

THERMAL RECTIFICATION BEHAVIOUR OF SOME SMALL QUANTUM
SYSTEMS

A THESIS SUBMITTED TO
THE GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES
OF
MIDDLE EAST TECHNICAL UNIVERSITY

BY

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IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR
THE DEGREE OF MASTER OF SCIENCE
IN
PHYSICS

SEPTEMBER 2021

Approval of the thesis:

THERMAL RECTIFICATION BEHAVIOUR OF SOME SMALL QUANTUM SYSTEMS

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ABSTRACT

THERMAL RECTIFICATION BEHAVIOUR OF SOME SMALL QUANTUM SYSTEMS

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September 2021, 44 pages

Thermal rectification behaviors for some small quantum systems are studied by using the Lindblad master equation. From the underlying Hamiltonian dynamics of the composite quantum systems consisting of small quantum systems and reservoirs, Lindblad master equations are obtained by using certain approximations. Optimum operation parameters are determined for a single two-level and two two-level quantum systems. It is shown that there is no thermal rectification behavior when the contact between two reservoirs is a single harmonic oscillator or two harmonic oscillators. Lindblad master equation and Hamiltonian dynamics is used separately to show that the zero rectification is due to the linearity of the dynamics of the oscillators and it is not the result of the approximations made when the Lindblad master equation is obtained.

Keywords: Lindblad master equation, thermal rectification, thermal diode, Ising coupling, Heisenberg coupling

ÖZ

BAZI KÜÇÜK KUANTUM SİSTEMLERİN ISIL DOĞRULTMA DAVRANIŞLARI

ZERVENT, SELAHİTTİN ATILAY

Yüksek Lisans, Fizik Bölümü

Tez Yöneticisi: Prof. Dr. Sadi Turgut

Eylül 2021 , 44 sayfa

Bazı küçük kuantum sistemleri için ısıl doğrultma davranışları Lindblad denklemi kullanılarak incelenmiştir. Küçük kuantum sistemleri ve rezervuarlardan oluşan bileşik kuantum sistemlerinin altında yatan Hamilton dinamiklerinden, belirli yaklaşımlarla Lindblad denklemleri elde edildi. Tek bir iki seviyeli ve iki iki seviyeli kuantum sistemleri için optimum çalışma parametreleri belirlendi. İki rezervuar arasındaki temas olarak harmonik osilatör ve iki harmonik osilatör için ısıl doğrultma davranışının olmadığı gösterilmiştir. Sıfır doğrultmanın Lindblad denklemini elde ettiğimizde yaptığımız yaklaşımların sonucu olmadığını göstermek için Hamilton dinamiğini kullandık.

Anahtar Kelimeler: Lindblad denklemi, ısıl doğrultma, ısıl diyot, Ising etkileşmesi, Heisenberg etkileşmesi

To my family

ACKNOWLEDGMENTS

I thank TÜBİTAK for their popular science books for kids, which encouraged me to be a scientist and for their financial support during my education through the 2210-A scholarship program.

TABLE OF CONTENTS

ABSTRACT	v
ÖZ	vi
ACKNOWLEDGMENTS	viii
TABLE OF CONTENTS	ix
LIST OF FIGURES	xi
CHAPTERS	
1 INTRODUCTION	1
2 LINDBLAD MASTER EQUATION	3
2.1 Density Matrices	3
2.1.1 Composite systems	4
2.1.2 Time evolution of a density matrix	5
2.2 Lindblad Master Equation from the Hamiltonian Dynamics	6
2.3 Master Equation for a Two-Level Atom in a Radiation Field	11
2.4 Master equation for the harmonic oscillator	14
2.5 Heat transfer expression	15
3 TWO-LEVEL SYSTEM	17
3.1 Master equation	17
3.2 Rectification behavior	20

4	TWO TWO-LEVEL SYSTEMS	25
4.1	Ising Coupling	25
4.1.1	Theory	25
4.1.2	Behaviour	27
4.2	Heisenberg Coupling	27
4.2.1	Theory	29
4.2.2	Behavior	30
5	HARMONIC OSCILLATOR	33
5.1	Master equation	33
5.2	Exact solution	35
5.3	Two harmonic oscillators	38
6	CONCLUSION	41
	REFERENCES	43

LIST OF FIGURES

FIGURES

Figure 3.1	Contact between the reservoirs. L corresponds to the left reservoir, R corresponds to the right reservoir, and S is the two-level system.	17
Figure 3.2	Heat transfer rates in the case $g_1 = 5, g_2 = 1$.	21
Figure 3.3	Rectification in the case $g_1 = 5, g_2 = 1$.	21
Figure 3.4	Rectification in the case $T_1/\omega = 1$	22
Figure 3.5	Rectification in the case $g_1 = 5, g_2 = 1$	23
Figure 4.1	Contact between the reservoirs. L corresponds to the left reservoir, R corresponds to the right reservoir, S_L is the left two-level system, and S_R is the right two-level system.	25
Figure 4.2	Transitions among the energy levels. The sequence represents the energy levels. The blue arrows correspond to the excitations or deexcitations done by the left reservoir, and the red arrows are the ones done by the right reservoir. The arrows on the left represent the heat flow from the left bath to the right bath, while the arrows on the right are the flow from the right bath to the left bath.	28
Figure 4.3	Heat transfer rate in the case $\omega_L = 11\omega_{LR}, \omega_R = 0$	28

Figure 4.4	Transitions among the energy levels. The sequence represents the energy levels. The blue arrows correspond to the excitations or decays done by the left reservoir, and the red arrows are the ones done by the right reservoir. The arrows on the left represent the heat flow from the left bath to the right bath, while the arrows on the right are the flow from the right bath to the left bath.	29
Figure 4.5	Rectification in the case $\omega_R = 0$, $T_L = \omega_{LR}$ and $T_R = 2\omega_{LR}$. $\omega_L = 0$ corresponds to the figure 4.4	29
Figure 4.6	Heat transfer rates in the case $\omega_L = 11\omega_{LR}$, $\omega_R = 0$	31
Figure 4.7	Rectification in the case $\omega_L = 11\omega_{LR}$, $\omega_R = 0$, $T_L = \omega_{LR}$ and $T_R = 2\omega_{LR}$	32
Figure 5.1	Contact between the reservoirs. L corresponds to the left reservoir, R corresponds to the right reservoir, and S is the harmonic oscillator.	33
Figure 5.2	Contact between the reservoirs. L corresponds to the left reservoir, R corresponds to the right reservoir, S_L is the left harmonic oscillator, and S_R is the right harmonic oscillator.	38
Figure 5.3	Contact between the reservoirs. L corresponds to the left reservoir, R corresponds to the right reservoir, S_1 is the first decoupled harmonic oscillator and S_2 is the second.	39

CHAPTER 1

INTRODUCTION

Humankind has recently begun to exploit quantum nature. The ability to manipulate individual molecules, atoms, and spins have led to the emergence of quantum devices.

However, those quantum devices are not isolated systems but open quantum systems which thermally interact with their environment. The stored quantum information leaks into the environment as the state of the system gradually approaches the thermal equilibrium state which is determined by the temperature of the environment. Therefore controlling the quantum devices also requires controlling their interaction with the environment. Thermal control in the nanoscale requires systems on nanoscale whose behaviors are governed by quantum mechanics. Therefore there is a need to study the thermal behaviour of quantum systems. Recently, such studies have been done[1, 2, 3, 4, 5, 6].

In this thesis, some basic well-known quantum systems are investigated for their thermal rectification behaviors when they are simultaneously in contact with two otherwise non-interacting thermal baths in the search for a possible quantum thermal diode. A thermal diode is the thermal analog of the electrical diode, which allows current to flow in one direction and restricts it when the opposite voltage difference is applied. In the thermal diode, heat is allowed to be transferred in one direction but restricted in the other direction.

Of course there is no rectification in the linear regime when the temperature difference between the reservoirs is small. For this reason, large temperature differences are treated in all of the calculations. For such large temperature differences, the steady-state quantum state of the thermal contact may diverge significantly from a canonical

thermal equilibrium state. For this reason, exact calculations of the state of the contact are necessary.

CHAPTER 2

LINDBLAD MASTER EQUATION

2.1 Density Matrices

Since we will deal with the thermal properties of quantum states, we have to deal with their statistics. And in order to characterize the statistical properties of a quantum system, we will use a density matrix.

Consider an ensemble of quantum states, each with its state vector. If we want to find the expectation value of an observable A , we have

$$\langle A \rangle = \sum_{\alpha} \frac{n_{\alpha}}{N} \langle \psi_{\alpha} | A | \psi_{\alpha} \rangle , \quad (2.1)$$

where n_{α} is the number of elements in the ensemble having state vector ψ_{α} . Inserting an identity operator, we have

$$\langle A \rangle = \sum_{\alpha, i} \frac{n_{\alpha}}{N} \langle \psi_{\alpha} | A | \phi_i \rangle \langle \phi_i | \psi_{\alpha} \rangle = \sum_{\alpha, i} \frac{n_{\alpha}}{N} \langle \phi_i | \psi_{\alpha} \rangle \langle \psi_{\alpha} | A | \phi_i \rangle , \quad (2.2)$$

where ϕ_i 's are orthonormal state vectors in an arbitrary base. If we define density matrix ρ as

$$\rho = \sum_{\alpha} p_{\alpha} | \psi_{\alpha} \rangle \langle \psi_{\alpha} | \quad (2.3)$$

where p_{α} 's are the classical probabilities of an element in the ensemble to be in state ψ_{α} ,

$$p_{\alpha} = \frac{n_{\alpha}}{N} . \quad (2.4)$$

Then the expectation value of an observable becomes

$$\langle A \rangle = \text{tr}(A\rho) . \quad (2.5)$$

Note that the state vectors can be represented in a particular basis as

$$|\psi_\alpha\rangle = \sum_i \langle\phi_i|\psi_\alpha\rangle|\phi_i\rangle = \sum_i c_{\alpha,i}|\phi_i\rangle. \quad (2.6)$$

Then the density matrix can be represented as

$$\rho = \sum_{\alpha,i,j} p_\alpha c_{\alpha,i} c_{\alpha,j}^\dagger |\phi_i\rangle\langle\phi_j| = \sum_{i,j} \rho_{i,j} |\phi_i\rangle\langle\phi_j|. \quad (2.7)$$

Therefore when the density matrix is represented in a particular basis, there are two probabilities to consider for the diagonal elements, the classical probability of the state to be the particular state in the ensemble, p_α and the quantum probability of that particular state to be in the base state, $|c_{\alpha,i}|^2$. The multiplication gives us the overall probability of finding the state in ϕ_i . Also, note that when we consider the density matrix in the energy basis, the diagonal elements of the matrix gives us the probabilities to find the state at the corresponding energies, therefore for a system in thermal equilibrium, there is no particular state for the system but particular diagonal elements of the density matrix. Therefore we need to work in the density matrix representation.

2.1.1 Composite systems

A system that consists of more than one quantum system is called a composite quantum system. Let us assume that a composite system is formed by a bath(B) and a system(S) coupled to it. When we want to find the expectation value of operator $A^{(S)}$ for the coupled system, we need to find the expectation value of the operator $A^{(S)} \otimes I^{(B)}$ where $A^{(S)}$ acts on the coupled system's Hilbert space and identity operator $I^{(B)}$ acts on the bath's.

Density matrix can be written as

$$\rho = \sum_{i,j,k,l} \rho_{ij,kl} |a_i b_j\rangle\langle a_k b_l|, \quad (2.8)$$

where

$$|a_i b_j\rangle = |a_i\rangle \otimes |b_j\rangle, \quad (2.9)$$

$|a_i\rangle$'s are in the system's Hilbert space and $|b_j\rangle$'s are in the bath's Hilbert space,

$|a_i b_j\rangle$'s are in the composite Hilbert space and $|a_i\rangle, |b_i\rangle, |a_i b_j\rangle$ are all orthonormal states. Then partial trace

$$\rho_s = \text{tr}_B(\rho) \quad (2.10)$$

becomes

$$\rho_s = \sum_{i,j,k,l} \rho_{ij,kl} \langle b_j | b_l \rangle |a_i\rangle \langle a_k| = \sum_{i,j,k} \rho_{ij,kj} |a_i\rangle \langle a_k|. \quad (2.11)$$

We use partial trace to characterize the statistics of a subsystem from the density matrix of the composite quantum system[7].

2.1.2 Time evolution of a density matrix

To obtain the time evolution of ρ_s in equation 2.10, we first write the Schrödinger equation for an arbitrary state $|\psi\rangle$ in the composite system's Hilbert space.

