Quantum Szilard Engine

by

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A thesis submitted in partial fulfillment of the requirements for the degree of

Master of Science

Department of Physics

Quaid-i-Azam University

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A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF MASTERS OF PHILOSOPHY IN PHYSICS AT THE QUAID-I-AZAM UNIVERSITY, ISLAMABAD 45320, PAKISTAN.
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RESEARCH COMPLETION CERTIFICATE

Certified that the research work contained in the thesis titled Quantum Szilard Engine has been carried out and completed by Mr. Sajid Majeed Roll No. 02182113001 under my supervision.

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DEDICATION

To

My Teachers

and

My Parents.

Acknowledgments

First and foremost, I would like to thank ALLAH Almighty for giving me the strength, knowledge, ability and opportunity to undertake this research study and to persevere and complete it satisfactorily. His continuous grace and mercy was with me throughout my life and ever more during the tenure of my research. Without His blessings, this achievement would not have been possible.

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Abstract

The Szilard engine, which is evocative of Maxwell's demon, offers an alluring method of transforming information into energy while appearing to go against the second Law of thermodynamics's basic tenets. Originally designed as a conventional thought experiment, Zurek later developed it and added a quantized treatment to the framework. This thesis explores the quantum Szilard engine, an innovative and beautiful concept that replaces the conventional rigid box (infinite potential well) with a harmonic potential. By using this alternate strategy, the scope of this model is greatly widened, allowing for a thorough analysis of its guiding principles and behaviors. The achievement of analytic calculations of the quantum Szilard engine is a noteworthy aspect of this research.

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Chapter 1

Introduction

1.1 Historical Review

The second law of thermodynamics is a fundamental law of physics as it provides insights into the behavior of entropy and the irreversibility of spontaneous or natural processes. For example flow of heat from a hot body to a cold body, mixing of gas, the dissipation of energy, the burning of a piece of paper and the breaking of glass are all irreversible processes. Before second law of thermodynamics, there were no explanation that why these processes are irreversible as the law of conservation of energy holds for all these processes in the reverse direction. Second law of thermodynamics states that:

"In any spontaneous or natural process, the total entropy of an isolated system always increases or remains constant"

$$\Delta S \geq 0.$$

Many challenges to the second law of thermodynamics involve a device widely known as a Maxwell's demon. Maxwell's demon is a hypothetical intelligent being (or a functionally equivalent device) capable of detecting and reacting to the motions of individual molecules. It has been about 150 years since Maxwell introduced the idea of this demon. The original concept of Maxwell's demon was conceived by James Clark Maxwell in 1867 to show the apparent violation of the second law of thermodynamics. In 1867 Maxwell wrote about his thought experiment for the first time in a letter to Peter Guthrie Tait. Before it was presented publicly, he wrote again a letter to John William in 1871 to discuss his idea. Finally, In 1872 Maxwell published his idea of "violating the second law by introducing the intelligent being in thermodynamical system" in his book[1] "Theory of Heat".

Maxwell assumed a container containing gas at a certain temperature. Corresponding to this temperature, average velocity of molecules has a particular value. Some of the molecules are moving at velocity greater than average velocity and some are moving at lower than average velocity. Then a partition is inserted in the middle of box, separating the box into container A and container B. A small size window is then constructed that could be closed or opened at will by a "being" to allow individual molecules of gas to pass through. By passing only fast-moving molecules from container A to container B and slow-moving molecules from B to A, the demon would bring about an effective flow from A to B of molecular kinetic energy. Thus container B and A will become hot and cold respectively. One can use this temperature difference to run an engine, when heat is allowed to flow from hot container towards cold one.

Another possible scenario [2] is that, the demon opens the door only when molecules are approaching the window from container B. In this way, all molecules will end up in container A. Hence a pressure difference is produced without any expenditure of energy or work. One can use this pressure difference to run an engine by hanging a load with a piston and allows the gas to push the piston to obtain useful work.

