Virtual Qubits and Quantum Thermal Machines

M.Sc project report submitted in partial fulfillment of the requirements for the degree of

Master of Science

by

Hrushikesh Gawali

216PH011

Under the supervision of

Dr. Deepak Vaid NIT Surathkal



Department of Physics National Institute of Technology, Surathkal Karnataka, India - 575025 December 2023

Declaration

I hereby declare that the Report of the P.G. Project Work entitled **Virtual Qubits and Quantum Thermal Machines** which is being submitted to the National Institute of Technology Karnataka Surathkal, in partial fulfilment of the requirements for the award of the Degree of Master of science in the department of Physics, is a bonafide report of the work carried out by me. The material contained in this Report has not been submitted to any University or Institution for the award of any degree.

Place : NITK, Surathkal Date:

Hrushikesh Gawali (216PH011)

Certificate

This is to certify that the P.G. Project Work Report entitled **Virtual Qubits** and Quantum Thermal Machines submitted by Hrushikesh Gawali, (216PH011) as the record of the work carried out by him, is accepted as the P.G. Project Work Report submission in partial fulfillment of the requirements for the award of degree of Master of Science in the Department of Physics.

Chairman-DPGC

Guide Dr. Deepak Vaid

Acknowledgement

It is a great pleasure to express my gratitude towards my supervisor Dr. Deepak Vaid for his invaluable advice, continuous support and patience. I am also grateful to him for allowing me to pursue problem of my own interest. I thank my fellow mates who have helped me throughout this project. Finally, I want to thank my parents for all there support and patience. Without them, this journey would have been incomplete.

Abstract

Thermal machines play an important role in thermodynamics. This project aims to study smallest thermal machines using virtual qubits. Virtual qubits are two level subsystems of two baths considered as a composite system. Thermal machines act on an external system. To understand the interaction with external system we move towards the field of open quantum systems, which provides master equation to do so. Particularly, we study Lindblad master equation.

Contents

1 Introduction		oduction	1
	1.1	Thermal machines and Qubits	1
	1.2	Quantum Mechanics basics	1
	1.3	Density Matrix	3
	1.4	Measurement	4
	1.5	Time evolution	5
	1.6	Composite System	6
	1.7	Open Quantum Systems	6
2	Line	lblad Master Equation	8
	2.1	Superoperator	8
	2.2	CPT Maps	8
		2.2.1 Condition for finding CPT maps	8
	2.3	Lindblad Master Equation	9
3	The	rmal Machine using Virtual Qubits	14
	3.1	Virtual Qubit and virtual temperature	14
	3.2	Constructing machine	15
		3.2.1 Machine Vitual Qubit	15
		3.2.2 Interaction Hamiltonian	16
A	Pro	of of expectation value in terms of density matrix	18
в	Pyt B.1 B.2	hon code Code for Von Neumann Time evolution	19 19 20

Chapter 1

Introduction

This chapter is mainly focused on the mathematical framework and basic concepts required for the project.

1.1 Thermal machines and Qubits

Thermal machines basically are devices that function as heat energy convertors. A typical thermal machine has two or more heat reserviour and a 'working fluid'. In classical thermodynamics, most common thermal machines are heat engines and refrigerators.[1] Carnot engine is an example of thermal machines which produces work, operating between two reserviours namely source and sink. It takes heat from the source converts it into work and remaining heat energy goes to sink. As shown in fig1.1 the engine extracts heat from the hot reserviour which is source, produces work and remaining heat is lost to sink (cold reserviour). Complete carnot cycle is studied using pressure volume diagram (PV diagram) as shown in fig 1.2.

This project focuses on thermal machines using virtual qubits. A qubit in simple words is quantum bit. As a classical bit has two state 0 and 1. A qubit has two energy states $|0\rangle$ and $|1\rangle$ where $|0\rangle$ is ground state and $|1\rangle$ is excited state. Thermal machine using qubits are smallest machines given its quantum nature.