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle, \quad (2.12)$$

where H is the Hamiltonian for the composite system. We can define the time evolution operator U as

$$U(t, t_0) |\psi(t_0)\rangle = |\psi(t)\rangle. \quad (2.13)$$

Since $|\psi_{t_0}\rangle$ is time-independent, the Schrödinger equation reduces to

$$i\hbar \frac{d}{dt} U(t, t_0) = H U(t, t_0) \quad (2.14)$$

for the time evolution operator, which results in

$$U(t, t_0) = e^{-i \frac{H(t-t_0)}{\hbar}}. \quad (2.15)$$

Since

$$\rho(t_0) = p_\alpha |\psi_\alpha(t_0)\rangle \langle \psi_\alpha(t_0)|, \quad (2.16)$$

the density matrix time evolution is therefore

$$\rho(t) = U(t, t_0) \rho(t_0) U^\dagger(t, t_0). \quad (2.17)$$

And from equation 2.15, the time derivative of the density matrix is

$$\dot{\rho}(t) = -\frac{i}{\hbar} [H, \rho(t)]. \quad (2.18)$$

And for the coupler system

$$\dot{\rho}_s(t) = \text{tr}_B\left(-\frac{i}{\hbar}[H, \rho(t)]\right). \quad (2.19)$$

Unfortunately this equation cannot be used in that form. In most of the cases, we are interested in the system only and we only know ρ_s . As a result, the right-hand side must be expressed entirely in terms of ρ_s . This cannot be done exactly. Therefore some approximations have to be used. If the right-hand side is expressed only in terms of a linear function of ρ_s at time t , then the equation is called a Markovian equation. In this approximation, all future values of the density matrix depends only on any chosen initial state (and not on any prior states).

2.2 Lindblad Master Equation from the Hamiltonian Dynamics

The dynamics of an open quantum system, in general, can not be represented with a unitary time evolution which does not explain the irreversibility, entropy increase, or relaxation to equilibrium. It is, instead, represented by a master equation for its density matrix. The dynamical map governed by the master equation should be a completely positive trace-preserving map to ensure that the time evolved density matrix conserve the properties of a density matrix. Moreover, if we neglect the memory effects in the evolution(We assume reservoir correlation functions decay so rapidly than the systematic evolution of the system), we can show that the master equation is in the Lindblad form[8].

$$\begin{aligned} \dot{\rho}_s(t) = & -\frac{i}{\hbar}[H, \rho_s(t)] \\ & + \sum_{k=1}^{N^2-1} \gamma_k \left[A_k \rho_s(t) A_k^\dagger - \frac{1}{2} \left\{ A_k^\dagger A_k, \rho_s(t) \right\} \right], \end{aligned} \quad (2.20)$$

where A_k 's are jump operators. Since equation 2.19 is generally very complicated to deal with, by making some approximations, we will obtain a master equation in the Lindblad form in which we obtain the jump operators from the underlying Hamiltonian evolution.

Following the footsteps of a classical textbook[8], we start with the time evolution of

the density matrix in the interaction picture for the whole system. The Hamiltonian of the whole system is

$$H = H_S + H_B + H_I , \quad (2.21)$$

where H_S is the system Hamiltonian, H_B is the bath Hamiltonian, and H_I is the Hamiltonian of the interaction between bath and the system. We write the Hamiltonian as

$$H = H_0 + H_I , \quad (2.22)$$

where

$$H_0 = H_S + H_B \quad (2.23)$$

is the unperturbed Hamiltonian and the interaction term, H_I , can be written as

$$H_I = \sum_{\alpha} A_{\alpha} \otimes B_{\alpha} , \quad (2.24)$$

where A_{α} and B_{α} are Hermitian operators where the former acts on the system and the latter acts on the reservoir. Here our aim is to relate the jump operators to A_{α} 's. The time evolution operator in the interaction picture is defined as

$$U_I(t, t_0) = U_0^{\dagger}(t, t_0)U(t, t_0) = e^{iH_0\frac{(t-t_0)}{\hbar}} e^{-iH\frac{(t-t_0)}{\hbar}} , \quad (2.25)$$

and the interaction picture state ket

$$U_I(t, t_0)|\psi(0)\rangle = |\psi(t)\rangle_I , \quad (2.26)$$

which makes the interaction picture density matrix as

$$\rho_I(t) = U_I(t, t_0)\rho(t_0)U_I^{\dagger}(t, t_0) . \quad (2.27)$$

Because

$$i\hbar\frac{d}{dt}U_I(t, t_0) = H_I(t)U_I(t, t_0) , \quad (2.28)$$

where

$$H_I(t) = U_0^{\dagger}(t, t_0)H_I U_0(t, t_0) , \quad (2.29)$$

the time derivative of the density matrix in the interaction picture becomes

$$\dot{\rho}_I(t) = -\frac{i}{\hbar} [H_I(t), \rho_I(t)] . \quad (2.30)$$

When equation 2.30 is integrated, the resulting density matrix as a function of time is

$$\rho(t)_I = \rho_I(0) - \frac{i}{\hbar} \int_0^t [H_I(s), \rho(s)] ds . \quad (2.31)$$

It could be substituted in equation 2.30 to obtain the time derivative of the density matrix again,

$$\dot{\rho}_I(t) = -\frac{i}{\hbar} [H_I(t), \rho_I(0)] - \frac{1}{\hbar^2} \int_0^t [H_I(t), [H_I(s), \rho_I(s)]] ds . \quad (2.32)$$

H_I in the interaction picture is

$$H_I(t) = \sum_{\alpha} A_{\alpha}(t) \otimes B_{\alpha}(t) . \quad (2.33)$$

If we apply the Born approximation for the density matrix by assuming the coupling between the system and reservoir is small enough to assume that the reservoir excitations are not affected by the system

$$\rho_I(t) = \rho_{I_s}(t) \otimes \rho_B , \quad (2.34)$$

and use equation 2.32, equation 2.33 has the following form

$$\begin{aligned} \dot{\rho}_{I_s}(t) = & \sum_{\alpha} (A_{\alpha}(t)\rho_{I_s}(t) - \rho_{I_s}(t)A_{\alpha}(t)) \text{tr}_B (B_{\alpha}(t)\rho_B) \\ & - \frac{1}{\hbar^2} \int_0^t ds \sum_{\alpha} \sum_{\beta} [A_{\alpha}(t)A_{\beta}(s)\rho_{I_s}(s) \text{tr}_B (B_{\alpha}(t)B_{\beta}(s)\rho_B) \\ & - A_{\beta}(s)\rho_{I_s}(s)A_{\alpha}(t) \text{tr}_B (B_{\beta}(s)\rho_B B_{\alpha}(t)) \\ & - A_{\alpha}(t)\rho_{I_s}(s)A_{\beta}(s) \text{tr}_B (B_{\alpha}(t)\rho_B B_{\beta}(s)) \\ & + \rho_{I_s}(s)A_{\beta}(s)A_{\alpha}(t) \text{tr}_B (\rho_B B_{\beta}(s)B_{\alpha}(t))] . \end{aligned} \quad (2.35)$$

Let us assume that

$$\text{tr}_B (B_{\alpha}(t)\rho_B) = 0 , \quad (2.36)$$

note that for any B operator we can add or subtract a constant times identity operator to B and accordingly modify H_S to have the same H consistent with equation 2.36.

Then, equation 2.35 can be written as

$$\begin{aligned} \dot{\rho}_{I_s}(t) = & -\frac{1}{\hbar^2} \int_0^t ds \sum_{\alpha, \beta} [\text{tr}_B (B_{\alpha}(t)B_{\beta}(s)\rho_B) (A_{\alpha}(t)A_{\beta}(s)\rho_{I_s}(s) - A_{\beta}(s)\rho_{I_s}(s)A_{\alpha}(t)) \\ & + \text{tr}_B (B_{\beta}(s)B_{\alpha}(t)\rho_{I_s}) (\rho_{I_s}(s)A_{\beta}(s)A_{\alpha}(t) - A_{\alpha}(t)\rho_{I_s}(s)A_{\beta}(s))] . \end{aligned} \quad (2.37)$$

Here the equation 2.37 is not a Markovian Master Equation which should be independent of the previous states of the system since it depends on the initial state at $t = 0$; But if it is assumed that the reservoir correlation functions,

$$\text{tr}_B (B_\alpha(t)B_\beta(s)\rho_B) = \langle B_\alpha(t)B_\beta(s) \rangle , \quad (2.38)$$

decay so rapidly that only the contribution around t is significant, then the limit at $t = 0$ can be changed to limit at $t = -\infty$. And if $-s + t$ is substituted for s , equation 2.37 becomes;

$$\begin{aligned} \dot{\rho}_{I_s} = & \frac{1}{\hbar^2} \int_0^\infty ds \sum_{\alpha,\beta} [\text{tr}_B(B_\alpha(t)B_\beta(t-s)\rho_B) (A_\alpha(t)A_\beta(t-s)\rho_{I_s}(t) \\ & - A_\beta(t-s)\rho_{I_s}(t)A_\alpha(t) \\ & + \text{tr}_B(B_\beta(t-s)B_\alpha(t)\rho_B (\rho_{I_s}(t)A_\beta(t-s)A_\alpha(t) - A_\alpha(t)\rho_{I_s}(t)A_\beta(t-s)))] . \end{aligned} \quad (2.39)$$

Now, define

$$A_\alpha(\omega) = \sum_{\epsilon' - \epsilon = \hbar\omega} \pi(\epsilon)A_\alpha\pi(\epsilon') , \quad (2.40)$$

where $\pi(\epsilon)$'s are the projection operators for the states having energy $\hbar\epsilon$. We can consider $\hbar = 1$ and Boltzmann constant $k = 1$ henceforth. It gives the results

$$\begin{aligned} e^{iH_S t} A_\alpha(\omega) e^{-iH_S t} &= e^{-i\omega t} A_\alpha(\omega) \\ e^{iH_S t} A_\alpha^\dagger(\omega) e^{-iH_S t} &= e^{i\omega t} A_\alpha^\dagger(\omega) , \end{aligned} \quad (2.41)$$

$$\begin{aligned} [H_S, A_\alpha(\omega)] &= -\omega A_\alpha(\omega) \\ [H_S, A_\alpha^\dagger(\omega)] &= \omega A_\alpha^\dagger(\omega) \\ A_\alpha^\dagger(\omega) &= A_\alpha(-\omega) , \end{aligned} \quad (2.42)$$

$$\begin{aligned} A_\beta(t-s) &= \sum_\omega e^{i\omega s} e^{-i\omega t} A_\beta(\omega) \\ &= \sum_\omega e^{-i\omega s} e^{i\omega t} A_\beta^\dagger(\omega) , \end{aligned} \quad (2.43)$$

$$\begin{aligned} A_\alpha(t) &= \sum_{\omega'} e^{i\omega' t} A_\alpha^\dagger(\omega') \\ &= \sum_{\omega'} e^{-i\omega' t} A_\alpha(\omega') . \end{aligned} \quad (2.44)$$

Substitute $A(t)$ in equation 2.39 accordingly,

$$\begin{aligned} \dot{\rho}_{I_S}(t) = & \sum_{\omega', \omega} \sum_{\alpha, \beta} e^{i(\omega' - \omega)t} \Gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_{I_S}(t) A_\alpha^\dagger(\omega') - A_\alpha^\dagger(\omega') A_\beta(\omega) \rho_{I_S}(t) \right) \\ & + e^{i(\omega - \omega')t} \Gamma_{\beta\alpha}(-\omega) \left(A_\alpha(\omega') \rho_{I_S}(t) A_\beta^\dagger(\omega) - \rho_{I_S}(t) A_\beta^\dagger(\omega) A_\alpha(\omega') \right), \end{aligned} \quad (2.45)$$

where $\Gamma_{\alpha\beta}$ is

$$\Gamma_{\alpha\beta}(\omega) = \int_0^\infty ds e^{i\omega s} \text{tr}_B (B_\alpha(t) B_\beta(t-s) \rho_B). \quad (2.46)$$

The fact that ρ_B and H_B commutes (since the bath is in a thermal state) and cyclic rearrangements in $\Gamma_{\alpha\beta}$ results in

$$\text{tr}_B \{ e^{iH_B t} B_\alpha e^{-iH_B t} e^{iH_B(t-s)} B_\beta e^{-iH_B(t-s)} \rho_B \} = \text{tr}_B \{ B_\alpha(s) B_\beta(0) \rho_B \}. \quad (2.47)$$