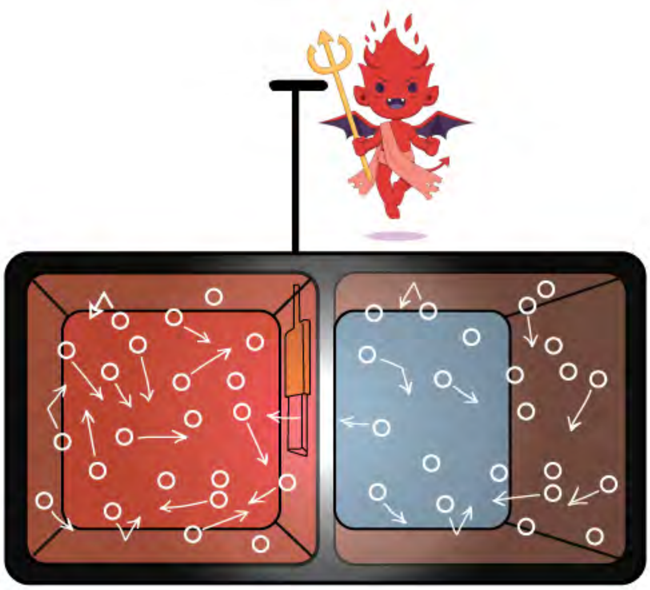

Figure 1.1: Temperature Demon.

Notice that Maxwell did not use the term "demon" in his debate and writing. In 1874, William Thomson (later Lord Kelvin) [3] gave this designation. This name "demon" has been stuck with Maxwell's imaginary character for about last 150 years. To be very honest, Thomson called it "Maxwell's intelligent demon". The introduction to the idea of Maxwell demon and all the above discussion happened at the end of 19th century, so there was no plausible justification about this apparent violation of the second law. Secondly, this experiment was beyond the ability of experiments at that time as there was no any device that could make such crucial measurements on individual molecules

1.2 Classical Szilard Engine

In 1929 [4], Leo Szilard gave a strong response to this apparent paradox. He was the first who related physical entropy and information. Basic motive of Szilard was to investigate the conditions that apparently violate the second law of thermodynamics and permit a perpetual motion machine. This was when concept of classical Szilard engine was given formally. Classical Szilard engine is a single molecule engine which consists of a single molecule trapped in a container of volume V attached to a thermal bath at temperature T. Molecule can move freely inside the container, partition is then inserted by the demon and the container is divided into two halves. Classical particle is localized by inserting the barrier. However, a measurement is performed to acquire the information whether particle is in the left or right half. Once the particle is located, it pushes the barrier towards the end of the container. Now if we connect a load with a wire and the other end of wire is connected to the frictionless barrier then useful work can be obtained by lifting the load when particle pushes the barrier.

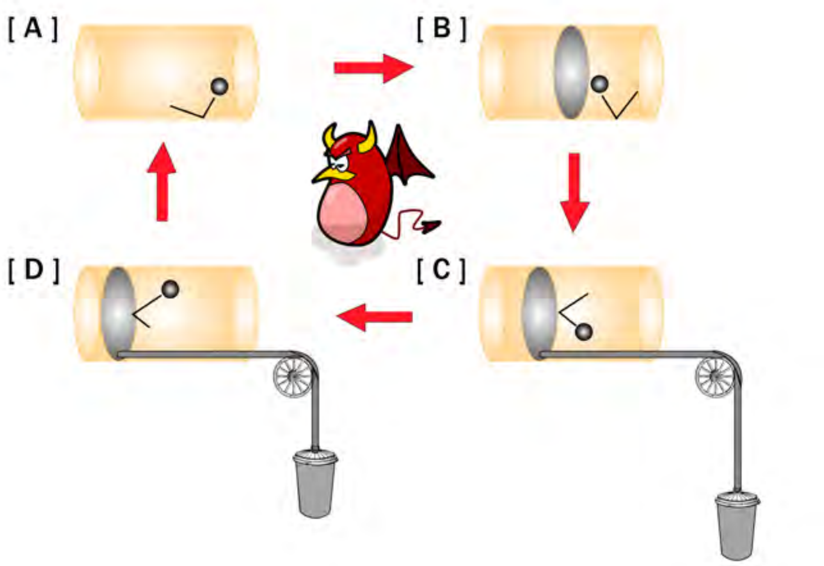

Figure 1.2: Classical Szilard Engine.

