T}$, that has no coherences and we consider it to be a state that maximizes the entropy of the whole system, then the resulting coherent steady state will according to our description have lower entropy. This applies, for example, also to models proposed in [28, 29].

2.2.2 The Role of Interaction in the Investigated Phenomenon: Physical Reasoning

But why does an interaction of the reservoir with the projection of the spin into the x-direction cause this strange behavior, while the same interaction in the z-direction does not? The only difference between the directions is that there is a magnetic field in the z-direction, and thus the spin energy depends on its projection into the z-direction. That does not leave much possibility as to what the reason might be. Specifically, the issue is that the interaction with the projection into the x-direction is pouring energy from the reservoir into the spin even in situations where it according to our description of entropy should not.

Let us look again first at the situation with $f_2 = 0$. In that case, the reservoir interacts only with the spin projection in the z-direction. Information about the z-direction will leak into the reservoir and thus decoherence will occur in the other two directions. When we look at (2.36), we see that this is what happens (plus precession, but this corresponds to free evolution and does not affect entropy). And by decoherence the entropy increases.

There are a few changes in (2.42) compared to (2.36). A new off-diagonal term is added, $\vec{b} \neq \vec{0}$, and the constant for the diagonal terms changes a bit. But the key change is that now into the reservoir leaks information about the projection into the x-direction, and thus "decoherence" (not in a literal sense, as v_3 describes populations, not coherences) also occurs in the z-direction. Thus when $v_3 < 0$ and the interaction of the reservoir with the projection into the x-direction reduces the magnitude of v_3, it is thereby increasing the energy of the spin. And this can occur even in cases when what we call "the entropy of the whole closed system" is thereby reduced.

We can thus imagine a discrete version of the engine we have proposed:

1. we let spin thermalize ($v_1(0) = v_2(0) = 0; v_3(0) = -\tanh\left(\frac{\omega_1}{2T}\right)$)
2. we increase ω by $\Delta\omega$ to get $W_{\text{out}} = -\Delta\omega v_3(0)$
3. we measure the projection of the spin in the x-direction, losing all information about the z-direction, so now $v_3 = 0$
4. we reduce ω to its original value, we do not need to do any work to do this, since $v_3 = 0$
5. we let the spin thermalize again

It would seem that this is just another implementation of the Quantum Szilard Engine. But the difference is greater than just that the measurement comes after the work is done, not before it (which is related to the fact that we are measuring in a direction perpendicular to the significant one). The main difference is that the work we get during one cycle is $-v_3(0)\Delta\omega$, while the work required to erase the memory where we store the information about the spin projection in the x-direction (which is the only measurement during the cycle) is $T\ln(2)$, which does not depend on $\Delta\omega$. That is, for every choice of the parameters T, ω_1, there exists a $\Delta\omega$ for which we get positive work from the cycle. Specifically, we need to increase the energy gap by

$$\Delta\omega > \frac{T\ln(2)}{\tanh\left(\frac{\omega_1}{2T}\right)} . \tag{2.45}$$

Note that we once again assume that $f_2 \neq 0$ here because otherwise, thermalization would not affect v_3, as we see from (2.37). In other words, the transition between the ground and excited state is forbidden for $f_2 = 0$.

Why would not this cycle behave like a perpetual motion machine in reality? Because there is more to fully considering the measurement process than just erasing information afterward. Generally, it is interaction with something outside of the system, and therefore the entropy of the system can decrease as a result of this interaction, as the system is not closed in the moment it happens.

However, when instead of measurement there is just an interaction between the reservoir and the projection of the spin to the x-direction, there is no interaction outside of the closed spin-reservoir system, so the total entropy of the spin-reservoir system should not decrease. Moreover, if we consider, that the full evolution of the spin-reservoir system is given by $\dot{\rho}_{\text{full}} = -i[H_{\text{full}}, \rho_{\text{full}}]$, the total entropy can not decrease regardless of the Hamiltonian [15]. Therefore we must conclude, that there is some problem in using thermodynamic limit, or weak coupling. For example, some assumption was made which is valid in the case when the reservoir interacts only with the projection of the spin to the z-direction but is not valid when we add interaction with projection to the x-direction.