1.2 Quantum Mechanics basics

Quantum mechanics emphasises that all possible states of a system exist in its own Hilbert space. So a state vector can describe the state of whole system. A state vector is analogous to algebraic vector. As new vector is



Figure 1.1: Carnot Engine



Figure 1.2: Carnot Engine pressure volume diagram



Figure 1.3: Bloch Sphere

formed by vector addition of basis vectors, similarly state vector is formed by addition basis states. General state can be represented by represented using dirac notation as

$$|\Psi\rangle = c_1 |\psi_1\rangle + c_2 |\psi_2\rangle + \dots + c_n |\psi_n\rangle \tag{1.1}$$

where $|\Psi\rangle$ is the state vector and $|\psi_n\rangle$ are basis vector with c_n as square root of probability.

So a general state of qubit can be given as

$$|\Psi\rangle = a |0\rangle + b |1\rangle \tag{1.2}$$

where a, $b \in \mathbb{C}$ satisfying $|a|^2 + |b|^2 = 1$. Any state of qubit can represented on the surface of a bloch sphere as shown 1.3.

1.3 Density Matrix

The theory of quantum mechanics is based on Hilbert space , as every system has its own state space. A unit vector in this state space is state vector of the system , which can describe state of a system. This implies can describe state of a system. This implies that all unit vector in state space are possible states of the system. These unit vectors are called pure states.

But experimentally we find system in on set of $\{|\psi_i\rangle\}$ with probabilities p_i . This is called mixed state where more than one p_i are non-zero. To

understand such systems we define density operator as

$$\rho \equiv \sum_{i} p_{i} \left| \psi_{i} \right\rangle \left\langle \psi_{i} \right| \tag{1.3}$$

Properties of density operator

- 1. has unit trace $Tr[\rho] = 1$
- 2. is a positive matrix $\rho > 0$
- 3. If $\text{Tr}[\rho^2] = 1$ for pure states and $\text{Tr}[\rho^2] < 1$ for mixed states. $\text{Tr}[\rho^2]$ is called as parity of states.
- 4. Diagonal elements are called populations where ρ_{ii} are real and $\sum_i \rho_{ii} = 1$. Off diagonal elements are called coherences with ρ_{ij} are complex and $\rho_{ij} = \rho_{ji}^*$.

1.4 Measurement

In Quantum Mechanics, every measurement is described by Hermitian operator, so such observable can be expanded as

$$O = \sum_{i} a_{i} |a_{i}\rangle \langle a_{i}| \tag{1.4}$$

where a_i are real eigenvalues and $\langle a_i |$ are real eigenvectors. The probability of finding observable O in a_i when in state $|\psi\rangle$ is given as

$$P(a_i) = |\langle \psi | a_i \rangle|^2 \tag{1.5}$$

For mixed states the probability is given in terms of density matrix

$$P(a_i) = Tr[|a_i\rangle \langle a_i| \rho] \tag{1.6}$$

The expectation value of the operator in a state $|\Psi\rangle$ is given as

$$\langle O \rangle = \langle \Psi | \, O \, | \Psi \rangle \tag{1.7}$$

In terms of density matrix, expectation values can be calculated as

$$\langle O \rangle = Tr[O\rho] \tag{1.8}$$

The subsequent derivation is given in Appendix A.



Figure 1.4: Time evolution of population where E = 1 and $\Omega = 1$

1.5 Time evolution

By Schrodinger equation, we have

$$\frac{d}{dt} |\Psi(t)\rangle = -i\hbar H |\Psi(t)\rangle \tag{1.9}$$

where H is hamiltonian of the system. But this equation is only valid iff $|\Psi(t)\rangle$ is pure state which implies the equation is valid for closed quantum system.

If at t=0, the state of a system is given by $|\Psi(t)\rangle$ at time t it will be

$$|\Psi(t)\rangle = e^{-i\hbar H} |\Psi(0)\rangle \tag{1.10}$$

For mixed state, time evolution is given by

$$\dot{\rho} = -i[H,\rho] \equiv \mathcal{L}\rho \tag{1.11}$$

which is Von-Neumann equation and \mathcal{L} is called Liouvillian Superoperator.[4]

Considering an example of space spanned by two basis vectors $|0\rangle$ and $|1\rangle$. The density matrix of the system is

$$\rho = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} = \rho_{00} |0\rangle \langle 0| + \rho_{01} |0\rangle \langle 1| + \rho_{10} |1\rangle \langle 0| + \rho_{11} |1\rangle \langle 1| \quad (1.12)$$

Assuming Hamiltonian as

$$H = E \left| 1 \right\rangle \left\langle 1 \right| + \Omega(\left| 0 \right\rangle \left\langle 1 \right| + \left| 1 \right\rangle \left\langle 0 \right| \right) \tag{1.13}$$

Using Von Neumann equation the variation in ρ_{00} and ρ_{11} with time is plotted in the fig 1.4. The associated code can be referred from Appendix B.1.