Work done by Classical Szilard Engine:

$$W = k_B ln \frac{V_f}{V_i},$$

$V_f = V$ and $V_i = \dfrac{V}{2}$

$$W = k_B T ln 2.$$

The ability to do work implies that entropy of system is decreasing.

Entropy Change:

$$dS = \frac{dQ}{T},$$

for isothermal process $dQ = -dW$

$$dS = -\frac{dW}{T},$$
$$dS = -k_B ln2.$$

This decrease in entropy leads to the violation of second law of thermodynamics.

To rescue the second law, Leo Szilard concluded that in order to measure the speed and position of molecule, demon needs to expend some energy. This simply means that information is obtained at cost of energy. As a result of expenditure of energy, entropy of demon will increase. Since demon is interacting with the gas, so the total entropy will be considered as a combined entropy of gas and demon such that:

$$dS_{total} = dS_{demon} + dS_{gas} \geq 0.$$

Hence according to Leo Szilard, demon entropy increases in such a way that it compensates the lowering of entropy of gas (entropic cost greater than thermodynamics profit) and prevents the second law of thermodynamics from being violated.

1.3 Arguments and Discussion

In 1948, Claude Shannon [5] developed classical information theory which laid the foundation for the study of information, data and communication. He introduced the concept of Information entropy known as Shannon entropy H. This theory defines entropy as the measure of randomness or uncertainty that can directly be related to the information gain. Complete uncertainty means that we have no information about the system, Shannon entropy will be zero in this case. Shannon entropy is defined as

$$H_s = -\sum_i p_i log p_i,$$

where p_i is the probability of an event i.

Many physicists have conducted calculations to show that the second law of thermodynamics remains intact when a complete analysis of the entire system including the demon is considered. The fundamental aspect of this physical argument involves performing calculations which establish that any such demon must inherently produce a greater amount of entropy while segregating molecules than the entropy it could possibly eliminate using the proposed method. In simpler terms, the energy expended in measuring the molecules velocities and selectively permitting their passage between points A and B is greater than the energy gained through the resulting temperature difference.

In 1961, Rolf Landauer [6] brought his deep insight to further resolve this paradox. In order to operate the Szilard engine in a cyclic process, it is necessary to come back to the initial state after each cycle. He realized that we need to erase information stored in demon's mind after each cycle to run the engine. When information is erased, Shannon entropy decreases leading to an increase in thermodynamics entropy. Energy (heat) required to erase 1-bit of information is equal to $k_B ln2$. This is known as Landauer principle. This minimum energy dissipated by erasing information was experimentally determined by Eric Lutz *et al*. in 2012. Furthermore, Lutz *et al* confirmed that the system must approach asymptotically zero processing speed in order to approach the Landauer's limit.

In 1982, Charles Bennett [7] further extended the idea of Landauer and provided further insight into the connection between information and thermodynamics. Actually John Earman and John D. Norton raised objections to Landauer's principle. In order to clarify, Bennet discussed in detail in his paper titled" Thermodynamics of Computation—a Review" that erasing information is associated with the dissipation of energy. Landauer and Bennett had reached the same conclusion as Szilard's 1929 paper, that the second law cannot be violated by Maxwell demon because entropy would be created.

Thus, the Szilard engine converts information into useful mechanical work, which shows that information can be used as a fuel. This prediction has been demonstrated by various experiments, both in classical [8, 9, 10, 11, 12] and quantum [13, 14, 15] regimes. Furthermore, a variety of molecular machines that act as Maxwell demons in living things have identified by biophysicist. [16].

1.4 Quantum Szilard Engine

Classical Szilard engine is based on classical mechanics and classical information theory. Barrier insertion localizes the particle, however measurement allows us to know where the particle is located. Quantum version of Szilard engine is based on quantum mechanics and quantum information theory. Quantum Szilard engine faces several challenges due to principle of superposition and probabilistic nature of quantum mechanics.

As the particle is in a superposition state, so the barrier insertion alone cannot localize the particle. To localize the particle, we need to perform quantum projective measurements on the system. Once the particle is projected to one of the eigenstates, it becomes localized and entropy reduces which leads to the apparent violation of second law. Quantum version of Szilard engine was developed by Zurek [17] for a particle trapped in an infinite potential well. His contribution to the understanding of the quantum Szilard engine has had a significant impact on the fields of quantum information theory, quantum thermodynamics, and quantum computation. A thorough investigation of the quantum harmonic Szilard engine is the focus of this thesis and we will discuss it in the next chapter.