And, therefore,

$$\begin{aligned} \dot{\rho}_{I_S}(t) = & \sum_{\omega, \omega'} \sum_{\alpha\beta} e^{i(\omega - \omega')t} \Gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_{I_S}(t) A_\alpha^\dagger(\omega') - A_\alpha^\dagger(\omega') A_\beta(\omega) \rho_{I_S}(t) \right) \\ & + e^{i(\omega - \omega')t} \Gamma_{\alpha\beta}^*(\omega) \left(A_\alpha(\omega') \rho_{I_S}(t) A_\beta^\dagger(\omega) - \rho_{I_S}(t) A_\beta^\dagger(\omega) A_\alpha(\omega') \right). \end{aligned} \quad (2.48)$$

Interchanging α and β for the second line does not change the equality,

$$\begin{aligned} \dot{\rho}_{I_S}(t) = & \sum_{\omega, \omega'} \sum_{\alpha, \beta} e^{i(\omega - \omega')t} \Gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_{I_S}(t) A_\alpha^\dagger(\omega') - A_\alpha^\dagger(\omega') A_\beta(\omega) \rho_{I_S}(t) \right) \\ & + e^{i(\omega - \omega')t} \Gamma_{\beta\alpha}^*(\omega) \left(A_\beta(\omega') \rho_{I_S}(t) A_\alpha^\dagger(\omega) - \rho_{I_S}(t) A_\alpha^\dagger(\omega) A_\beta(\omega') \right). \end{aligned} \quad (2.49)$$

The time scale for the intrinsic evolution of the system, τ_S is typically $|\omega' - \omega|^{-1}$. If the relaxation time of the open system τ_R is large compared to the τ_S , the terms which have $\omega \neq \omega'$ results in rapidly oscillating terms in the τ_R scale. Therefore they can be neglected, and we are left with the terms in which $\omega = \omega'$. Rearranging terms

$$\begin{aligned} \dot{\rho}_{I_S}(t) = & \sum_{\alpha, \beta, \omega} \left(\Gamma_{\alpha\beta}(\omega) + \Gamma_{\beta\alpha}^*(\omega) \right) \left(A_\beta(\omega) \rho_{I_S}(t) A_\alpha^\dagger(\omega) - \frac{1}{2} \{ A_\alpha^\dagger(\omega) A_\beta(\omega), \rho_{I_S}(t) \} \right) \\ & - \left(\Gamma_{\alpha\beta}(\omega) - \Gamma_{\beta\alpha}^*(\omega) \right) \frac{1}{2} [A_\alpha^\dagger(\omega) A_\beta(\omega), \rho_{I_S}(t)]. \end{aligned} \quad (2.50)$$

Eventually, equation 2.50 can be written as

$$\begin{aligned} \dot{\rho}_{I_S}(t) = & -i [H_{LS}, \rho_{I_S}(t)] \\ & + \sum_{\alpha, \beta, \omega} \gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_{I_S}(t) A_\alpha^\dagger(\omega) - \frac{1}{2} \{ A_\alpha^\dagger(\omega) A_\beta(\omega), \rho_{I_S}(t) \} \right), \end{aligned} \quad (2.51)$$

where

$$H_{LS} = \sum_{\alpha, \beta, \omega} \frac{\hbar}{2i} (\Gamma_{\alpha\beta}(\omega) - \Gamma_{\beta\alpha}(\omega)) A_{\alpha}^{\dagger}(\omega) A_{\beta}(\omega), \quad (2.52)$$

and

$$\gamma_{\alpha\beta}(\omega) = \Gamma_{\alpha\beta}(\omega) + \Gamma_{\beta\alpha}(\omega). \quad (2.53)$$

Now we need to find the Schrödinger picture evolution of the density matrix. Since

$$\rho = e^{-iH_S t} \rho_{I_S} e^{iH_S t}, \quad (2.54)$$

the time evolution of ρ becomes

$$\dot{\rho} = -iH_S \rho + i\rho H_S + e^{-iH_S t} \dot{\rho}_{I_S} e^{iH_S t}. \quad (2.55)$$

And, since

$$[H_S, A_{\alpha}^{\dagger}(\omega) A_{\beta}(\omega)] = 0, \quad (2.56)$$

and

$$e^{-iH_S t} A_{\alpha}^{\dagger}(\omega) \rho_{I_S} A_{\beta}(\omega) e^{iH_S t} = A_{\alpha}^{\dagger}(\omega) \rho A_{\beta}(\omega), \quad (2.57)$$

$$e^{-iH_S t} A_{\alpha}(\omega) \rho_{I_S} A_{\beta}^{\dagger}(\omega) e^{iH_S t} = A_{\alpha}(\omega) \rho A_{\beta}^{\dagger}(\omega), \quad (2.58)$$

we have

$$\begin{aligned} \dot{\rho}_s(t) = & -i [H_{LS} + H_S, \rho_s(t)] \\ & + \sum_{\alpha, \beta, \omega} \gamma_{\alpha\beta}(\omega) \left(A_{\beta}(\omega) \rho_s(t) A_{\alpha}^{\dagger}(\omega) - \frac{1}{2} \{ A_{\alpha}^{\dagger}(\omega) A_{\beta}(\omega), \rho_s(t) \} \right). \end{aligned} \quad (2.59)$$

2.3 Master Equation for a Two-Level Atom in a Radiation Field

Since giving a physical example makes our assumptions clearer and concrete, the coupling of a radiation field in free space, which is at a thermal state, with an electric dipole of a two-level atom will simulate the reservoir and a two-level quantum system coupling in the following sections. The Hamiltonian for radiation field is

$$H_B = \sum_{\vec{k}} \sum_{\lambda=1,2} \omega_k b_{\lambda}^{\dagger}(\vec{k}) b_{\lambda}(\vec{k}). \quad (2.60)$$

It is possible to write the interaction Hamiltonian as

$$H_I = -\vec{D} \cdot \vec{E}, \quad (2.61)$$

where \vec{E} is the electric field operator and \vec{D} is the dipole moment.

From [8],

$$\vec{E} = i \sum_{\vec{k}} \sum_{\lambda=1,2} \sqrt{\frac{2\pi\omega_k}{V}} \vec{e}_\lambda(\vec{k}) \left(b_\lambda(\vec{k}) - b_\lambda^\dagger(\vec{k}) \right), \quad (2.62)$$

where

$$\begin{aligned} \vec{k} \cdot \vec{e}_\lambda(\vec{k}) &= 0 \\ \vec{e}_\lambda(\vec{k}) \cdot \vec{e}_{\lambda'}(\vec{k}) &= \delta_{\lambda\lambda'} \end{aligned} \quad (2.63)$$

Since the expectation value of E is zero for a thermal bath, the approximation in equation 2.36 is validated.

Electric field operator in interaction picture reads as

$$E_\alpha(t) = e^{i \sum_{k,\lambda} \omega_k b_\lambda^\dagger(\vec{k}) b_\lambda(\vec{k}) t} i \sum_{\vec{k},\lambda} \sqrt{\frac{2\pi\omega_k}{V}} e_\lambda^\alpha(\vec{k}) \left(b_\lambda(\vec{k}') - b_\lambda^\dagger(\vec{k}') \right) e^{-i \sum_{k,\lambda} \omega_k b_\lambda^\dagger(\vec{k}) b_\lambda(\vec{k}) t}. \quad (2.64)$$

From the relations of

$$e^{i\omega_k b^\dagger b t} b e^{-i\omega_k b^\dagger b t} = e^{i\omega_k b^\dagger b t} e^{-i\omega_k b b^\dagger t} b = e^{-i\omega_k t} b, \quad (2.65)$$

$$e^{i\omega_k b^\dagger b t} b^\dagger e^{-i\omega_k b^\dagger b t} = b^\dagger e^{i\omega_k b b^\dagger t} e^{-i\omega_k b^\dagger b t} = e^{i\omega_k t} b^\dagger, \quad (2.66)$$

we have equation 2.64 as

$$E^\alpha(t) = i \sum_{\vec{k},\lambda} \sqrt{\frac{2\pi\omega_k}{V}} e_\lambda^\alpha(\vec{k}) \left(e^{-i\omega_k t} b_\lambda(\vec{k}') - e^{i\omega_k t} b_\lambda^\dagger(\vec{k}') \right). \quad (2.67)$$

Then,

$$\begin{aligned} \Gamma_{\alpha\beta} = \sum_{\vec{k},\vec{k}',\lambda,\lambda'} \frac{2\pi}{V} \sqrt{\omega_k \omega_{k'}} e_\lambda^\alpha(\vec{k}) e_{\lambda'}^\beta(\vec{k}') \int_0^\infty ds e^{i\omega_k s} [& - e^{-i\omega_k s} \langle b_\lambda(\vec{k}) b_{\lambda'}(\vec{k}') \rangle \\ & + e^{-i\omega_k s} \langle b_\lambda(\vec{k}) b_{\lambda'}^\dagger(\vec{k}') \rangle \\ & + e^{+i\omega_k s} \langle b_\lambda^\dagger(\vec{k}) b_{\lambda'}(\vec{k}') \rangle \\ & - e^{+i\omega_k s} \langle b_\lambda^\dagger(\vec{k}) b_{\lambda'}^\dagger(\vec{k}') \rangle]. \end{aligned} \quad (2.68)$$

Here we need to find the expectation values. Since we used thermal reservoirs throughout the thesis, the density matrix of the baths are those of thermal state's

$$\rho_B = \frac{1}{Z} e^{-\beta H_B}, \quad (2.69)$$

where Z is the partition function.

$$Z = \text{tr}_B (e^{-\beta H_B}) \quad (2.70)$$

From [9],

$$\rho_B = \prod_{\vec{k}, \lambda} (1 - e^{-\beta \omega_k}) e^{-\beta \omega_k b_\lambda^\dagger(\vec{k}) b_\lambda(\vec{k})} . \quad (2.71)$$

Therefore,

$$\langle b_\lambda(\vec{k}) b_{\lambda'}(\vec{k}') \rangle = \text{tr}_B (b_\lambda(\vec{k}) b_{\lambda'}(\vec{k}') \rho_0) = 0 \quad (2.72)$$

and

$$\begin{aligned} \langle b_\lambda^\dagger(\vec{k}) b_{\lambda'}(\vec{k}') \rangle &= \delta_{\lambda\lambda'} \delta_{\vec{k}\vec{k}'} (1 - e^{-\beta \omega_k}) \sum_{n=0}^{\infty} n e^{-\beta \omega_k n} \\ &= \delta_{\lambda\lambda'} \delta_{\vec{k}\vec{k}'} N(\omega_k) , \end{aligned} \quad (2.73)$$

where

$$N(\omega_k) = \frac{e^{-\beta \omega_k}}{1 - e^{-\beta \omega_k}} . \quad (2.74)$$

Then,

$$\langle b_\lambda(\vec{k}) b_{\lambda'}(\vec{k}') \rangle = \delta_{\lambda\lambda'} \delta_{\vec{k}\vec{k}'} (1 + N(\omega_k)) , \quad (2.75)$$

and

$$\Gamma_{\alpha\beta}(\omega) = \sum_{\vec{k}, \lambda} \frac{2\pi}{V} \omega_k e_\lambda^\alpha(\vec{k}) e_\lambda^\beta(\vec{k}) \int_0^\infty ds [e^{i(\omega+\omega_k)s} N(\omega_k) + e^{i(\omega-\omega_k)s} (N(\omega_k) + 1)] . \quad (2.76)$$

It is possible to approximate the summation over \vec{k} as an integral

$$\sum_{\vec{k}} = \int d^3n = \int \frac{V}{(2\pi)^3} d^3k , \quad (2.77)$$

and

$$\int d^3k = \frac{1}{c^3} \int_0^\infty \omega_k^2 d\omega_k \int d\Omega . \quad (2.78)$$

The integrand for the solid angle integration is the vectors under λ summation

$$\sum_{\lambda} e_\lambda^\alpha(\vec{k}) e_\lambda^\beta(\vec{k}) = \delta_{\alpha\beta} - \frac{k_\alpha k_\beta}{k^2} , \quad (2.79)$$

Therefore, it reads as

$$\int d\Omega (\delta_{\alpha\beta} - \cos^2 \theta) = \frac{8\pi}{3} \delta_{\alpha\beta} . \quad (2.80)$$