1.6 Composite System

Consider a state space of N subsystems, then state space of the composite system is given as $\mathcal{H}_n = \mathcal{H}_1 \otimes \mathcal{H}_2 \cdots \otimes \mathcal{H}_N$ where \mathcal{H}_i is state space of i^{th} subsystem. Therefore, if we have i^{th} subsystem in $|\psi_i\rangle$ state the total state is given as $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_n\rangle$. Same concept is applied to composite mixed state if mixed state of i^{th} system is ρ_i then for state density matrix is given as $\rho = \rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_n$.

If these states can be written as $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$ then these are called as separable states. The states that cannot be separated are called entangled states.

If there are two system a and b forming composite system $\mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b$ and we are interested in properties of system a. To study the properties of subsystem a we take partial trace of density matrix ρ over subspace b given as

$$\rho_a \equiv Tr_b[\rho] \tag{1.14}$$

where ρ_a is known as reduced density matrix. Expanding in terms of basis vectors we get

$$\rho_{a} \equiv Tr_{b} \left[\sum_{i,j,k,l} |a_{i}\rangle \langle a_{j}| \otimes |b_{k}\rangle \langle b_{l}| \right]$$
(1.15)

$$\equiv \sum_{i,j} |a_i\rangle \langle a_j| Tr\left[\sum_{k,l} |b_k\rangle \langle b_l|\right]$$
(1.16)

In open quantum system, tracing out helps to isolate properties of system from the environment.[4]

1.7 Open Quantum Systems

The field of open quantum system deals with quantum systems having interaction with quantum systems interaction with environment. As no quantum system is completely isolated system, so a complete description of a quantum system requires the inclusion of environment. These interaction changes the dynamics of the system and can cause quantum dissipation. The main approach of open quantum system is as follows

- 1. Choosing a system of interest.
- 2. Considering environment interaction, dividing the total system in system of interest and environment.

CHAPTER 1. INTRODUCTION

3. Finding the equation of motion of total system and then finding reduced equation equation of the system of interest.

Chapter 2

Lindblad Master Equation

This chapter deals with Lindblad Master Equation and mathematical framework needed to understand it.

2.1 Superoperator

We define a Fock Liouville space(FLS). It is similar to Hilbert space, but here matrices act as vectors. So, density matrix is a vector in FLS represented as $\rho \rightarrow |\rho\rangle\rangle$. The scalar product in this space of two matrices ρ and ϕ is given as $\langle\langle \phi | \rho \rangle \rangle \equiv Tr[\phi^{\dagger}\rho]$. The operators acting in this space on the matrices are called Liouville superoperator.[4] For example, density matrix of two level system in FLS is given as

$$|\rho\rangle\rangle = \begin{pmatrix} \rho_{00}\\ \rho_{01}\\ \rho_{10}\\ \rho_{11} \end{pmatrix}$$
(2.1)

2.2 CPT Maps

Consider Hilbert space \mathcal{H} formed by density matrix. A map $\mathcal{V} : \rho(\mathcal{H}) \to \rho(\mathcal{H})$ in this space that doesn't change the properties namely trace preservance and complete positivity are called a complete positive and trace preserving map (CPT map).[4]

2.2.1 Condition for finding CPT maps

For finding CPT maps for density matrix, the necessary and sufficient condition is provided by two theorems. **Theorem 1 (Choi's theorem)** A linear map $\mathcal{V} : B(\mathcal{H}) \to B(\mathcal{H} \text{ is com$ pletely positive iff it can be expressed as

$$V_{\rho} = \sum_{i} V_{i}^{\dagger} \rho V_{i} \tag{2.2}$$

with $V_i \in B(\mathcal{H})$.