There are two possibilities for when this could happen. One option is a projection of the dynamics of the full system onto the spin subsystem. The second option is, that what we defined as entropy is not actual entropy, and therefore it may decrease in time, even though entropy does not decrease in time. Let us first discuss this second option and then come back to the first one.

What are some of the conditions, that some function $\tilde{S}$ must satisfy, to be considered entropy of the system, if the time evolution was calculated accurately? In the case when $f_1 = 0, f_2 \neq 0$ state $\vec{v_T}$ (with no coherences) is maximizing the $\tilde{S}$ (at least locally) for $t \to \infty$ because all initial states are converging to this state. However, $\vec{v_T}$ can not be maximizing the $\tilde{S}$ for all times, because if we choose $\vec{v_T}$ to be the initial state, the state of the spin will still evolve nontrivially, before converging back to the initial state. In the case of $f_1 \neq 0, f_2 \neq 0$ the state, that maximizes $\tilde{S}$ for $t \to \infty$ must be the steady state with spin having non-zero coherences, but again, this can not be the same for general time, as the evolution is not trivial even in the case if we choose this state to be the initial. So we see, that the function $\tilde{S}$ can not depend only on the Bloch vector, but the state of the system has to be defined also by some other quantity (perhaps the time). The form of $\tilde{S}$ must also depend on both coupling constants f_1, f_2, as the resulting steady state depends on their product, and the behavior of the system is quite different in the case when just $f_1 = 0$ compared to the case when just $f_2 = 0$. This makes sense, as these constants describe the reservoir (similarly to for example temperature).

We were not able to find the generalization of entropy that would satisfy these conditions. It can be however interesting research topic, that can bring useful insights into the role of coherences in quantum thermodynamics.

Now back to the other option. If the problem is not in the definition of entropy, it would have to be in the equation of motion for the reduced system. This was obtained from the evolution of the full system (which conserves the entropy) by projecting it onto the spin. We will explore what could be inconsistent in this process, in the next subsection.

2.2.3 Redfield approximation

Not many assumptions have been made during the projection of the full evolution onto the reduced system (as we already mentioned, Born-Markov and secular approximations were not used). If we do not want to question weak coupling itself, it leaves just the so-called Redfield limit [15]

$$\begin{aligned} \partial_t \rho(t) &= -\int_0^t \mathrm{d}s\, \mathrm{Tr}_{\mathrm{R}}[H_{\mathrm{I}}(t), [H_{\mathrm{I}}(s), \rho(s) \otimes \rho_{\mathrm{R}}]] \rightarrow \\ \partial_t \rho(t) &= -\int_0^t \mathrm{d}s\, \mathrm{Tr}_{\mathrm{R}}[H_{\mathrm{I}}(t), [H_{\mathrm{I}}(s), \rho(t) \otimes \rho_{\mathrm{R}}]] \,. \end{aligned} \tag{2.46}$$

This approximation changes the time argument of the reduced density matrix on the right-hand side of its equation of motion, so the time derivative depends only on the current state and not the previous ones. This approximation is therefore necessary for Bloch equations to be local in time.

According to [30, 31] this approximation assumes, that the characteristic relaxation time of the reservoir τ_{R} is much shorter than the characteristic time over which the state of the spin varies significantly τ_{S}. It is straightforward to assume, that $\tau_{\mathrm{R}} \sim 1/T$ and $\tau_{\mathrm{S}} \sim 1/\omega$. Then the assumption used in deriving the Redfield limit (2.46) can be cast symbolically as

$$\begin{aligned} \tau_{\mathrm{R}} &\ll \tau_{\mathrm{S}} \\ \omega &\ll T \,. \end{aligned} \tag{2.47}$$

We see that upon using this assumption, all of the apparent conflicts with the Second law of thermodynamics vanish. Namely:

- In (2.2.1) to show, that the time derivative in entropy (2.44) can be negative we first show that the first bracket is negative and then assume, that prefactor ω/T can be arbitrarily large. But according to (2.47), this factor is quite small.

- In [19] the steady-state coherences vanish.