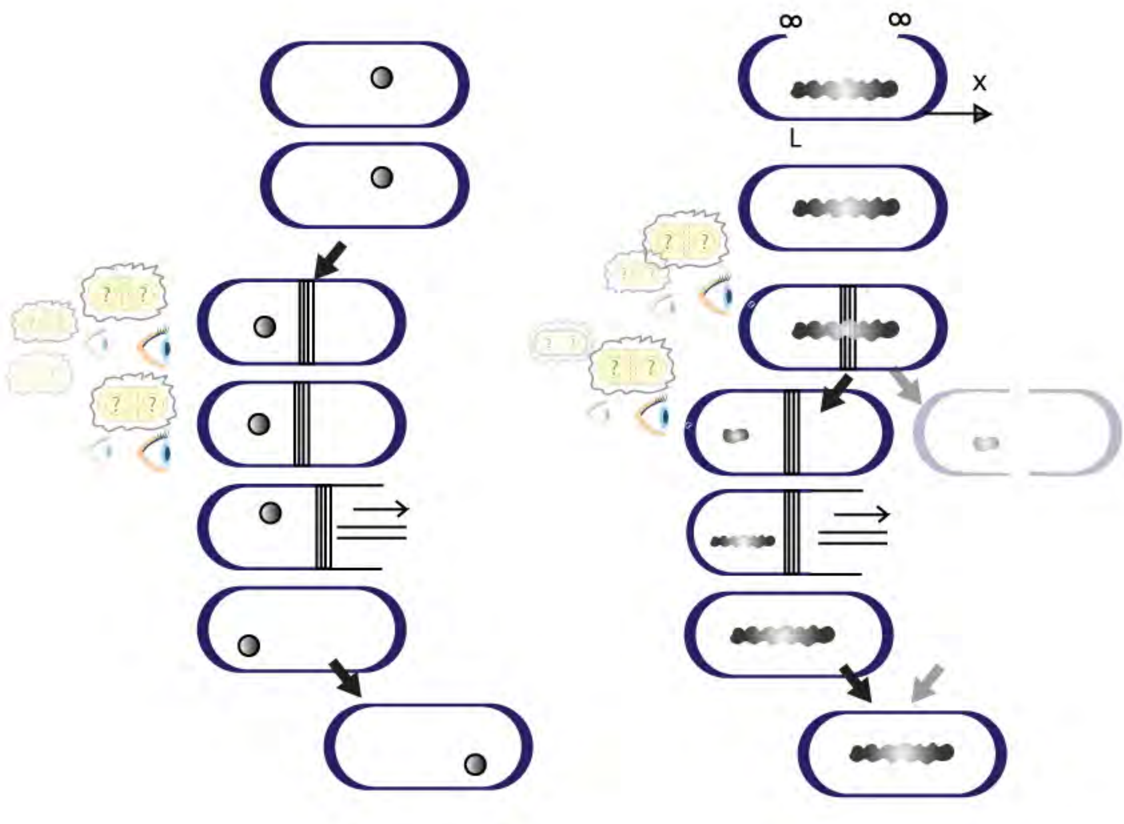

Figure 1.3: Comparison of Quantum and Classical Szilard Engine.

1.5 Multiparticle Szilard Engine

Multiparticle [32] Szilard engine shown in Figure 1.4 is a further generalization of Szilard engine. Instead of single particle trapped in a container, more than one particle is involved. We can allow the particles to interact making it more complex. At high temperature we don't need to take care whether the particles are bosons or fermions, however, at low temperature(especially close to *zero Kelvin*) nature(bosonic or fermionic) of particle affects the efficiency of engine. At low temperature quantum nature of particles becomes more significant which treats bosons and fermions differently.