Theorem 2 (Choi-Krauss Theorem) A linear map $\mathcal{V} : B(\mathcal{H}) \to B(\mathcal{H})$ is completely positive and trace preserving iff it can be expressed as

$$\mathcal{V}\rho = \sum_{l} V_{l}^{\dagger}\rho V_{l} \tag{2.3}$$

with $V_l \in B(\mathcal{H})$ fulfilling

$$\sum_{l} V_{l} V_{l}^{\dagger} = \mathbb{1}_{\mathcal{H}}$$
(2.4)

Krauss operators are operators which satisfy the condition $\sum V_l V_l^{\dagger} = \mathbb{1}_{\mathcal{H}}$. So CPT map can also be represented using Krauss operators. These CPT maps help us to prove Lindblad master equation.[4]

2.3 Lindblad Master Equation

Lindblad master equation is essentially an equation that governs time evolution of density matrix of a subsystem of a complicated system. While the density matrix time evolution of total system is given by Von Neumann equation.[4]

To get an idea of lindblad form, it is essential to understand its formulation. Time evolution of density matrix can be expressed by equation

$$\frac{d}{dt}\rho(t) = \mathcal{L}\rho(t) \tag{2.5}$$

where \mathcal{L} is superoperator acting on density matrix which equivalent to its time derivative. Finding this superoperator necessarily gives the time evolution of density matrix.

This time derivative can expressed in limit format

$$\frac{d\rho}{dt} = \lim_{\Delta t \to 0} \frac{1}{\Delta t} (\mathcal{V}(\Delta t)\rho - \rho)$$
(2.6)

where $\mathcal{V}(\Delta t)$ is a map. This map is Krauss operator which in Fock Louville space can be expanded as

$$V_l(t) = \sum_{i=1}^{d^2} \langle \langle F_i | V_l(t) \rangle \rangle | F_j \rangle \rangle$$
(2.7)

where $|F_i\rangle\rangle$ are orthonormal basis vectors. By Choi's theorem,

$$\mathcal{V}(t)\rho = \sum_{l} \left[\sum_{i=1}^{d^2} \langle \langle F_i | V_l(t) \rangle \rangle F_i \rho \sum_{j=1}^{d^2} F_j^{\dagger} \langle \langle V_l(t) | F_j \rangle \rangle \right] = \sum_{i,j=1}^{d^2} c_{ij}(t) F_i \rho F_j^{\dagger}$$
(2.8)

where $c_{ij}(t) = \sum_{l} \langle \langle F_i | V_l \rangle \rangle \langle \langle V_l | F_j \rangle \rangle$. Using this (2.6) becomes $d\rho = 1$ (1.6)

$$\frac{d\rho}{dt} = \lim_{\Delta t \to 0} \frac{1}{\Delta t} (\mathcal{V}_{\rho}(\Delta t) - \rho)
= \lim_{\Delta t \to 0} \left[\sum_{i,j=1}^{d^2} c_{ij}(\Delta t) F_i \rho F_j^{\dagger} - \rho \right]
= \lim_{\Delta t \to 0} \left\{ \sum_{i,j=1}^{d^2 - 1} c_{ij}(\Delta t) F_i \rho F_j^{\dagger} + \sum_{i=1}^{d^2 - 1} c_{i,d^2}(\Delta t) F_i \rho F_{d^2}^{\dagger}
+ \sum_{j=1}^{d^2 - 1} c_{d^2,j}(\Delta t) F_{d^2} \rho F_j^{\dagger} + c_{d^2,d^2}(\Delta t) F_{d^2} F_{d^2}^{\dagger} - \rho \right\}$$

Assuming $F_{d^2} = \frac{1}{\sqrt{d}} \mathbb{1}$, therefore the equation becomes

$$\frac{d\rho}{dt} = \lim_{\Delta t \to 0} \left[\sum_{i,j=1}^{d^2-1} c_{ij}(\Delta t) F_i \rho F_j^{\dagger} + \sum_{i=1}^{d^2-1} c_{i,d^2}(\Delta t) F_i \rho F_{d^2}^{\dagger} + \sum_{j=1}^{d^2-1} c_{d^2,j}(\Delta t) F_{d^2} \rho F_j^{\dagger} + \frac{1}{d} c_{d^2,d^2}(\Delta t) \rho - \rho \right]$$
(2.9)