Redfield limit assumes condition (2.47) in the sense that it is a sufficient condition, but not a necessary one. Therefore we can not be sure, wheater the results derived using the Redfield limit are valid also for cases when (2.47) does not hold. However, it is possible that the coherence-inducing heat bath is only artifact caused by plugging in values that are incompatible with assumptions, that were used to derive the equations of motion.

But if this was the actual problem all along, we should ask the following question: why coupling of the reservoir with the projection of the spin to the

z-direction was not causing a decrease in entropy as well? The reasons for this are similar to what we indicated in subsection 2.2.2. By approximation (2.46) we speed up the rate at which the information about the projection of the spin into a given direction is escaping into the reservoir (at least that is how it works in the case of z-direction). We try to illustrate why this happens in figure 2.3. If the direction, with which the reservoir is interacting is the z-axis, this only speeds up decoherence. But if this is true also for the x-axis and the projection of spin into z-direction is negative, a similar mechanism might induce a heat current from the reservoir to the spin, which might be non-physical.

To sum up this subsection: the Redfield approximation was used in the derivation of the equations of motion in [19]. This approximation was derived in [30] with the assumption we recast for this model as (2.47). All of the supposed conflicts with the Second law of thermodynamics vanish upon applying this assumption. However, we did not find any direct proof, that it is this approximation that causes the counterintuitive behavior of the model presented in paper [19], so it might all be just a coincidence. The best way to find out, wheater the equations of motion derived in [19] describe the evolution of the system would be to compare their predictions with some experimental data. However, no one has constructed a system with Hamiltonian (2.1) in a laboratory yet, so this question remains open.

2.3 Summary

In this chapter, we investigated the phenomena of coherence-inducing heat bath that was introduced in [19]. We studied a model proposed in [19] that has a steady state with non-zero coherences, and discussed what role these coherences play in extracting work from the reservoir. It turned out, that in the case of fast thermodynamic cycles with single heat bath coherences provide an advantage over incoherent states.

However, it also seems, that it is possible to extract work from this system periodically with only one (coherence-inducing) heat reservoir needed. In other words, it is possible to construct an engine, which is forbidden by the Kelvin-Planck statement of the Second law of thermodynamics. Upon further investigation, it turned out, that we can also anticipate, that any system, that converges into a steady state with non-zero coherences from all initial states, seemingly decreases the entropy of the whole system. We can see it from the following construction: we prepare the reservoir in a state of thermal equilibrium and the reduced system in such a state, that has the same populations as the final state but zero coherences. Then the final steady state of the reduced system will have lower von Neumann entropy than the initial one. And according to assumptions of weak coupling the reservoir should be in the same state as it was at the beginning (as there are no correlations between the reservoir and the reduced system, and the reduced system has the same energy). Then the sum of the von Neumann entropy of the reduced system and the entropy of the reservoir has decreased over time.

We discussed two possible solutions for this supposed conflict with the Second law. One is, that what we called entropy is not the actual entropy of the whole closed system, and one has to generalize the entropy for this system. We came up