Eventually,

$$\Gamma_{\alpha\beta}(\omega) = \frac{2\delta_{\alpha\beta}}{3\pi c^3} \int_0^\infty d\omega_k \omega_k^3 \left[N(\omega_k) \int_0^\infty e^{i(\omega+\omega_k)s} ds \right. \\ \left. + (N(\omega) + 1) \int_0^\infty e^{-i(\omega_k-\omega)s} ds \right], \quad (2.81)$$

and

$$\gamma_{\alpha\beta}(\omega) = \frac{2\delta_{\alpha\beta}}{3\pi c^3} \int_0^\infty d\omega_k \omega_k^3 \left[N(\omega_k) \int_{-\infty}^\infty e^{i(\omega+\omega_k)s} ds \right. \\ \left. + (N(\omega_k) + 1) \int_{-\infty}^\infty e^{i(\omega-\omega_k)s} ds \right]. \quad (2.82)$$

The integrals are Dirac delta functions. Therefore,

$$\text{For } \omega > 0 \quad \gamma_{\alpha\beta} = \delta_{\alpha\beta} \frac{4\omega^3}{3c^3} (N(\omega) + 1) \\ \text{For } \omega < 0 \quad \gamma_{\alpha\beta} = \delta_{\alpha\beta} \frac{4\omega^3}{3c^3} N(\omega) \\ = \delta_{\alpha\beta} \frac{4|\omega|^3}{3c^3} (N(|\omega|) + 1). \quad (2.83)$$

And the master equation reads as

$$\dot{\rho}_s(t) = -\frac{i}{\hbar} [H_{LS}, \rho_s(t)] + D(\rho_s(t)), \quad (2.84)$$

where $D(\rho_s(t))$ is called the dissipator,

$$D(\rho_s(t)) = \sum_{\omega>0} \frac{4\omega^3}{3c^3} (1 + N(\omega)) \left[D_\alpha(\omega) \rho_s(t) D_\alpha^\dagger(\omega) - \frac{1}{2} \{ D_\alpha^\dagger(\omega) D_\alpha(\omega), \rho_s(t) \} \right] \\ + \sum_{\omega>0} \frac{4\omega^3}{3c^3} N(\omega) \left[D_\alpha^\dagger(\omega) \rho_s(t) D_\alpha(\omega) - \frac{1}{2} \{ D_\alpha(\omega) D_\alpha^\dagger(\omega), \rho_s(t) \} \right]. \quad (2.85)$$

2.4 Master equation for the harmonic oscillator

Here the Hamiltonians read as

$$H_I = \sum_n g_n (a + a^\dagger) (b_n + b_n^\dagger) \\ H_S = \omega a^\dagger a \\ H_B = \sum_n \Omega_n b_n^\dagger b_n, \quad (2.86)$$

where n is the number of oscillators in the bath. The equation 2.40 becomes

$$A(\omega) = \sum_{\varepsilon' - \varepsilon = \hbar\omega} \pi(\varepsilon)(a + a^\dagger)\pi(\varepsilon') . \quad (2.87)$$

When the ω is larger than zero, the creation operator gives zero therefore

$$A(\omega) = \sum_{\varepsilon' - \varepsilon = \hbar\omega} \pi(\varepsilon)a\pi(\varepsilon') = a . \quad (2.88)$$

When the ω is less than zero, the annihilation operator gives zero and

$$A(\omega) = \sum_{\varepsilon' - \varepsilon = \omega} \pi(\varepsilon)a^\dagger\pi(\varepsilon') = a^\dagger . \quad (2.89)$$

Then, following the previous calculation's footsteps, we obtain

$$\begin{aligned} \dot{\rho}_s = & \gamma(N_1 + 1) \left[a_s \rho_s a^\dagger - \frac{1}{2} a^\dagger a \rho_s - \frac{1}{2} \rho_s a^\dagger a \right] \\ & \gamma(N_1) \left[a^\dagger \rho_s a - \frac{1}{2} a a^\dagger \rho_s - \frac{1}{2} \rho_s a a^\dagger \right] , \end{aligned} \quad (2.90)$$

where

$$\gamma = \sum_n g_n^2 \int_{-\infty}^{\infty} e^{i(\omega - \Omega_n)s} ds . \quad (2.91)$$

2.5 Heat transfer expression

Now we find the heat transfer expression. We formulate the energy transfer rate as the rate of change of the expectation value of the system Hamiltonian due to the interaction with the bath,

$$q = \frac{d}{dt} \langle H_s \rangle = \text{tr}(\dot{\rho}_s H_s) . \quad (2.92)$$

After this point, we will not include $[H_{LS} + H_S, \rho_s(t)]$ in our calculations since the dynamics it generated do not contribute to the energy transfer because

$$[H_S, H_{LS}] = 0 , \quad (2.93)$$

and

$$\text{tr}([H_{LS} + H_S, \rho_s] H_s) = \text{tr}([H_S, H_S + H_{LS}] \rho_s) = 0 . \quad (2.94)$$

CHAPTER 3

TWO-LEVEL SYSTEM

Now we will investigate the heat transfer rate for a two-level quantum system as the coupler between the reservoirs. Here we first derive the Lindblad master equation for the system and two reservoirs coupling. Then we will find the steady-state case, and from the steady-state density matrix and the master equation, we will find the heat transfer rate and the thermal rectification characteristics.

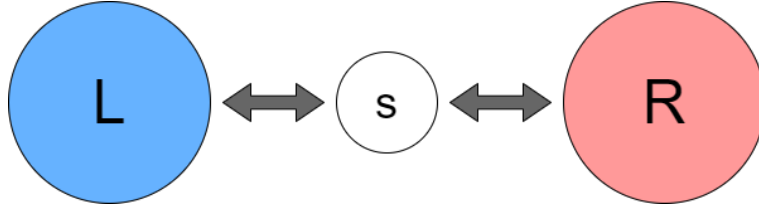


Figure 3.1: Contact between the reservoirs. L corresponds to the left reservoir, R corresponds to the right reservoir, and S is the two-level system.

3.1 Master equation

The coupling is

$$H_I = \sum_{\alpha, \lambda} \vec{D}_\alpha \cdot g_\lambda \vec{E}_{\alpha, \lambda}. \quad (3.1)$$

α 's are the indices for three dimensions, λ 's are the indices for the reservoirs, and there are only two possible ω values that correspond to the raising and lowering energies of the two-level system. For ω 's positive value,

$$D(\omega) = |g\rangle\langle g|D_\alpha|e\rangle\langle e| = \langle g|D_\alpha|e\rangle\sigma_-, \quad (3.2)$$

where $|g\rangle$ is the ground state and $|e\rangle$ is the excited state for the two-level atom. Substituting equation 3.1 in equation 2.85,

$$\begin{aligned} \dot{\rho}_s(t) = & \frac{4\omega_0^3}{3c^3} (g_1^2(1 + N_1) + g_2^2(1 + N_2)) \sum_{\alpha} |\langle g | D_{\alpha} | e \rangle|^2 [\sigma_- \rho_s(t) \sigma_+ \\ & - \frac{1}{2} \sigma_+ \sigma_- \rho_s(t) - \frac{1}{2} \rho_s(t) \sigma_+ \sigma_-] \\ & + \frac{4\omega_0^3}{3c^3} (g_1^2 N_1 + g_2^2 N_2) \sum_{\alpha} |\langle g | D_{\alpha} | e \rangle|^2 [\sigma_+ \rho_s(t) \sigma_- \\ & - \frac{1}{2} \sigma_- \sigma_+ \rho_s(t) - \frac{1}{2} \rho_s(t) \sigma_- \sigma_+] . \end{aligned} \quad (3.3)$$

We will not be interested in the off-diagonal terms of ρ_s in the energy basis since they will not contribute to the energy calculation of the system, therefore the energy transfer rate. This reduces the unknowns to two from four. The corresponding equations for the steady-state case are the following

$$\begin{aligned} (g_1^2(1 + N_1) + g_2^2(1 + N_2)) \rho_{11} - (g_1^2 N_1 + g_2^2 N_2) \rho_{00} &= 0 \\ (g_1^2 N_1 + g_2^2 N_2) \rho_{00} - (g_1^2(1 + N_1) + g_2^2(1 + N_2)) \rho_{11} &= 0 , \end{aligned} \quad (3.4)$$

where ρ_0 and ρ_1 are the diagonal elements of the density matrix corresponding to the ground and excited-state probabilities. These are two dependent equations in two variables. We will first find the steady-state solution to find the heat transfer rate. To solve the equations, we will need an extra constraint of normalization,

$$\rho_{00} + \rho_{11} = 1 . \quad (3.5)$$

The results are the following

$$\rho_{00} = \frac{g_1^2(1 + N_1) + g_2^2(1 + N_2)}{g_1^2(1 + 2N_1) + g_2^2(1 + 2N_2)} , \quad (3.6)$$

$$\rho_{11} = \frac{g_1^2 N_1 + g_2^2 N_2}{g_1^2(1 + 2N_1) + g_2^2(1 + 2N_2)} . \quad (3.7)$$

Here one might check the temperature of the two-level system from the probabilities in equations 3.6 and 3.7,

$$T = -\omega \ln \frac{g_1^2 N_1 + g_2^2 N_2}{g_1^2(1 + N_1) + g_2^2(1 + N_2)} . \quad (3.8)$$

Here, if we denote

$$T_2 = T_1 + \Delta T , \quad (3.9)$$

then, if we consider T in equation 3.8 as $T(T_1, T_2)$ and we expand $T(T_1, T_2)$ for T_2 around T_1 expands as

$$T = T_1 + \frac{g_2^2}{g_1^2 + g_2^2} \Delta T + \dots , \quad (3.10)$$

in which the first two terms are the expected classical results. Steady-state solution is the result of canceling effects of the two reservoirs on the system. Now we will investigate the heat transfer rate. It can be found by considering a single reservoir's effect on the system. The reservoir causes a change in the energy level density changes the expectation value of the system's energy. Since it will be in the steady-state case, the other reservoir will have the opposite effect on the densities. Therefore, there will be a net flow rate of energy from one reservoir to another. The heat flow rate from the first reservoir becomes

$$q = \text{tr} (D_1 (\rho_{s,steady}) H_s) , \quad (3.11)$$

where ρ_{steady} is the density matrix at steady-state $D_1(\rho_{steady})$ is the dissipator in the master equation resulting from the contact with the first reservoir. Then the heat transfer rate becomes

$$q = \omega \left(\frac{d}{dt} \rho_{11,steady} \right)_{1^{st}bath} , \quad (3.12)$$

where $1^{st}bath$ near the parenthesis indicates the rate of change due to the first reservoir only The master equation involving a single reservoir results in

$$\begin{aligned} \dot{\rho}_{00} &= \gamma g_1^2 (1 + N_1) \rho_{11} - \gamma g_1^2 N_1 \rho_{00} \\ \dot{\rho}_{11} &= \gamma g_1^2 N_1 \rho_{00} - \gamma g_1^2 (1 + N_1) \rho_{11} , \end{aligned} \quad (3.13)$$

where γ is a constant

$$\gamma = \frac{4\omega_0^3}{3c^3} \sum_{\alpha} | \langle g | D_{\alpha} | e \rangle |^2 \quad (3.14)$$

Here, we assumed the ground state has zero energy, substitute the steady-state solution, and find its effect on the energy change rate of the system,

$$q = \omega \gamma g_1^2 g_2^2 \frac{(N_1 - N_2)}{g_1^2 (1 + 2N_1) + g_2^2 (1 + 2N_2)} . \quad (3.15)$$

One can check the heat flow for the second reservoir as well,

$$\begin{aligned} \dot{\rho}_{00} &= \gamma g_2^2 (1 + N_2) \rho_{11} - \gamma g_2^2 N_2 \rho_{00} \\ \dot{\rho}_{11} &= \gamma g_2^2 N_2 \rho_{00} - \gamma g_2^2 (1 + N_2) \rho_{11} . \end{aligned} \quad (3.16)$$

And the heat transfer rate becomes

$$q = \omega\gamma g_1^2 g_2^2 \frac{(N_2 - N_1)}{g_1^2(1 + 2N_1) + g_2^2(1 + 2N_2)} . \quad (3.17)$$

It is the heat flow of the first reservoir with an additional minus sign which should be the case since the heat flows from one reservoir to the other reservoir. Here, the effects of reservoirs on the system cancel each other and result in a net heat transfer rate between the reservoirs with a steady-state system

3.2 Rectification behavior

To analyze the rectification behaviour, we need to express it mathematically. There are more than one ways to express it. We will use

$$R = \frac{Q(T_1, T_2) + Q(T_2, T_1)}{Q(T_1, T_2) - Q(T_2, T_1)} , \quad (3.18)$$

where $Q(T_1, T_2)$ corresponds to the heat flow from the first reservoir when the first reservoir is at temperature T_1 and the second reservoir is at T_2 . Here R takes values between $+1$ and -1 . The limiting values correspond to maximum rectification. The value 0 will be the no rectification case when the heat flow rate changes sign when the temperatures are exchanged. Note that the amount of rectification is actually characterized by the absolute value of R . It can have its negative value if one considers the other reservoir as the first reservoir.