To eliminate time dependence, the following constants are defined

$$g_{i,j} = \lim_{\Delta t \to 0} \frac{c_{i,j}(\Delta t)}{\Delta t} \qquad (i,j < d^2)$$
(2.10)

$$g_{i,d^2} = \lim_{\Delta t \to 0} \frac{c_{i,d^2}(\Delta t)}{\Delta t} \quad (i,j < d^2)$$

$$(2.11)$$

$$g_{d^2,j} = \lim_{\Delta t \to 0} \frac{c_{d^2}(\Delta t)}{\Delta t} \qquad (i < d^2)$$

$$(2.12)$$

$$g_{d^2,d^2} = \lim_{\Delta t \to 0} \frac{c_{i,d^2}(\Delta t) - d}{\Delta t}$$

$$(2.13)$$

Putting coefficient in equation

$$\frac{d\rho}{dt} = \sum_{i,j=1}^{d^2-1} g_{i,j} F_i \rho F_j^{\dagger} + \frac{1}{\sqrt{d}} \sum_{i=1}^{d^2-1} g_{i,d^2} F_i \rho + \frac{1}{\sqrt{d}} \sum_{j=1}^{d^2-1} g_{d^2,j} \rho F_j^{\dagger} + \frac{g_{d^2,d^2}}{d} \rho \quad (2.14)$$

Let operator F be the sum of all Krauss operators

$$F = \frac{1}{\sqrt{d}} \sum_{i=1}^{d^2 - 1} g_{i,d^2} F_i$$
(2.15)

Therefore equation can be rewritten as

$$\frac{d\rho}{dt} = \sum_{i,j=1}^{d^2-1} g_{i,j} F_i \rho F_j^{\dagger} + F\rho + \rho F^{\dagger} + \frac{g_{d^2,d^2}}{d}\rho$$
(2.16)

Splitting operator F into Hermitian and anti Hermitian part

$$F = \frac{F + F^{\dagger}}{2} + i\frac{F - F^{\dagger}}{2i} = G - iH$$
 (2.17)

On putting in equation

$$\frac{d\rho}{dt} = g_{i,j}F_i\rho F_j^{\dagger} + \{G,\rho\} - i[H,\rho] + \frac{g_{d^2,d^2}}{d}\rho$$
(2.18)

Let $G_2 = G + \frac{g_{d^2, d^2}}{2d}$

$$\frac{d\rho}{dt} = g_{i,j}F_i\rho F_j^{\dagger} + \{G_2, \rho\} - i[H, \rho]$$
(2.19)

To ensure the complete positivity of maps

$$Tr\left[\frac{d\rho}{dt}\right] = Tr\left[\sum_{i,j=1}^{d^2-1} F_j^{\dagger} F_i \rho + 2G_2 \rho\right] = 0$$
(2.20)

Therefore G_2 should fulfill

$$G_2 = \frac{1}{2} \sum_{i,j=1}^{d^2 - 1} g_{i,j} F_j^{\dagger} F_i \rho$$
(2.21)

Applying this condition equation

$$\frac{d\rho}{dt} = -i[H,\rho] + \sum_{i,j=1}^{d^2-1} g_{i,j} \left[F_i \rho F_j^{\dagger} - \frac{1}{2} \{ F_j^{\dagger} F_i, \rho \} \right]$$
(2.22)



Figure 2.1: Population dynamics under pure coherent dynamics

By diagonalising it, the diagonal form of the Lindblad master equation

$$\frac{d\rho}{dt} = -i[H,\rho] + \sum_{k} \Gamma_k \left[L_k \rho l_k^{\dagger} - \frac{1}{2} \{ L_k L_k^{\dagger}, \rho \} \right] \equiv \mathcal{L}_{\rho}$$
(2.23)