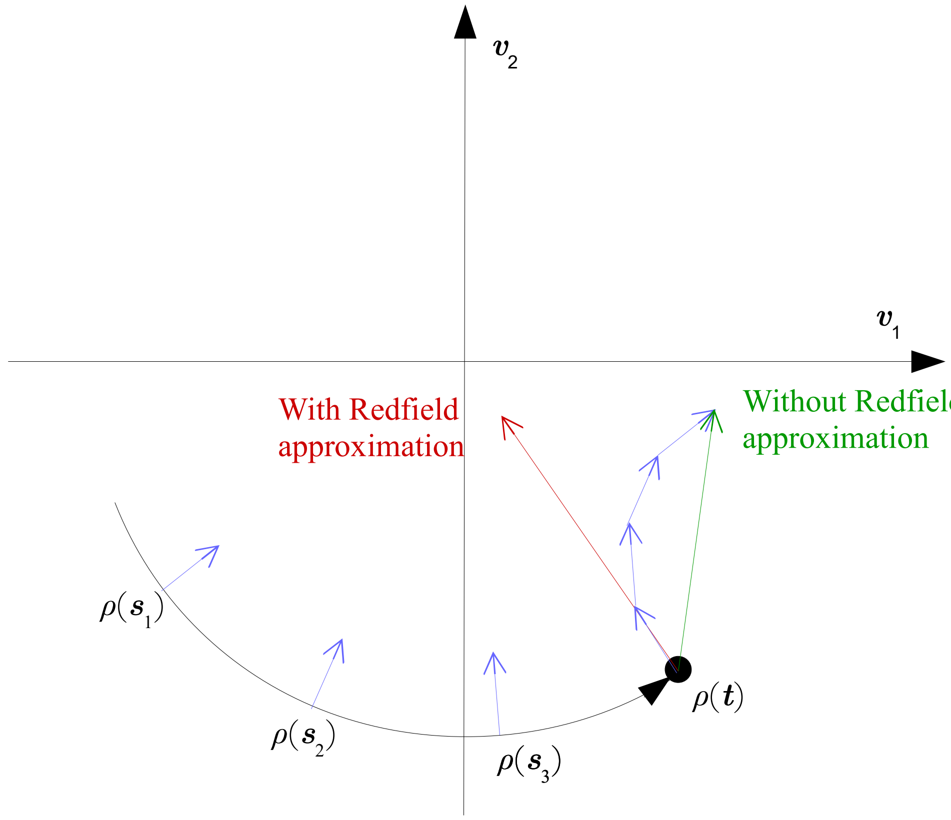

Figure 2.3: Figure aims to show why the Redfield limit speeds up the rate at which information about the projection of spin into a given direction is escaping into the reservoir. We illustrate this in the case for $f_1 \neq 0, f_2 = 0$, in this case, it is equivalent to speeding up the decoherence. Matrix M that contains derivatives from Bloch equation derived using Redfield limit for this case is (2.36). Because $\dot{v}_3 = 0$, we ignore the z-direction in this figure. We see that free evolution is precession with angular frequency ω_0, in the figure it is represented by the black curved dart. Decoherence induced by the reservoir contributes to evolution by time derivative, which is proportional (with a negative constant) to the current state. The current state is the black circle, this effect on it is represented by the red dart. This is the result of the Redfield limit. If we want to calculate the effect of the reservoir without using this approximation, we have to integrate along the whole black dart. We represent the integration by adding several discrete contributions (blue darts). We assume that each contribution is proportional to the state at that time, we also drew them to have the same size, which is not completely accurate, as they have to decrease as we go more to the past. But the point is, that when we add these contributions, the result (green dart) is not pointing straight to the center. Therefore, the state will converge faster if we apply the Redfield limit. Or in other words, the Redfield limit can speed up the rate at which information leaks into the reservoir. It is also clear, why in this case this effect grows with ω_0: state changes more during the same time, therefore without the Redfield limit, we get contributions that are more different. And as the temperature is inversely proportional to the relaxation time, the length of the black dart, along which we have to integrate is proportional to ω_0/T.

with some conditions, that this entropy has to satisfy to describe the evolution of the system, but we were unable to find an explicit expression for such entropy.

Another option we discussed is, that assumption of the Redfield limit made during the derivation of the equation of motion of the reduced system, might be incompatible with the values that are being substituted into those equations of motion. It is true, that upon assuming values that are compatible with the derivation of approximations, all "conflicts with the Second law of thermodynamics" vanish. However, this is not a proof, that the Redfield limit gives inconsistent results outside of the scope of assumptions made during its derivation. Also, we only explained, how the Redfield limit speeds up decoherence, and suggested, that similarly, it can induce some non-physical heat currents, but this once again does not prove, that it happens in this case. The surest way to tell, wheater the equations of motion are accurate or not, would be to observe experimentally a physical version of this system and compare its behavior to predictions of these equations.

There is a third option, that the assumption of the weak coupling is inconsistent with the classical thermodynamics in the first place. However, this would just mean that both equations of motion and the definition of entropy can be inconsistent with the classical thermodynamics. Therefore we did not discuss this option.

Although we were not able to narrow down the reasons for the counterintuitive behavior of this system to one, we believe, that we provided a solid base for a further investigation upon this intriguing issue. We also believe that it is important to fully understand what causes this behavior, as this system is pushing the boundaries of our current understanding of quantum thermodynamics.