When the system is a two-level quantum system, and when the coupling constants are equal there is left-right exchange symmetry in the system. If the temperatures of the reservoirs are exchanged, overall coupling does not change. Therefore the rectification will be zero. However, if the coupling constants are different, it results in a non-zero rectification.

In figure 3.2 it can be seen from the heat flow rates that there is a rectification behavior with the two-level system as a coupling between two reservoirs.

Now we will investigate the rectification behavior to find how to obtain the optimal conditions which maximize the thermal rectification. There are five degrees of freedom in the system, which are the temperatures of the reservoirs, the coupling

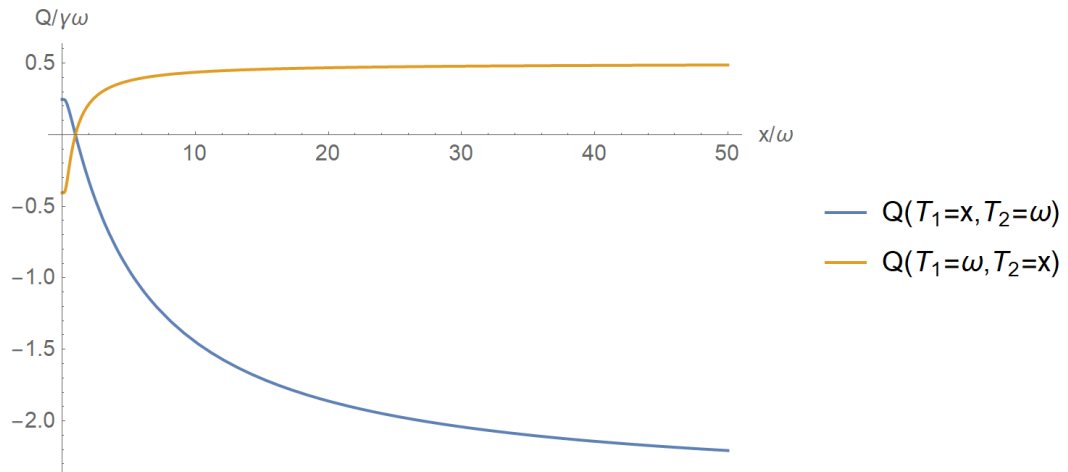


Figure 3.2: Heat transfer rates in the case $g_1 = 5$, $g_2 = 1$.

constants, and the energy difference between the two levels. We first investigate the lower temperature's effect on the rectification with a constant temperature for the hot reservoir.

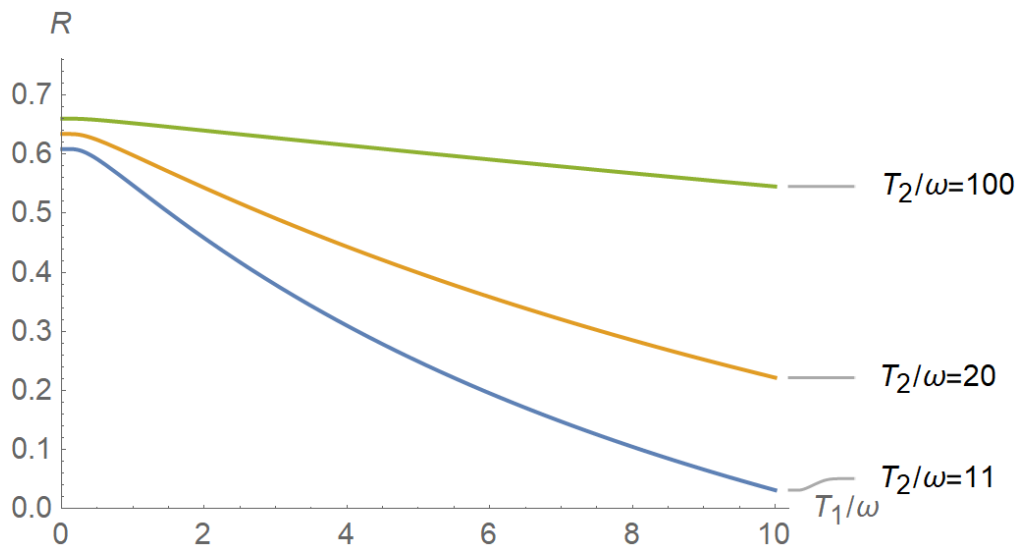


Figure 3.3: Rectification in the case $g_1 = 5$, $g_2 = 1$.

The rectification is reduced with the increasing temperature of the colder reservoir and increased with the increasing temperature of the hot reservoir, as can be seen in figure 3.3. Therefore having the colder bath as cold as possible and having the reservoir as hot as possible will increase the thermal rectification.

Now we investigate the coupling constant's effect on the rectification. However, we just investigate the effect of their ratio but not their individual values since their strength changes the heat transfer rate equally on both directions. Here, as the ratio increases, the rectification increases too as expected since it increases the asymmetric character of the coupling. To maximize the rectification, one should have the most asymmetric condition possible in the coupling constants.

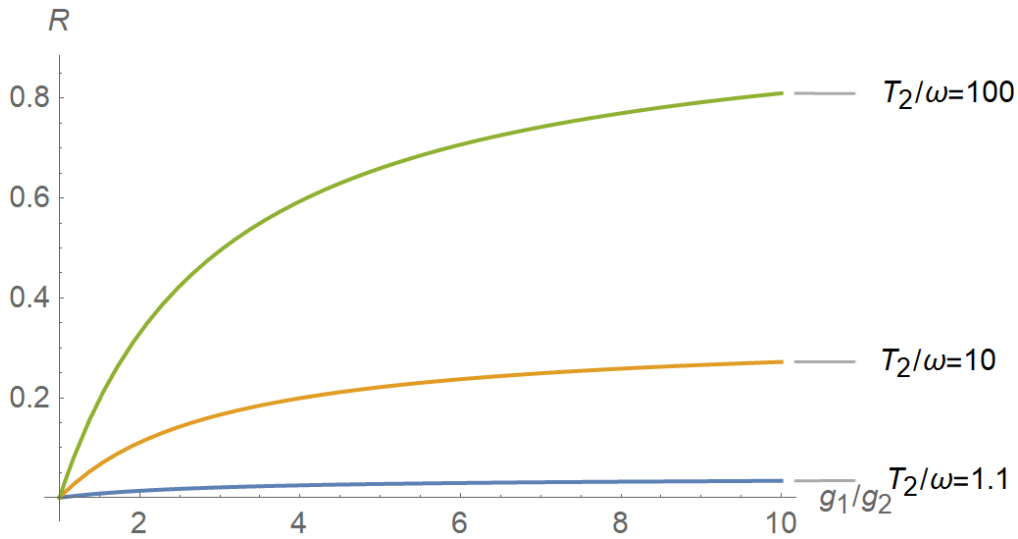


Figure 3.4: Rectification in the case $T_1/\omega = 1$

The last variable is the excitation energy of the two-level system. The effect can be seen in figure 3.5. As the energy increases, the rectification is reduced.

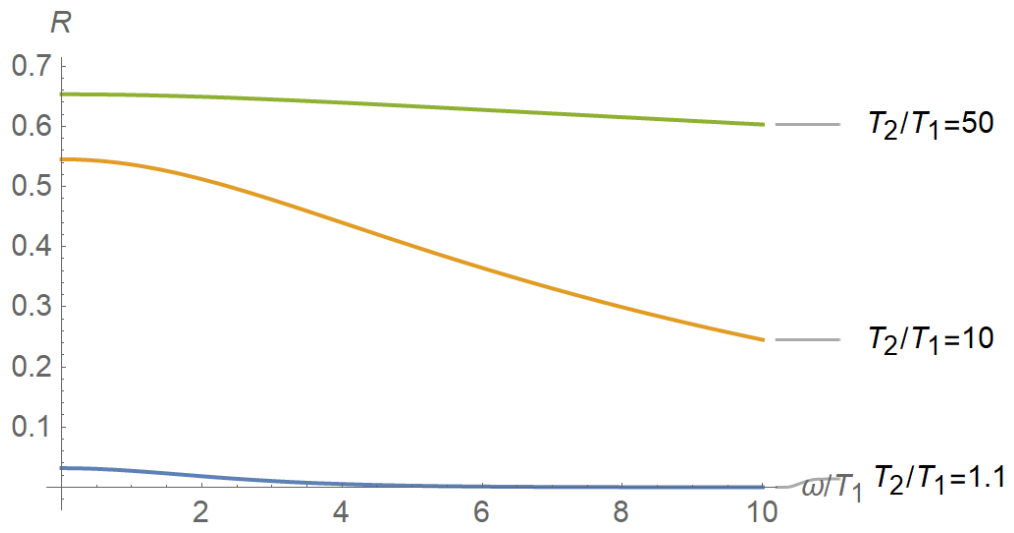


Figure 3.5: Rectification in the case $g_1 = 5, g_2 = 1$

CHAPTER 4

TWO TWO-LEVEL SYSTEMS

Now we investigate a system consisting of a two two-level system as a contact between reservoirs. The left reservoir is in contact with the left two-level system, and the right reservoir is in contact with the right two-level system only while the two-level systems interact.

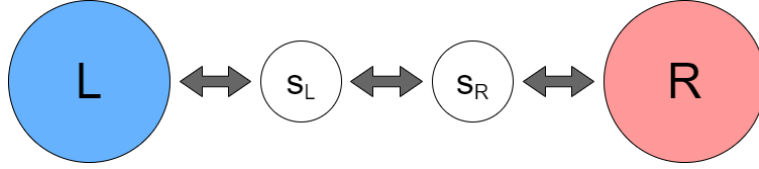


Figure 4.1: Contact between the reservoirs. L corresponds to the left reservoir, R corresponds to the right reservoir, S_L is the left two-level system, and S_R is the right two-level system.

4.1 Ising Coupling

4.1.1 Theory

The Hamiltonian of the whole system is

$$H = H_S + H_L + H_R + \sum_i g_{L,i}(a_{L,i}^\dagger + a_{L,i})\sigma_x^L + \sum_j g_{R,j}(a_{R,j}^\dagger + a_{R,j})\sigma_x^R, \quad (4.1)$$

where

$$H_S = \frac{\omega_L}{2}\sigma_z^L + \frac{\omega_R}{2}\sigma_z^R + \frac{\omega_{LR}}{2}\sigma_z^L\sigma_z^R, \quad (4.2)$$

and L, R denotes the left and right reservoirs. The coupling between the two-level atoms is called the Ising coupling. Here, we assumed the coupling constants are

equal for both reservoirs since the rectification we will investigate is not due to the asymmetric coupling constants. Then

$$\begin{aligned}
\dot{\rho}_s(t) = & \gamma(\omega)(1 + N_L(\omega))[\sigma_+^L \rho_s(t) \sigma_+^L - \frac{1}{2} \sigma_+^L \sigma_-^L \rho_s(t) - \frac{1}{2} \rho_s(t) \sigma_+^L \sigma_-^L] \\
& + \gamma(\omega) N_L(\omega)[\sigma_+^L \rho_s(t) \sigma_-^L - \frac{1}{2} \sigma_-^L \sigma_+^L \rho_s(t) - \frac{1}{2} \rho_s(t) \sigma_-^L \sigma_+^L] \\
& + \gamma(\omega)(1 + N_R(\omega))[\sigma_-^R \rho_s(t) \sigma_+^R - \frac{1}{2} \sigma_+^R \sigma_-^R \rho_s(t) - \frac{1}{2} \rho_s(t) \sigma_+^R \sigma_-^R] \\
& + \gamma(\omega) N_R(\omega)[\sigma_-^R \rho_s(t) \sigma_-^R - \frac{1}{2} \sigma_-^R \sigma_+^R \rho_s(t) - \frac{1}{2} \rho_s(t) \sigma_-^R \sigma_+^R] .
\end{aligned} \tag{4.3}$$