This final form of Lindblad master equation where L_k operators are called Lindblad operators. The second term in the equation takes into account the dissipation to the environment. On removing dissipative term reduces the equation to Von Neumann equation.[5][4]

To understand the variation in the density matrix with time using Lindblad master equation, we consider Lindbladian of the form

$$\frac{d\rho}{dt} = -i[H,\rho] + \Gamma \left[\sigma^{-}\rho\sigma^{+} - \frac{1}{2}\{\sigma^{+}\sigma^{-},\rho\}\right]$$
(2.24)

Assuming the initial state of the qubit is $|1\rangle$ which means $\rho_{11} = 1$ with no coherence. The figure 2.1 represent the system with no coherent dynamics $(\Omega = 0)$ but decay. Figure 2.2 represent the system with coherent driving $(\Omega = 1)$ and decay. The subsequent code is given in Appendix B.2



Figure 2.2: Population dynamics under both coherent and incoherent dynamics

Chapter 3

Thermal Machine using Virtual Qubits

Quantum thermal machines are fundamentally thermal machines at quantum scale which makes it possibly the smallest thermal machine. In this chapter, we will construct a quantum thermal machine using basics of quantum mechanics and thermodynamics. The machine of particular interest is made using the concept of 'Virtual Qubit' and 'Virtual Temperature'.

3.1 Virtual Qubit and virtual temperature

Consider two thermal bath with T_1 and T_2 respectively. These two bath are isolated from each other. Assuming that each bath has two energy states with energy difference \mathcal{E}_1 and \mathcal{E}_2 for bath 1 and bath 2 respectively. Therefore first bath energy states can be given as $|g\rangle_{B_1}$ and $|e\rangle_{B_1}$ and for second bath $|g\rangle_{B_2}$ and $|e\rangle_{B_2}$. On forming a composite system of these two baths, energy states becomes $|g\rangle_{B_1} |g\rangle_{B_2}$, $|e\rangle_{B_1} |g\rangle_{B_2}$, $|g\rangle_{B_1} |e\rangle_{B_2}$ and $|g\rangle_{B_1} |e\rangle_{B_2}$. A virtual qubit is constructed using two states $|e\rangle_{B_1} |g\rangle_{B_2}$ and $|g\rangle_{B_1} |e\rangle_{B_2}$. If $\mathcal{E}_2 \geq \mathcal{E}_1$, then energy difference for vitual qubit is $\mathcal{E}_v = \mathcal{E}_2 - \mathcal{E}_1$. So the two states of virtual qubit are

$$|G\rangle_{B_v} = |e\rangle_{B_1} |g\rangle_{B_2} \qquad |E\rangle_{B_v} = |g\rangle_{B_1} |e\rangle_{B_2} \qquad (3.1)$$

Using Boltzmann distribution, the population of each bath are related as

$$p_1^e = p_1^g e^{-\mathcal{E}_1/T_1} \qquad p_2^e = p_2^g e^{-\mathcal{E}_2/T_2}$$
(3.2)

So for virtual qubit, the population will be

$$p_v^E = p_1^g p_2^e = p_1^g p_2^g e^{-\mathcal{E}_2/T_2} \qquad p_v^G = p_1^e p_2^g = p_1^g p_2^g e^{-\mathcal{E}_1/T_1}$$
(3.3)



Figure 3.1: Virtual Qubit

We define virtual temperature (T_v) of this virtual qubit using Boltzmann distribution between the states

$$p_v^E = p_v^G e^{-\mathcal{E}_v/T_v} \tag{3.4}$$

Therefore,

$$e^{-\mathcal{E}_v/T_v} = \frac{e^{-\mathcal{E}_2/T_2}}{e^{-\mathcal{E}_1/T_1}} \tag{3.5}$$

The virtual temperature is given by

$$T_v = \frac{\mathcal{E}_2 - \mathcal{E}_1}{\frac{\mathcal{E}_2}{T_2} - \frac{\mathcal{E}_1}{T_1}} \tag{3.6}$$

3.2 Constructing machine

A machine is contructed using two qubits, with each qubit in thermal contact with thermal bath. Considering qubit 1 is in contact with bath 1 and qubit 2 with bath 2. An interaction Hamiltonian is introduced which promotes the interaction of qubits with each other and external system.[2][3]

3.2.1 Machine Vitual Qubit

We choose qubit 1 with energy difference between states as E_1 and qubit 2 with energy difference E_2 . Without an interactive Hamiltonian the qubits will only interact with the bath, attaining equilibrium with bath temperature. The main assumption is that only energy conserving interactions take place between machine and bath.