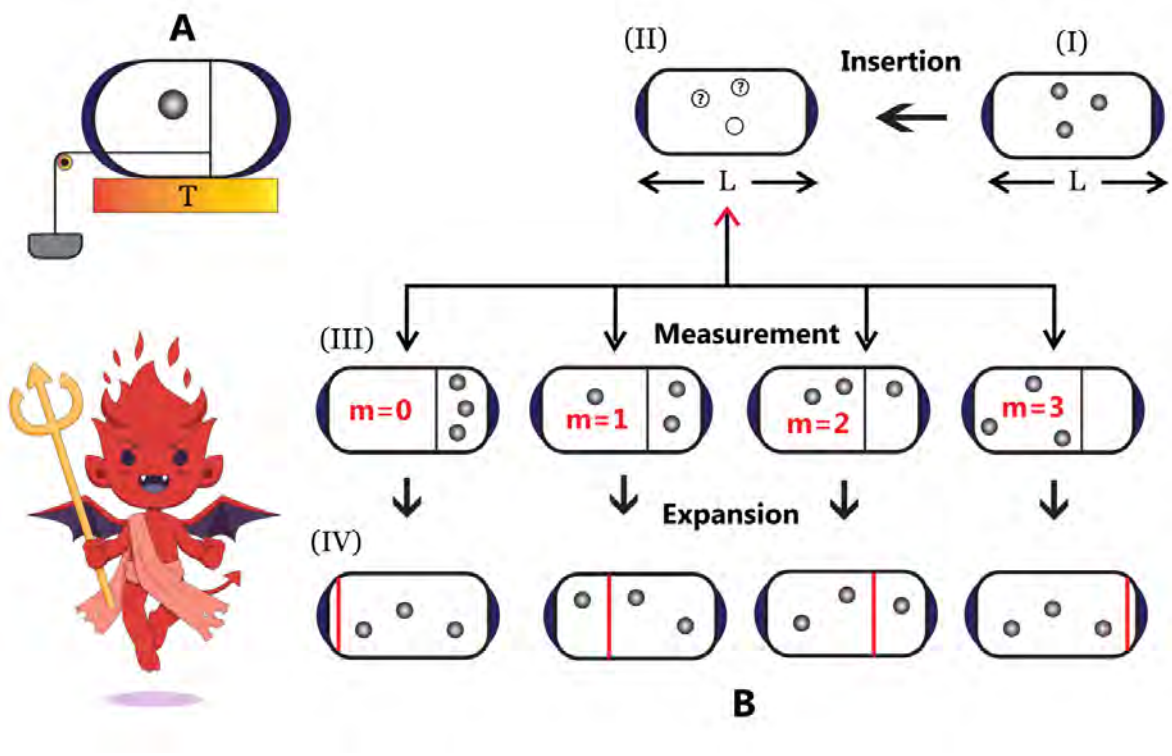

Figure 1.4: Multiparticle Szilard Engine

Bosonic Szilard engine is more efficient than fermionic Szilard engine. It is also found that classical Szilard engine is more efficient than fermionic Szilard engine, while the case is different for bosonic Szilard engine because bosons clump together at *zero Kelvin*[33].

Chapter 2

Fundamental Concepts

2.1 Density Operator

Density operator formalism is a mathematical framework which is used to describe the state of a quantum system. It gives more general description of quantum system utilizing the concept of mixed state. In quantum mechanics, state vectors are used to describe a pure state. However, in many practical cases, quantum system is a statistical combination of multiple pure states known as a mixed state. For mixed states, we use density operator to represent the quantum system.

Density operator acts on the Hilbert space of the system and is represented by symbol $\hat{\rho}$ as

$$\hat{\rho} = \sum_{n=0}^{\infty} p_n |\psi_n\rangle\langle\psi_n|, \tag{2.1}$$

where $|\psi_n\rangle$ is a basis vector in Hilbert space and p_n is the probability of the system being in the state $|\psi_n\rangle$ such that:

$$\sum_{n=0}^{\infty} p_n = 1.$$

2.1.1 Properties of Density Operator

Density operators satisfy following properties:

Hermiticity

It is a Hermitian operator which means that it is equal to its Hermitian conjugate.

$$\hat{\rho} = \hat{\rho}^\dagger.$$

Normalization

It is normalized operator which means that trace of density operator is always equal to 1.

$$Tr\left[\hat{\rho}\right] = 1.$$

Positivity
It is positive semi definite operator which means that all of its eigenvalues are non-zero.

$$\hat{\rho} \geq 0.$$

2.2 Pure and Mixed States

Density matrix can be used to represent both pure and mixed states. Pure and mixed state differ from one another.