Note that γ is a function of ω here since there is more than one transition energy. Let us denote the eigenkets of the system as

$$|\uparrow\uparrow\rangle \rightarrow |\psi_1\rangle , \tag{4.4}$$

$$|\uparrow\downarrow\rangle \rightarrow |\psi_2\rangle , \tag{4.5}$$

$$|\downarrow\uparrow\rangle \rightarrow |\psi_3\rangle , \tag{4.6}$$

$$|\downarrow\downarrow\rangle \rightarrow |\psi_4\rangle . \tag{4.7}$$

Now we consider our bath is an Ohmic bath[1] in which

$$\gamma(\omega) = \gamma_0 \omega . \tag{4.8}$$

Then, the Lindbladian results in the following equations for the diagonal elements of the density matrix in energy basis at the steady state;

$$\begin{aligned}
[-(E_1 - E_2)(N_{12} + 1) - (E_1 - E_3)(N_{13} + 1)] \rho_{11} + (E_1 - E_2) N_{12} \rho_{22} \\
+ (E_1 - E_3) N_{13} \rho_{33} = 0
\end{aligned} \tag{4.9}$$

$$\begin{aligned}
(E_1 - E_2)(N_{12} + 1) \rho_{11} + [-(E_1 - E_2) N_{12} - (E_2 - E_4)(N_{24} + 1)] \rho_{22} \\
+ (E_2 - E_4) N_{24} \rho_{44} = 0
\end{aligned} \tag{4.10}$$

$$\begin{aligned}
(E_1 - E_3)(N_{13} + 1) \rho_{11} + [-(E_4 - E_3) N_{43} - (E_1 - E_3) N_{13} \rho_{33} \\
+ (E_4 - E_3)(N_{43} + 1) \rho_{44} = 0
\end{aligned} \tag{4.11}$$

$$(E_2 - E_4) (N_{24} + 1) \rho_{22} + (E_4 - E_3) N_{43} \rho_{33} + [- (E_4 - E_3) (N_{43} + 1) - (E_2 - E_4) N_{24}] \rho_{44} = 0 , \quad (4.12)$$

where

$$N_{ij} = \frac{1}{e^{\beta\alpha(E_i - E_j)} - 1} , \quad (4.13)$$

and alpha denotes the corresponding reservoir which induces the level changes in the system. The equations combined with the normalization of the density matrix has a unique solution whose exact expression can be found in [2].

The heat flow of the right reservoir is

$$q = \gamma_0 (E_1 - E_2) [(N_{12} + 1) \rho_{11} - N_{12} \rho_{22}] (E_1 - E_2 + E_4 - E_3) . \quad (4.14)$$

4.1.2 Behaviour

The probabilities' flow among the energy eigenstates forms a loop and each flow between two eigenstates is done by a specific reservoir. This loop can be arranged like in figure 4.1 so that it involves an excitation done by the cold reservoir, which acts as an impediment in the flow. However, when the baths are interchanged, there will be no excitation done by the cold reservoir but a deexcitation by the hot reservoir, which always has a finite rate at any temperature. If you arrange the energies like in figure 4.2 and require an excitement by the cold reservoir in the loop, this will cause a significant rectification effect since the opposite loop does not require such a thing.

If you arrange the levels so that the cold reservoir's excitation becomes a decay and all transition have the same energy as in figure 4.4, then the system acts as a two-level system, and the rectification becomes zero with equal coupling strengths as expected. The behavior of rectification in figure 4.5 indicates the rectification is done by the cold reservoir's excitation, like in figure 4.2.

4.2 Heisenberg Coupling

Now we will consider the coupler consists of two-level atoms coupled by the Heisenberg coupling.

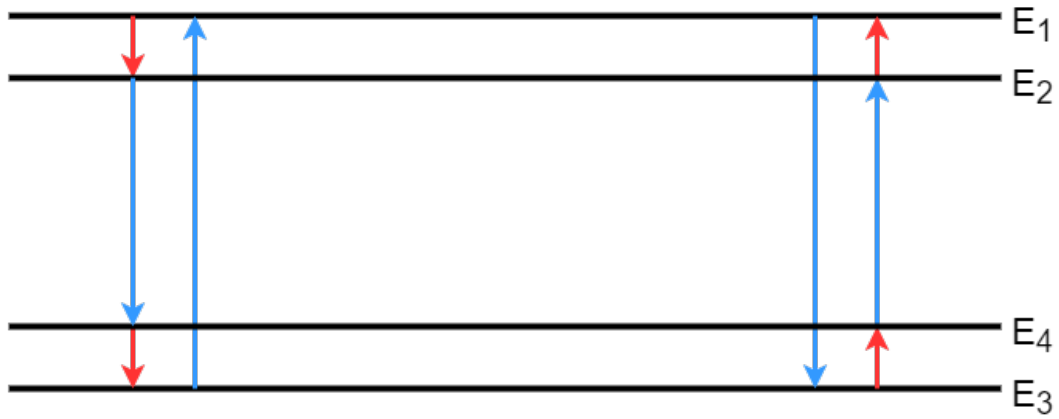


Figure 4.2: Transitions among the energy levels. The sequence represents the energy levels. The blue arrows correspond to the excitations or deexcitations done by the left reservoir, and the red arrows are the ones done by the right reservoir. The arrows on the left represent the heat flow from the left bath to the right bath, while the arrows on the right are the flow from the right bath to the left bath.

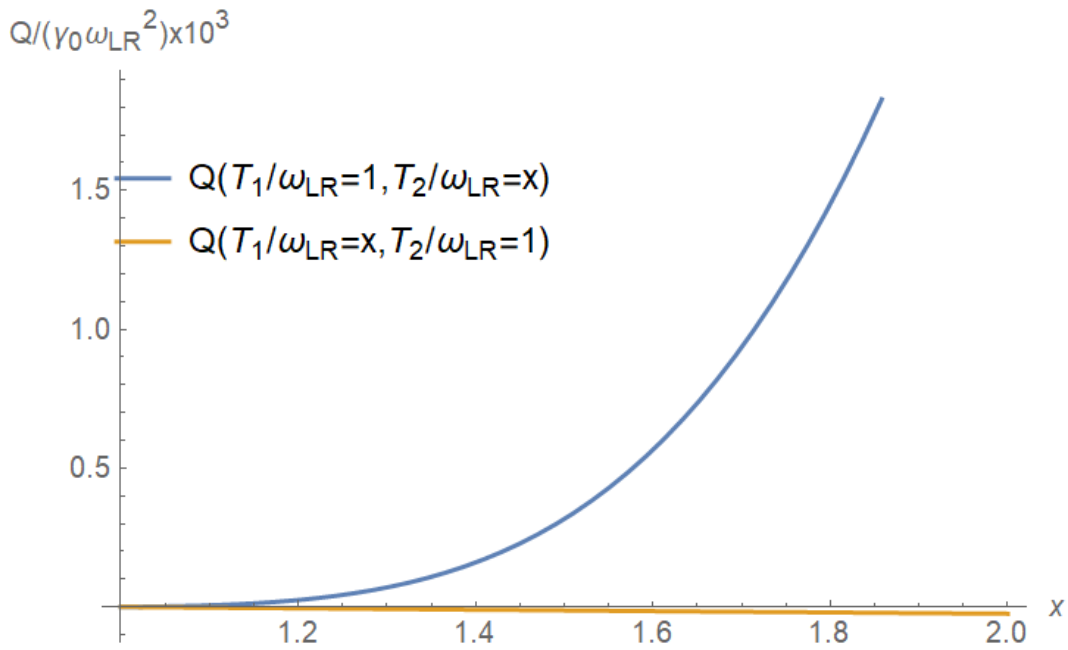


Figure 4.3: Heat transfer rate in the case $\omega_L = 11\omega_{LR}, \omega_R = 0$

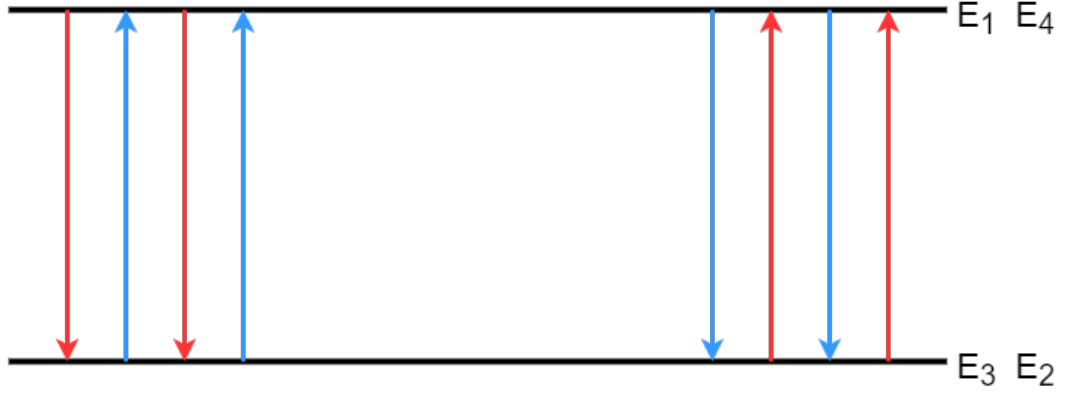


Figure 4.4: Transitions among the energy levels. The sequence represents the energy levels. The blue arrows correspond to the excitations or decays done by the left reservoir, and the red arrows are the ones done by the right reservoir. The arrows on the left represent the heat flow from the left bath to the right bath, while the arrows on the right are the flow from the right bath to the left bath.

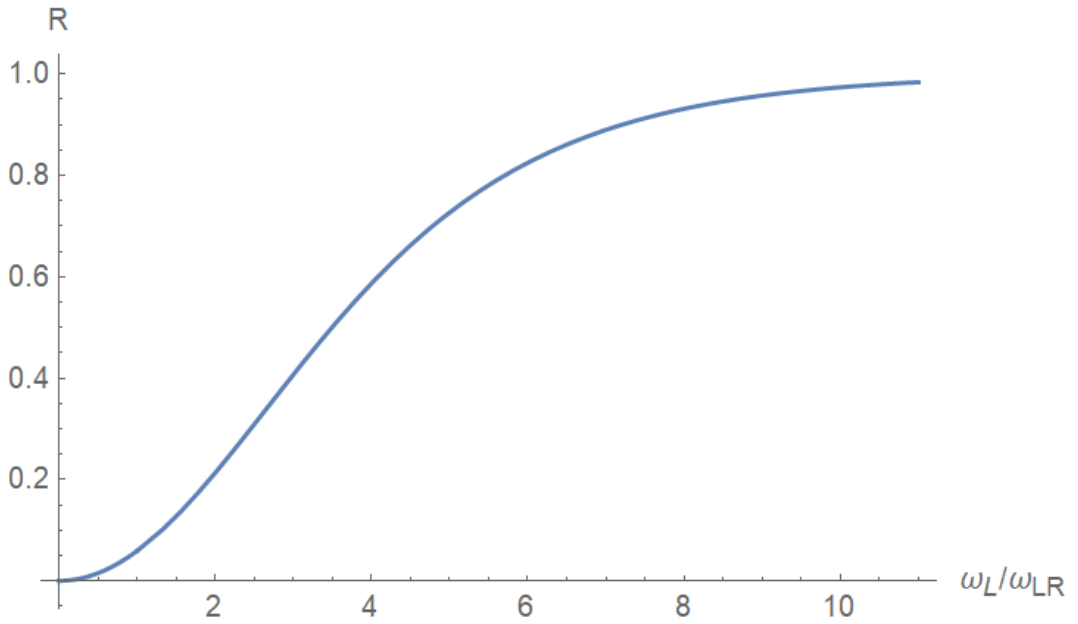


Figure 4.5: Rectification in the case $\omega_R = 0$, $T_L = \omega_{LR}$ and $T_R = 2\omega_{LR}$. $\omega_L = 0$ corresponds to the figure 4.4

4.2.1 Theory

Hamiltonian for the whole system is

$$H = H_S + H_L + H_R + \sum_i (a_{L,i}^\dagger + a_{L,i}) \sigma_x^L + \sum_j (a_{R,j}^\dagger + a_{R,j}) \sigma_x^R, \quad (4.15)$$

where

$$H_S = \frac{\omega_L}{2}\sigma_z^L + \frac{\omega_R}{2}\sigma_z^R + \frac{\omega_{LR}}{2}\sigma_x^L\sigma_x^R + \frac{\omega_{LR}}{2}\sigma_y^L\sigma_y^R + \frac{\omega_{LR}}{2}\sigma_z^L\sigma_z^R, \quad (4.16)$$

where ω_L , ω_R , and ω_{LR} are real. First we obtain the energy eigenstates of the system.