Considering the process in which qubit reaches equilibrium with bath, the energy states of two qubits are $|0\rangle_1 |0\rangle_2$, $|0\rangle_1 |1\rangle_2$, $|1\rangle_1 |0\rangle_2$ and $|1\rangle_1 |1\rangle_2$. A machine virtual qubit is introduced with two states

$$|0\rangle_{v} = |1\rangle_{1} |0\rangle_{2} \qquad |0\rangle_{v} = |1\rangle_{1} |0\rangle_{2} \qquad (3.7)$$



Figure 3.2: Machine Virtual Qubit

The energy difference between two states is $E_v = E_2 - E_1$. Using previous calculation, the virtual temperature attained by machine virtual qubit is

$$T_v = \frac{E_2 - E_1}{\frac{E_2}{T_2} - \frac{E_1}{T_1}}$$
(3.8)

There is very selective coupling between machine and virtual qubit with $\mathcal{E}_1 = E_1$ and $\mathcal{E}_2 = E_2$ because of resonant interaction. So the machine is engineered using E_1 and E_2 values.

3.2.2 Interaction Hamiltonian

As mentioned earlier, the machine acts on external system. A simple case can be considered where external system is also virtual qubit with energy difference $E_2 - E_1 = E_3$. The interaction between this machine and external



Figure 3.3: Machine interacting with external system

system is acheived using interaction Hamiltonian.[2]

$$H_{int} = g(|0\rangle_1 |1\rangle_2 |0\rangle_{31} \langle 1|_2 \langle 0|_3 \langle 1| + |1\rangle_1 |0\rangle_2 |1\rangle_{31} \langle 0|_2 \langle 1|_3 \langle 0|)$$
(3.9)

$$= g(|1\rangle_{v} |0\rangle_{3v} \langle 1|_{3} \langle 0| + |0\rangle_{v} |1\rangle_{3v} \langle 1|_{3} \langle 0|$$
(5.10)

All interaction Hamiltonian does is to swap between two degenerate energy states $|0\rangle_v |1\rangle_3 \leftrightarrow |1\rangle_v |0\rangle_3$.

Appendix A

Proof of expectation value in terms of density matrix

The expectation value of operator O is defined as

$$\langle O \rangle = \langle \Psi | \, O \, | \Psi \rangle \tag{A.1}$$

On expanding $|\Psi\rangle$ in terms of basis vectors as $\sum_k c_k |\psi_k\rangle$ the expectation value can be given as

$$\langle O \rangle = \sum_{k} p_k \langle \psi_k | O | \psi_k \rangle \tag{A.2}$$

Using completeness theorem, $\mathbb{1} = \sum_{i} |i\rangle \langle i|$ where $|i\rangle$ are basis states span over the Hilbert space. So the trace of operator O is

$$tr[O] = \sum_{i} \langle i | O | i \rangle \tag{A.3}$$

Applying the concept of completeness theorem in A.2

$$\begin{aligned} \langle O \rangle &= \sum_{k} p_{k} \langle \psi_{k} | \ \mathbb{1}O\mathbb{1} | \psi_{k} \rangle \\ &= \sum_{k} p_{k} \sum_{ij} \langle \psi_{k} | i \rangle \langle i | O | j \rangle \langle j | \psi_{k} \rangle \\ &= \sum_{ij} \sum_{k} p_{k} \langle j | \psi_{k} \rangle \langle \psi_{k} | i \rangle \langle i | O | j \rangle \\ &= \sum_{ij} \langle j | \left\{ \sum_{k} p_{k} | \psi_{k} \rangle \langle \psi_{k} | \right\} | i \rangle \langle i | O | j \rangle = \sum_{ij} \langle j | \rho O | j \rangle = tr[\rho O] \end{aligned}$$