2.2.1 Pure States

A quantum state is said to be a pure state if it can be represented by a single ket in a Hilbert space.

$$|\psi\rangle = \sum_{m=1} b_m |u_m\rangle.$$

Density operator for a pure state $|\psi\rangle$ can be written as

$$\hat{\rho} = |\psi\rangle\langle\psi|. \tag{2.2}$$

Here we can see that $p = 1$ which means that there is only one eigenvalue of density operator if state is pure. Pure state has only quantum uncertainties.

Purity Test

$$Tr\left[\rho^2\right] = 1.$$

This is because there is on only eigenstate state with probability $p = 1$.

2.2.2 Mixed States

State which represents the statistical mixture of pure states is known as mixed state. It occurs when quantum system is in probabilistic or uncertain state. We cannot represent the mixed state using a single ket vector, it is necessary to use the notion of density operators to represent the mixed state. We can use the linear combination of pure states to represent the mixed state.

$$\hat{\rho}_{mix} = \sum_{n=0} p_n \hat{\rho}_n^{pure},$$

where $\hat{\rho}_n^{pure} = |\psi_n\rangle\langle\psi_n|$.

Therefore

$$\hat{\rho}_{mix} = \sum_{n=0} p_n |\psi_n\rangle\langle\psi_n| \tag{2.3}$$

such that:

$$\sum_{n=0} p_n = 1$$

Purity Test

$$Tr\left[\rho_{mix}^2\right] < 1.$$

This is because there are more than one pure state with $0 \leq p_n < 1$ that contribute to form a mixed state.

2.3 Expectation Value

Average or expectation value of an operator $\hat{A}$ for a given density operator can be written as

$$\langle\hat{A}\rangle = Tr\left[\hat{\rho}\hat{A}\right].$$

Proof:

From the elementary quantum mechanics

$$\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle,$$

where

$$|\psi\rangle = \sum_{m=1} b_m |u_m\rangle,$$

$$\langle\psi| = \sum_{m=1} b_m^* \langle u_m|,$$

so

$$\langle\hat{A}\rangle = \sum_{n=1} b_n^* \langle u_n|\hat{A} \sum_{m=1} b_m |u_m\rangle,$$

$$\langle\hat{A}\rangle = \sum_{n,m=1} b_m b_n^* \langle u_n|\hat{A}|u_m\rangle.$$

Recall

$$b_m = \langle u_m|\psi\rangle,$$

$$b_m^* = \langle \psi|u_m\rangle,$$

so

$$\langle \hat{A}\rangle = \sum_{n,m=1} \langle u_m|\psi\rangle\langle\psi|u_n\rangle\langle u_n|\hat{A}|u_m\rangle,$$

where from Eq. (2.2)

$$\hat{\rho} = |\psi\rangle\langle\psi|,$$

so

$$\langle \hat{A}\rangle = \sum_{n,m=1} \langle u_m|\hat{\rho}|u_n\rangle\langle u_n|\hat{A}|u_m\rangle,$$

$$\langle \hat{A}\rangle = \sum_{m=1}\langle u_m|\hat{\rho}\left(\sum_{n=1}|u_n\rangle\langle u_n|\right)\hat{A}|u_m\rangle,$$

using completeness relation i.e.

$$\sum_{n=1}|u_n\rangle\langle u_n| = 1,$$

$$\langle \hat{A}\rangle = \sum_{m=1}\langle u_m|\hat{\rho}\hat{A}|u_m,\rangle$$

$$\Rightarrow \boldsymbol{\langle \hat{A}\rangle = Tr\left[\hat{\rho}\hat{A}\right]}. \tag{2.4}$$

This relation is valid whether the state is mixed or pure, because the expectation value of an operator $\hat{A}$ for mixed state can be written as well i.e.

$$\langle \hat{A}\rangle_{mix} = \sum_{n=1} p_n\langle\psi_n|\hat{A}|\psi_n\rangle. \tag{2.5}$$