Conclusion

In chapter 1, we studied a model of coherence-enhanced currents proposed in [14]. At first, we studied the model mathematically and calculated the moment-generating function for the heat current and entropy production of coherence-enhanced heat current in the model with a single heat bath in contact with a two-level degenerate system. Based on these mathematical results, we have presented a new physical insight about the cause of this coherence-induced enhancement: probability current through a given channel is proportional to a probability of a system being in a suitable state. Superposition enables a system to flow through many channels while being in a single quantum state. And the probability of the system being in this quantum state is therefore larger than in the case when the system is just in a mixture of more states.

Then we used these results to show, that work done by a cyclic heat engine utilizing coherence-enhanced heat current can be greater than its fluctuations even in case of limit, when the two-level system is always close to the equilibrium with a heat reservoir it is currently interacting with.

Furthermore, we proposed a generalization of the model from [14], that was using coherences to enhance current between two particle reservoirs. We used this model to create a heat engine, that does work while being in a nonequilibrium steady state. We also derived a condition that determines with how fast decoherence coherent-enhanced current still provides a significant quantum advantage.

In chapter 2, we studied a model proposed in [19], in which spin in a magnetic field forms coherences just by interaction with the reservoir. At first, we have shown, that coherences generated this way really provide the quantum advantage in the extraction of work. Then we show, that we can extract work from the reservoir proposed in [19] periodically without any other reservoir needed. That seems to contradict the Kelvin-Planck statement of the Second law of thermodynamics. Therefore we studied the production of entropy induced by the interaction of the spin and the reservoir.

However, it turned out, that either our formula for entropy is incomplete, or the equations of motion of the spin derived in [19] are not consistent with the used values for temperature T and energy gap ω. We were not able to find out which of these options can be used to explain the behavior of this system. So we discussed both of these options and hopefully provided a solid base for further exploration of this remarkable model.

Results presented in our work provide useful physical insights into the theory of quantum coherence and its applications. Therefore our results are potentially useful in all areas of quantum physics, that try to exploit quantum coherences to gain the quantum advantage, particularly in quantum thermodynamics and quantum optics, as in our work we were mostly discussing papers concerning these two fields.

Bibliography

[1] Alexander Streltsov, Gerardo Adesso, and Martin B. Plenio. Colloquium: Quantum coherence as a resource. *Rev. Mod. Phys.*, 89:041003, Oct 2017.

[2] Yu-Han Ma, C. L. Liu, and C. P. Sun. Works with quantum resource of coherence, 2021.

[3] Eric Chitambar and Gilad Gour. Critical examination of incoherent operations and a physically consistent resource theory of quantum coherence. *Phys. Rev. Lett.*, 117:030401, Jul 2016.

[4] David Deutsch and Richard Jozsa. Rapid solution of problems by quantum computation. *Proceedings of the Royal Society of London. Series A: Mathematical and Physical Sciences*, 439(1907):553–558, 1992.

[5] Charles H. Bennett and Gilles Brassard. Quantum cryptography: Public key distribution and coin tossing. *Theoretical Computer Science*, 560:7–11, 2014. Theoretical Aspects of Quantum Cryptography – celebrating 30 years of BB84.

[6] Vittorio Giovannetti, Seth Lloyd, and Lorenzo Maccone. Quantum-enhanced measurements: Beating the standard quantum limit. *Science*, 306(5700):1330–1336, 2004.

[7] Adolfo del Campo, Aurélia Chenu, Shujin Deng, and Haibin Wu. *Friction-Free Quantum Machines*, pages 127–148. Springer International Publishing, Cham, 2018.

[8] Kay Brandner, Michael Bauer, and Udo Seifert. Universal coherence-induced power losses of quantum heat engines in linear response. *Phys. Rev. Lett.*, 119:170602, Oct 2017.

[9] Stefan Aimet and Hyukjoon Kwon. Engineering a heat engine purely driven by quantum coherence. *Phys. Rev. A*, 107:012221, Jan 2023.

[10] Shunsuke Kamimura, Hideaki Hakoshima, Yuichiro Matsuzaki, Kyo Yoshida, and Yasuhiro Tokura. Quantum-enhanced heat engine based on superabsorption. *Phys. Rev. Lett.*, 128:180602, May 2022.