If we express the coupling operators in the energy basis, we get

$$\sigma_x^L = \begin{pmatrix} 0 & 0 & -\frac{\frac{a+b}{c}}{\sqrt{1+(\frac{a+b}{c})^2}} & -\frac{\frac{a-b}{c}}{\sqrt{1+(\frac{a-b}{c})^2}} \\ 0 & 0 & \frac{1}{\sqrt{1+(\frac{a+b}{c})^2}} & \frac{1}{\sqrt{1+(\frac{a-b}{c})^2}} \\ -\frac{\frac{a+b}{c}}{\sqrt{1+(\frac{a+b}{c})^2}} & \frac{1}{\sqrt{1+(\frac{a+b}{c})^2}} & 0 & 0 \\ -\frac{\frac{a-b}{c}}{\sqrt{1+(\frac{a-b}{c})^2}} & \frac{1}{\sqrt{1+(\frac{a+b}{c})^2}} & 0 & 0 \end{pmatrix}, \quad (4.17)$$

and

$$\sigma_x^R = \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{1+(\frac{a+b}{c})^2}} & \frac{1}{\sqrt{1+(\frac{a-b}{c})^2}} \\ 0 & 0 & -\frac{\frac{a+b}{c}}{\sqrt{1+(\frac{a+b}{c})^2}} & -\frac{\frac{a-b}{c}}{\sqrt{1+(\frac{a-b}{c})^2}} \\ \frac{1}{\sqrt{1+(\frac{a+b}{c})^2}} & -\frac{\frac{a+b}{c}}{\sqrt{1+(\frac{a+b}{c})^2}} & 0 & 0 \\ \frac{1}{\sqrt{1+(\frac{a+b}{c})^2}} & -\frac{\frac{a-b}{c}}{\sqrt{1+(\frac{a-b}{c})^2}} & 0 & 0 \end{pmatrix}, \quad (4.18)$$

where

$$a = \omega_R - \omega_L, \quad (4.19)$$

$$c = 2\omega_{LR}, \quad (4.20)$$

$$b = \sqrt{a^2 + c^2}. \quad (4.21)$$

4.2.2 Behavior

The matrices mean that both left and right reservoirs are responsible for the transitions $1 \leftrightarrow 3$, $3 \leftrightarrow 2$, $2 \leftrightarrow 4$, and $4 \leftrightarrow 1$. The transitions in the loop can be done by both reservoirs. This prevents an impediment like in the Ising coupling case in the energy flow since there is no excitation done by the cold reservoir only. Therefore the rectification is greatly reduced for similar parameters to figure 4.3 as can be seen in figure 4.6.

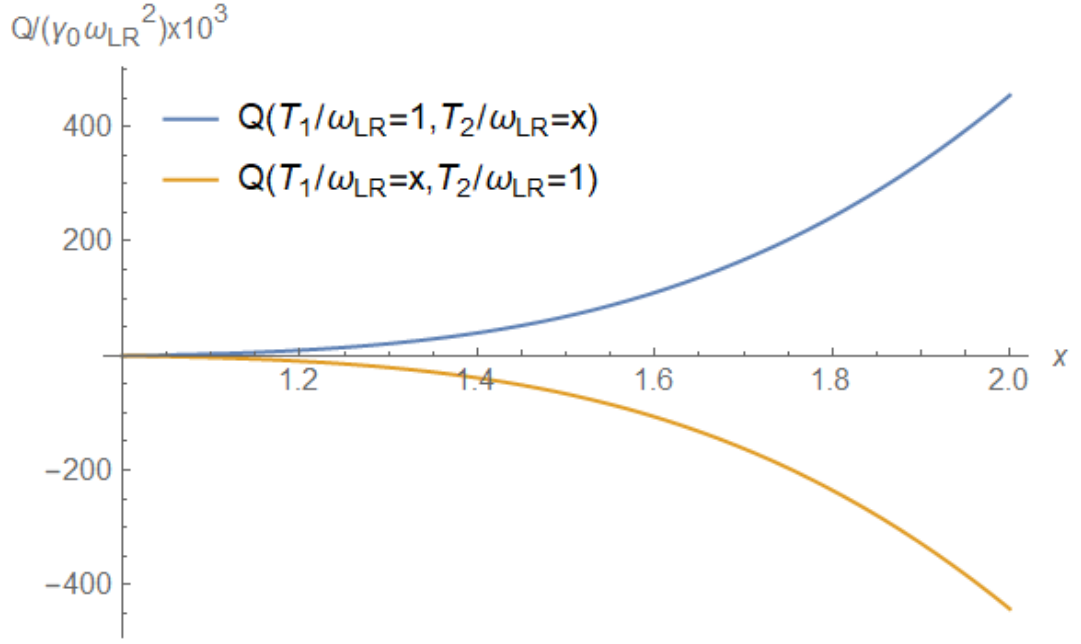


Figure 4.6: Heat transfer rates in the case $\omega_L = 11\omega_{LR}$, $\omega_R = 0$

We can express our system Hamiltonian as

$$H_S = \frac{\omega_L}{2}\sigma_z^L + \frac{\omega_R}{2}\sigma_z^R + \frac{\omega_{XY}}{2}\sigma_x^L\sigma_x^R + \frac{\omega_{XY}}{2}\sigma_y^L\sigma_y^R + \frac{\omega_{LR}}{2}\sigma_z^L\sigma_z^R, \quad (4.22)$$

which is called the XXZ model. The case $\omega_{XY} = 0$ is the Ising coupling, and $\omega_{XY} = \omega_{LR}$ is the Heisenberg coupling. Then we can plot the rectification as a function of ω_{XY} in figure 4.7. It can be seen how the rectification is reduced with increasing ω_{XY} term.

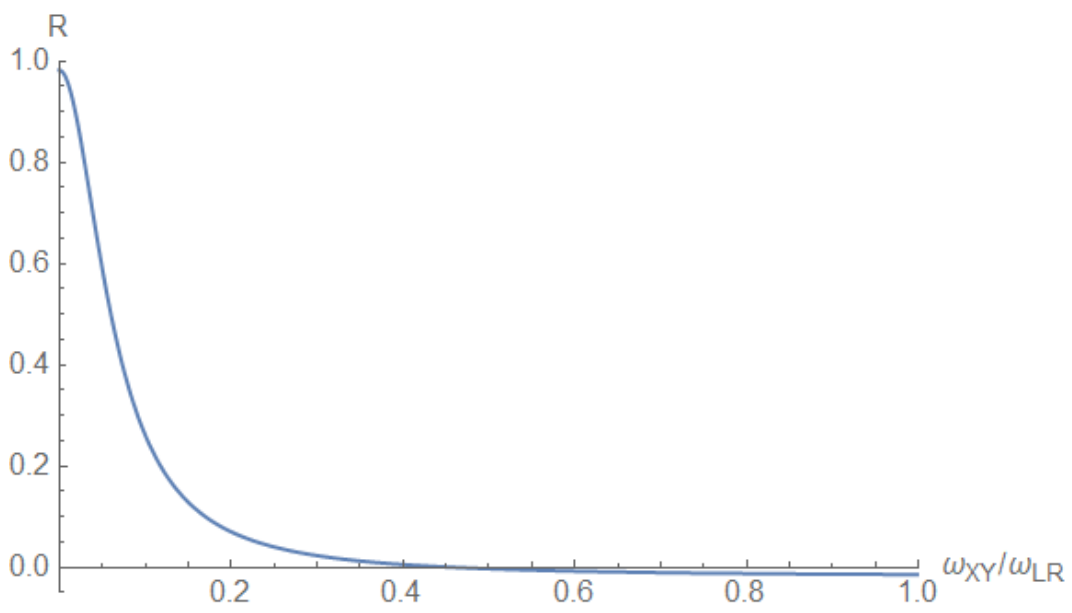


Figure 4.7: Rectification in the case $\omega_L = 11\omega_{LR}$, $\omega_R = 0$, $T_L = \omega_{LR}$ and $T_R = 2\omega_{LR}$

CHAPTER 5

HARMONIC OSCILLATOR

Now we will investigate the thermal rectification behavior of a harmonic oscillator as the coupler between the reservoirs.

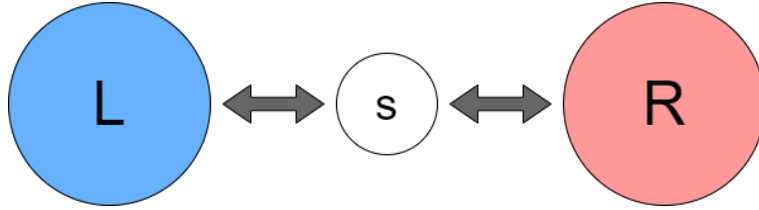


Figure 5.1: Contact between the reservoirs. L corresponds to the left reservoir, R corresponds to the right reservoir, and S is the harmonic oscillator.

5.1 Master equation

Hamiltonian of the whole system is

$$\begin{aligned} H = & \omega a^\dagger a + \sum_x \Omega_1 b_x^\dagger b_x + \sum_y \Omega_2 b_y^\dagger b_y \\ & + \sum_x g_x (a^\dagger + a) (b_x^\dagger + b_x) + \sum_y g_y (a^\dagger + a) (b_y^\dagger + b_y) \end{aligned} \quad (5.1)$$

With two reservoirs, equation 2.90 becomes

$$\begin{aligned}
\dot{\rho}_s = & \gamma_1 (N_1 + 1) \left[a \rho_s a^\dagger - \frac{1}{2} a^\dagger a \rho_s - \frac{1}{2} \rho_s a^\dagger a \right] \\
& + \gamma_1 (N_1) \left[a^\dagger \rho_s a - \frac{1}{2} a a^\dagger \rho_s - \frac{1}{2} \rho_s a a^\dagger \right] \\
& + \gamma_2 (N_2 + 1) \left[a \rho_s a^\dagger - \frac{1}{2} a^\dagger a \rho_s - \frac{1}{2} \rho_s a^\dagger a \right] \\
& + \gamma_2 (N_2) \left[a^\dagger \rho_s a - \frac{1}{2} a a^\dagger \rho_s - \frac{1}{2} \rho_s a a^\dagger \right] .
\end{aligned} \tag{5.2}$$

There are infinitely many elements in the diagonal terms of the density matrix. However, we look for a general solution. For the n^{th} element of the density matrix, we have the following relation.

$$\begin{aligned}
\dot{\rho}_n = & \gamma_1 (N_1 + 1) (n + 1) \rho_{n+1} - \gamma_1 (N_1 + 1) n \rho_n \\
& + \gamma_1 N_1 n \rho_{n-1} - \gamma_1 N_1 (n + 1) \rho_n \\
& + \gamma_2 (N_2 + 1) (n + 1) \rho_{n+1} - \gamma_2 (N_2 + 1) n \rho_n \\
& + \gamma_2 N_2 n \rho_{n-1} - \gamma_2 N_2 (n + 1) \rho_n .
\end{aligned} \tag{5.3}$$

When we check for the $n = 0$, we see the following relation.

$$\begin{aligned}
\dot{\rho}_0 = & \gamma_1 (N_1 + 1) \rho_1 - \gamma_1 N_1 \rho_0 \\
& + \gamma_2 (N_2 + 1) \rho_1 - \gamma_2 N_2 \rho_0 ,
\end{aligned} \tag{5.4}$$

which results in

$$\rho_1 = \frac{\gamma_1 N_1 + \gamma_2 N_2}{\gamma_1 (N_1 + 1) + \gamma_2 (N_2 + 1)} \rho_0 , \tag{5.5}$$

and the general relation becomes

$$\rho_n = \frac{\gamma_1 N_1 + \gamma_2 N_2}{\gamma_1 (N_1 + 1) + \gamma_2 (N_2 + 1)} \rho_{n-1} . \tag{5.6}$$

Then the general solution for ρ_n is

$$\rho_n = r^n \rho_0 , \tag{5.7}$$

where

$$r = \frac{\gamma_1 N_1 + \gamma_2 N_2}{\gamma_1 (N_1 + 1) + \gamma_2 (N_2 + 1)} . \tag{5.8}$$

From the normalization of the density matrix,

$$\rho_n = r^n (1 - r) . \tag{5.9}$$

Then, from one reservoir's dissipator

$$\begin{aligned}\dot{\rho}_n = & \gamma_1 (N_1 + 1) (n + 1) \rho_{n+1} - \gamma_1 (N_1 + 1) n \rho_n \\ & + \gamma_1 N_1 n \rho_{n-1} - \gamma_1 N_1 (n + 1) \rho_n .\end{aligned}\quad (5.10)$$

Then, the energy flow becomes

$$\begin{aligned}q = & - \sum_{n=0}^{\infty} \omega \gamma_1 (1 - r) [(N_1 + 1) (n + 1) n r^{n+1} \\ & - (N + 1) n^2 r^n + N_1 n^2 r^{n-1} - N_1 (n + 1) n r^n] .\end{aligned}\quad (5.11)$$

And, the flow becomes

$$q = \omega \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} (N_1 - N_2) . \quad (5.12)$$

This is an interesting situation. If one looks at the equation, it is symmetric with respect to coupling constants. If one interchanges them, the result is not affected, which means zero rectification. We need further analysis without the approximations of our Lindblad approach to check the rectification is precisely zero or resulted from our approximations.