Appendix B

Python code

B.1 Code for Von Neumann Time evolution

```
from qutip import *
import numpy as np
import matplotlib.pyplot as plt
#defining basis vectors
vec_0 = Qobj([[1],[0]])
vec_1 = Qobj([[0],[1]])
#defining hamiltonian
E = 1
omeg = 1
H = E*vec_1*vec_1.dag() + omeg*(vec_0*vec_1.dag() + vec_1*vec_0.dag())
#for evolution
times = np.linspace(0, 5, 100)
result = mesolve(H, vec_1, times, [],[])
states = result.states
#Extracting values
rho_{00} = []
rho_11 = []
for state in states:
    dm = state*state.dag()
    #for rho_00
    val_00 = vec_0.dag()*(dm*vec_0)
```

```
rho_00.append(val_00[0][0][0])
#for rho_11
val_11 = vec_1.dag()*(dm*vec_1)
rho_11.append(val_11[0][0][0])
```

```
#for potting the graph
plt.plot(times, rho_00, color='orange', label='rho_00')
plt.plot(times, rho_11, color='blue', label='rho_11')
plt.legend()
plt.xlabel('Time')
plt.ylabel('Population')
```

B.2 Code for Population dynamics using Lindblad Master Equation

```
from qutip import *
import numpy as np
import matplotlib.pyplot as plt
#defining basis vectors
vec_0 = Qobj([[1],[0]])
vec_1 = Qobj([[0],[1]])
def plotter(val):
    #defining constants
    E = 1
    omeg = val
    #defining Hamiltonian
    H = E*vec_1*vec_1.dag() + omeg*(vec_0*vec_1.dag() + vec_1*vec_0.dag())
    #collapse operator
    c_{ops} = [0.3*destroy(2)]
    #solving equation
    times = np.linspace(0, 10, 100)
    result = mesolve(H, vec_1, times, c_ops,[])
    states = result.states
```

```
#retrieving values
    rho_{00} = []
    rho_11 = []
    for state in states:
        dm = state*state.dag()
        #for rho_00
        val_00 = vec_0.dag()*(dm*vec_0)
        rho_00.append(val_00[0][0][0])
        #for rho_11
        val_11 = vec_1.dag()*(dm*vec_1)
        rho_11.append(val_11[0][0][0])
    #plotting values
    plt.plot(times, rho_00, color='orange', label='rho_00')
    plt.plot(times, rho_11, color='blue', label='rho_11')
    plt.legend()
    plt.xlabel('Time')
    plt.ylabel('Population')
#for incoherent dynamics
plotter(0)
#for coherent driving and decay
plotter(1)
```

References

- Sourav Bhattacharjee and Amit Dutta. "Quantum thermal machines and batteries". In: *The European Physical Journal B* 94.12 (Dec. 2021), p. 239. ISSN: 1434-6036. DOI: 10.1140/epjb/s10051-021-00235-3. URL: https://doi.org/10.1140/epjb/s10051-021-00235-3.
- [2] Nicolas Brunner et al. "Virtual qubits, virtual temperatures, and the foundations of thermodynamics". In: *Physical Review E* 85.5 (May 2012). DOI: 10.1103/physreve.85.051117. URL: https://doi.org/10.1103%2Fphysreve.85.051117.
- [3] Noah Linden, Sandu Popescu, and Paul Skrzypczyk. "How Small Can Thermal Machines Be? The Smallest Possible Refrigerator". In: *Physical Review Letters* 105.13 (Sept. 2010). DOI: 10.1103/physrevlett. 105.130401. URL: https://doi.org/10.1103%2Fphysrevlett.105. 130401.
- [4] Daniel Manzano. "A short introduction to the Lindblad master equation". In: AIP Advances 10.2 (Feb. 2020), p. 025106. DOI: 10.1063/1. 5115323. URL: https://doi.org/10.1063%2F1.5115323.
- Bei Zeng et al. Quantum Information Meets Quantum Matter. Springer New York, 2019. DOI: 10.1007/978-1-4939-9084-9. URL: https: //doi.org/10.1007/978-1-4939-9084-9.