Proof:

$$\langle \hat{A}\rangle_{mix} = Tr\left[\hat{\rho_{mix}}\hat{A}\right],$$

$$\langle \hat{A}\rangle_{mix} = Tr\left[\sum_{n=1} p_n|\psi_n\rangle\langle\psi_n|\hat{A}\right],$$

$$\langle\hat{A}\rangle_{mix} = \sum_{m}\langle m|\left(\sum_{n=1}p_n|\psi_n\rangle\langle\psi_n|\hat{A}\right)|m\rangle,$$

$$\langle\hat{A}\rangle_{mix} = \sum_{m.n=1} p_n\langle m|\psi_n\rangle\langle\psi_n|\hat{A}|m\rangle,$$

$$\langle\hat{A}\rangle_{mix} = \sum_{n=1}p_n\langle\psi_n|\hat{A}|\left(\sum_{m=1}|m\rangle\langle m|\right)|\psi_n\rangle,$$

using completeness relation. i.e.

$$\sum_{m=1}|m\rangle\langle m| = \hat{I},$$

$$\langle\hat{A}\rangle_{mix}=\sum_{n=1}p_n\langle\psi_n|\hat{A}|\psi_n\rangle.$$

Hence, Eq. (2.5) has proved. So we can write Eq. (2.4) for mixed states as

$$\boldsymbol{\langle\hat{A}\rangle_{mix} = Tr\left[\hat{\rho_{mix}}\hat{A}\right].}$$

2.4 Time Evolution of Density Operator

Using the Schrodinger wave equation, we can find time evolution of density operator is given by von Neumann-Liouville equation.

Schrodinger wave equation is

$$i\frac{\partial}{\partial t}|\psi_n\rangle = \hat{H}|\psi_n\rangle, \tag{2.6}$$

and its complex conjugate is

$$-i\frac{\partial}{\partial t}\langle\psi_n| = \langle\psi_n|\hat{H}. \tag{2.7}$$

Now let us differentiate Eq. (2.1) with respect to time

$$\frac{\partial}{\partial t}\hat{\rho} = \frac{\partial}{\partial t}\left(\sum_{n=0}^{\infty} p_n|\psi_n\rangle\langle\psi_n|\right),$$

$$\frac{\partial}{\partial t}\hat{\rho} =\sum_{n=0}^{\infty} p_n\left(\frac{\partial}{\partial t}|\psi_n\rangle\right)\langle\psi_n|+\sum_{n=0}^{\infty} p_n|\psi_n\rangle\left(\frac{\partial}{\partial t}\langle\psi_n|\right),$$

from Eq. (2.6) and (2.7)

$$\frac{\partial}{\partial t}\hat{\rho} =\sum_{n=0}^{\infty} p_n\left(-i\hat{H}|\psi_n\rangle\right)\langle\psi_n|+\sum_{n=0}^{\infty} p_n|\psi_n\rangle\left(i\langle\psi_n|\hat{H}\right),$$

$$\frac{\partial}{\partial t}\hat{\rho} = -i\left(\hat{H}\sum_{n=0}^{\infty} p_n|\psi_n\rangle\langle\psi_n| - \sum_{n=0}^{\infty} p_n|\psi_n\rangle\langle\psi_n|\hat{H}\right),$$

from Eq. (2.1)

$$i\frac{\partial}{\partial t}\hat{\rho} = \left(\hat{H}\hat{\rho} - \hat{\rho}\hat{H}\right),$$

$$i\frac{\partial}{\partial t}\hat{\rho} = \left[\hat{H}, \hat{\rho}\right]. \tag{2.8}$$

This is the equation of motion of density operator known as **von Neumann equation**. It gives us the time evolve state at a later time t if density operator is known to us at earlier time t_o.