[11] Paul Menczel, Eetu Loisa, Kay Brandner, and Christian Flindt. Thermodynamic uncertainty relations for coherently driven open quantum systems. *Journal of Physics A: Mathematical and Theoretical*, 54(31):314002, jul 2021.

[12] Naoto Shiraishi and Hiroyasu Tajima. Efficiency versus speed in quantum heat engines: Rigorous constraint from lieb-robinson bound. *Phys. Rev. E*, 96:022138, Aug 2017.

[13] C. L. Latune, I. Sinayskiy, and F. Petruccione. Thermodynamics from indistinguishability: Mitigating and amplifying the effects of the bath. *Phys. Rev. Res.*, 1:033192, Dec 2019.

[14] Hiroyasu Tajima and Ken Funo. Superconducting-like heat current: Effective cancellation of current-dissipation trade-off by quantum coherence. *Phys. Rev. Lett.*, 127:190604, Nov 2021.

[15] Heinz-Peter Breuer and Francesco Petruccione. *The Theory of Open Quantum Systems*. 01 2006.

[16] Lorenza Viola, Emanuel Knill, and Seth Lloyd. Dynamical decoupling of open quantum systems. *Phys. Rev. Lett.*, 82:2417–2421, Mar 1999.

[17] Peter W. Shor. Scheme for reducing decoherence in quantum computer memory. *Phys. Rev. A*, 52:R2493–R2496, Oct 1995.

[18] Carole Addis, Gregoire Brebner, Pinja Haikka, and Sabrina Maniscalco. Coherence trapping and information backflow in dephasing qubits. *Phys. Rev. A*, 89:024101, Feb 2014.

[19] Giacomo Guarnieri, Michal Kolář, and Radim Filip. Steady-state coherences by composite system-bath interactions. *Phys. Rev. Lett.*, 121:070401, Aug 2018.

[20] Naoto Shiraishi, Keiji Saito, and Hal Tasaki. Universal trade-off relation between power and efficiency for heat engines. *Phys. Rev. Lett.*, 117:190601, Oct 2016.

[21] Armen E. Allahverdyan, Karen V. Hovhannisyan, Alexey V. Melkikh, and Sasun G. Gevorkian. Carnot cycle at finite power: Attainability of maximal efficiency. *Phys. Rev. Lett.*, 111:050601, Aug 2013.

[22] T. Baumgratz, M. Cramer, and M. B. Plenio. Quantifying coherence. *Phys. Rev. Lett.*, 113:140401, Sep 2014.

[23] Gregory Bulnes Cuetara, Massimiliano Esposito, and Gernot Schaller. Quantum thermodynamics with degenerate eigenstate coherences. *Entropy*, 18(12), 2016.

[24] Hugo Touchette. The large deviation approach to statistical mechanics. *Physics Reports*, 478(1-3):1–69, jul 2009.

[25] Michele Campisi, Peter Hänggi, and Peter Talkner. Colloquium: Quantum fluctuation relations: Foundations and applications. *Rev. Mod. Phys.*, 83:771–791, Jul 2011.

[26] Mischa P. Woods, Ralph Silva, and Jonathan Oppenheim. Autonomous quantum machines and finite-sized clocks. *Annales Henri Poincaré*, 20(1):125–218, oct 2018.

[27] Suriyanarayanan Vaikuntanathan and Christopher Jarzynski. Modeling maxwell's demon with a microcanonical szilard engine. *Phys. Rev. E*, 83:061120, Jun 2011.

[28] Artur Slobodeniuk, Tomáš Novotný, and Radim Filip. Extraction of autonomous quantum coherences. *Quantum*, 6:689, Apr 2022.

[29] Ricardo Román-Ancheyta, Michal Kolář, Giacomo Guarnieri, and Radim Filip. Enhanced steady-state coherence via repeated system-bath interactions. *Phys. Rev. A*, 104:062209, Dec 2021.

[30] A. G. Redfield. On the theory of relaxation processes. *IBM Journal of Research and Development*, 1(1):19–31, 1957.

[31] Karl Blum. *Density Matrix Theory and Applications*, volume 64 of *Springer Series on Atomic, Optical and Plasma Physics*. Springer, Berlin, Heidelberg, 2012.