5.2 Exact solution

We consider the special case when the composite system is formed from linear oscillators. In that case, it can be shown that the rectification is always zero. Below we are going to prove that this is the case. The Hamiltonian can be written in the form

$$H = \sum_{ij} \hbar W_{ij} b_i^\dagger b_j , \quad (5.13)$$

where

$$W_{ij} = W_{ij}^* . \quad (5.14)$$

Since W is a Hermitian matrix, we can diagonalize it

$$W_{ij} = \sum_{\alpha} U_{i\alpha} \omega_{\alpha} \bar{U}_{j\alpha} , \quad (5.15)$$

and obtain the Hamiltonian as

$$H = \sum_{\alpha} \hbar \omega_{\alpha} c_{\alpha}^\dagger c_{\alpha} , \quad (5.16)$$

where

$$\begin{aligned} c_\alpha^\dagger &= \sum_i U_{i\alpha} b_i^\dagger \\ c_\alpha &= \sum_j \bar{U}_{j\alpha} b_j . \end{aligned} \quad (5.17)$$

Now, define N_{ij} as

$$N_{ij}(t) = \langle b_j^\dagger b_i \rangle_t = \sum_{\alpha, \beta} \bar{U}_{j\alpha} \langle c_\alpha^\dagger c_\beta \rangle_t U_{i\beta} . \quad (5.18)$$

Then, from the Heisenberg picture c 's

$$c_\alpha(t) = e^{-i\omega_\alpha t} c_\alpha \quad c_\alpha^\dagger(t) = e^{i\omega_\alpha t} c_\alpha^\dagger , \quad (5.19)$$

we have

$$N_{ij}(t) = \bar{U}_{j\alpha} e^{i\omega_\alpha t - i\omega_\beta t} \langle c_\alpha^\dagger c_\beta \rangle_0 U_{i\beta} . \quad (5.20)$$

From

$$\langle c_\alpha^\dagger c_\beta \rangle_0 = U_{k\alpha} \langle b_k^\dagger b_l \rangle_0 \bar{U}_{l\beta} , \quad (5.21)$$

N_{ij} becomes

$$N_{ij}(t) = \sum_{\alpha, \beta, k, l} \bar{U}_{j\alpha} e^{i\omega_\alpha t} U_{k\alpha} N_{kl}(0) U_{i\beta} e^{-i\omega_\beta t} \bar{U}_{l\beta} . \quad (5.22)$$

By using the relation

$$e^{i\omega_\alpha t} = (e^{i\Omega t})_{\alpha\alpha} , \quad (5.23)$$

where Ω matrix is the diagonal matrix in which

$$\Omega_{\alpha\alpha} = \omega_\alpha , \quad (5.24)$$

N_{ij} can be written as a multiplication of matrices

$$N_{ij}(t) = (U e^{-i\Omega t} U^\dagger)_{il} N_{lk}(0) (U e^{i\Omega t} U^\dagger)_{kj} . \quad (5.25)$$

Since

$$W = U \Omega U^\dagger , \quad (5.26)$$

we can write

$$N_{ij}(t) = (e^{-iWt})_{il} N_{lk}(0) (e^{iWt})_{kj} . \quad (5.27)$$

Eventually,

$$N(t) = e^{-iWt} N(0) e^{iWt} . \quad (5.28)$$

We are looking for the heat transfer rate expression, which is the rate of change in the expectation value of one of the reservoirs,

$$q = \frac{d\langle H_L \rangle}{dt} = \frac{-i}{\hbar} \langle [H, H_{LL}] \rangle , \quad (5.29)$$

where Hamiltonian is

$$H = H_{LL} + H_{RR} + H_{SS} + H_{SL} + H_{LS} + H_{RS} + H_{SR} . \quad (5.30)$$

The only terms which do not commute with H_{LL} are H_{SL} and H_{LS}

$$q = \frac{i}{\hbar} \langle [H_{LL}, H_{SL} + H_{LS}] \rangle , \quad (5.31)$$

where

$$H_{LL} = \sum_x \hbar \omega_x^L b_x^\dagger b_x , \quad (5.32)$$

$$H_{SL} = \sum_{ix} G_{ix}^L b_i^\dagger b_x , \quad (5.33)$$

$$H_{LS} = H_{SL}^\dagger . \quad (5.34)$$

From the relations

$$\begin{aligned} [b_x^\dagger b_x, b_i^\dagger b_x] &= -b_i^\dagger b_x \\ [b_x b_x, b_x^\dagger b_i] &= b_x^\dagger b_i , \end{aligned} \quad (5.35)$$

the heat flow becomes

$$q = \frac{i}{\hbar} \sum_{ix} -G_{ix}^L \omega_x^L \langle b_i^\dagger b_x \rangle + h.c. , \quad (5.36)$$

where *h.c.* corresponds to Hermitian conjugate. Now we have

$$q = \frac{-i}{\hbar} \text{tr} \{ (G^L \omega^L) N(t) \} . \quad (5.37)$$

When we substitute equation 5.28 for $N(t)$

$$q = \frac{-i}{\hbar} \text{tr} \{ e^{iWt} (G^L \omega^L) e^{-iWt} N(0) \} . \quad (5.38)$$

Here the information of temperatures is given in the initial reservoirs' expectation values of the energy of the individual oscillators, in other words, in $N(0)$ terms for the corresponding reservoir's corresponding oscillators. Since there are separate terms for separate reservoirs, the terms that the temperatures appear are separable,

$$q = f_L(T_L) + g_R(T_R) . \quad (5.39)$$

If the temperatures are the same, we know that the heat flow is zero, therefore

$$f_L(x) = -g_R(x) . \quad (5.40)$$

Then

$$q = f_L(T_L) - f_L(T_R) , \quad (5.41)$$

which makes the thermal rectification zero. Note that there will be a transient regime after the contact is initiated. However, we are interested in the regime where there is steady heat flow from one reservoir to the other, and our equation still governs that part of the regime as well as the transient part.

5.3 Two harmonic oscillators

Now we consider a coupling consists of two harmonic oscillators where each oscillator is coupled to only one reservoir and the the other oscillator.

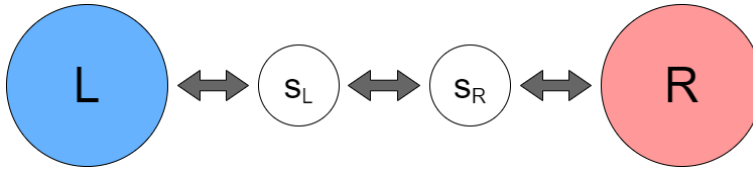


Figure 5.2: Contact between the reservoirs. L corresponds to the left reservoir, R corresponds to the right reservoir, S_L is the left harmonic oscillator, and S_R is the right harmonic oscillator.

When the Hamiltonian of the system without the reservoirs is in the form

$$H = \omega_1 a^\dagger a + \omega_2 b^\dagger b + \omega_{12} a^\dagger b + \omega_{21} b^\dagger a , \quad (5.42)$$

where

$$\omega_{12}^* = \omega_{21} . \quad (5.43)$$

As shown in [10] it can be written in the form

$$H = \begin{pmatrix} a^\dagger & b^\dagger \end{pmatrix} \begin{pmatrix} \omega_1 & \omega_{12} \\ \omega_{21} & \omega_2 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} , \quad (5.44)$$

where the ω matrix is a Hermitian matrix. That means we can diagonalize it. The diagonalized form is

$$H = \Omega_+ c_1^\dagger c_1 + \Omega_- c_2^\dagger c_2, \quad (5.45)$$

where

$$\Omega_\pm = \frac{(\omega_1 + \omega_2) \pm \sqrt{(\omega_1 - \omega_2)^2 + 4\omega_{12}\omega_{21}}}{2}, \quad (5.46)$$

and

$$c_1 = a \cos(\alpha) - b \sin(\alpha), \quad (5.47)$$

$$c_2 = a \sin(\alpha) + b \cos(\alpha), \quad (5.48)$$

where

$$\tan(\alpha) = \frac{2\omega_{21}}{(\omega_1 - \omega_2) - \sqrt{4\omega_1\omega_2 + (\omega_1 - \omega_2)^2}}, \quad (5.49)$$

and c_α are the annihilation operators of the new oscillators

When one considers the couplings between the reservoirs and the system as in the previous section, they become

$$(a^\dagger + a) = \cos(\alpha)(c_1^\dagger + c_1) + \sin(\alpha)(c_2^\dagger + c_2), \quad (5.50)$$

$$(b^\dagger + b) = -\sin(\alpha)(c_1^\dagger + c_1) + \cos(\alpha)(c_2^\dagger + c_2). \quad (5.51)$$

We have two independent harmonic oscillators, each coupled to both reservoirs with

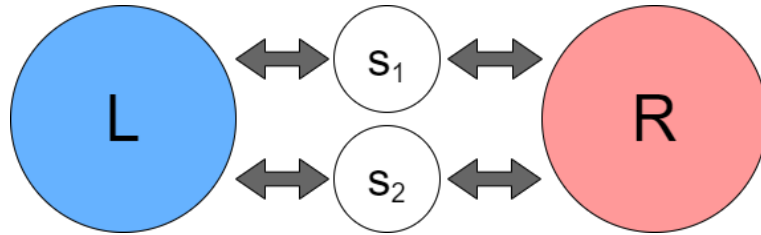


Figure 5.3: Contact between the reservoirs. L corresponds to the left reservoir, R corresponds to the right reservoir, S_1 is the first decoupled harmonic oscillator and S_2 is the second.

distinct coupling constants. From chapter 4, we know how an oscillator results in a non-rectifying coupling, and therefore, we have zero rectification again with a double harmonic oscillator case

CHAPTER 6

CONCLUSION

Thermal rectification behaviors of some small quantum systems which are used as a contact between reservoirs are investigated.

If the contact between reservoirs is a two-level system and the coupling constants with reservoirs are different, rectification occurs. It is shown that the rectification is optimized when the transition energy of the two-level atom is low, higher temperature is as high as possible, lower temperature is low as possible, and the coupling constants are as asymmetric as possible. Note that, higher rectification does not guarantee higher heat flow rates. Lower coupling constants and transitions energies means lower heat transfer rate. They should be optimized.

If the contact is two two-level systems, each one is in contact with a different reservoir and the other two level system, a much higher rectification than a single two-level system can be obtained with the appropriate parameters. When the interaction between the two-level systems is through the Ising coupling, the energy states of the double system are the same states which single reservoirs' coupling operators cause shifts. This causes in the loop of the transitions to transfer energy from one reservoir to the other, individual transitions are done by particular reservoirs. Therefore, by arranging the parameters, one can require a high energy excitation done by the cold reservoir and create an impediment in the loop. Note that this excitation becomes a high energy decay done by the hot reservoir, which always has a finite rate. Therefore a rectification effect is obtained. As the excitation energy goes higher, the rectification effect increases. Other energy levels should be optimized for the ideal heat transfer rate. If the coupling is Heisenberg coupling both reservoirs are responsible for all the transitions. Therefore, the rectification effect is greatly reduced.

If a harmonic oscillator is used as a contact, it is shown that there is no rectification effect even though there are asymmetric coupling constants. It is checked that whether it is a result caused by the approximations we did to obtain the Lindblad Master equation. However, without the approximations, we were able to show that there should be zero rectification since we were able to obtain the heat transfer rate as two separate functions of the temperatures of the reservoirs.

If the contact is a double harmonic oscillator, each one in contact with a different reservoir and the other oscillator system again results in a zero rectification effect since we can show that this coupling is equivalent to two independent harmonic oscillators each in contact with both reservoirs.

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