We can also evolve density operator over time by applying a unitary time-evolution operator $\hat{U}(t - t_o)$,

$$\hat{U}(t - t_o) = e^{-i\hat{H}(t-t_o)}, \tag{2.9}$$

where $\hat{H}$ is the time-independent Hamiltonian.

$$\hat{U}^{\dagger}(t - t_o) = e^{-i\hat{H}(t-t_o)},$$

$$\hat{U}\hat{U}^{\dagger} = I. \tag{2.10}$$

Using this operator we can connect the density operator at time t to t_o:

$$\hat{\rho}(t) = \hat{U}(t - t_o)\left[\hat{\rho}(t_o)\right]\hat{U}^{\dagger}(t - t_o). \tag{2.11}$$

Trace is preserved during unitary evolution.

$$Tr\left(\hat{\rho}(t)\right) = Tr\left[\hat{U}(t - t_o)\left[\hat{\rho}(t_o)\right]\hat{U}^{\dagger}(t - t_o)\right],$$

using cyclic properties of trace & Eq. (2.10)

$$Tr\left(\hat{\rho}(t)\right) = Tr\left[\hat{U}(t - t_o)\hat{U}^{\dagger}(t - t_o)\hat{\rho}(t_o)\right],$$

$$\boldsymbol{Tr\left[\hat{\rho}(t)\right] = Tr\left[\hat{\rho}(t_o)\right]}.$$

Purity is also preserved during unitary evolution.

$$Tr\left[\hat{\rho}^2(t)\right] = Tr\left[\hat{U}(t - t_o)\hat{\rho}\hat{U}^{\dagger}(t - t_o)\hat{U}(t - t_o)\hat{\rho}\hat{U}^{\dagger}(t - t_o)\right],$$

using cyclic properties of trace & Eq. (2.10)

$$Tr\left[\hat{\rho}^2(t)\right] = Tr\left[\hat{\rho}\hat{U}^\dagger(t-t_o)\hat{U}(t-t_o)\hat{\rho}\hat{U}^\dagger(t-t_o)\hat{U}(t-t_o)\right],$$

$$Tr\left[\hat{\rho}^2(t)\right] = Tr\left[\hat{\rho}\hat{\rho}\right],$$

$$\boldsymbol{Tr\left[\hat{\rho}^2(t)\right] = Tr\left[\hat{\rho}^2\right]}.$$

2.5 Composite System

In elementary quantum mechanics, we usually deal with single particle in isolation. In many cases, it becomes necessary to deal with multiparticle state or composite system which can be define as:

If our system is made up of two or more individual systems, then the entire system is known as a composite system.

In order to construct the state of composite system mathematically in quantum mechanics, first we need to develop the composite Hilbert Space $\mathcal{H}$.

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2,$$

$\mathcal{H}$ is the Hilbert space of composite system with N the dimensions of space such that

$$N = N_1 \times N_2$$

$\mathcal{H}_1$is the Hilbert space of subsystem-1 with N_1 dimensions of space.

$\mathcal{H}_2$ is the Hilbert space of subsystem-2 with N_2 dimensions of space.

$\otimes$ represents the Kronecker product or tensor product.

Let $|\phi\rangle$ belong to $\mathcal{H}_1$ and $|\chi\rangle$ belong to $\mathcal{H}_2$. We can construct $|\psi\rangle$ that belongs to $\mathcal{H}$ using tensor product:

$$|\psi\rangle = |\phi\rangle \otimes |\chi\rangle,$$

where $|\psi\rangle$ is a composite state.

Example:

Let

$$|\phi\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$|\chi\rangle = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},$$

Then

$$|\psi\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},$$

$$|\psi\rangle = \begin{pmatrix} 1\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} & 0\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \\ 0\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} & 1\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{pmatrix},$$

$$|\psi\rangle = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}.$$

Here, we can see that if $|\phi\rangle$ and $|\chi\rangle$ are 2×2 matrices then $|\psi\rangle$ is a 4×4 matrix.

Properties of Tensor product:

1. $|\phi\rangle \otimes (|\chi_1\rangle + |\chi_2\rangle) = |\phi\rangle \otimes |\chi_1\rangle + |\phi\rangle \otimes |\chi_2\rangle$
2. $(|\chi_1\rangle + |\chi_2\rangle) \otimes |\phi\rangle = |\chi_1\rangle \otimes |\phi\rangle + |\chi_2\rangle \otimes |\phi\rangle$
3. $|\phi\rangle \otimes (\alpha|\chi\rangle) = \alpha|\phi\rangle \otimes |\chi\rangle$
4. $|\phi\rangle \otimes 0 = 0 \otimes |\phi\rangle = 0$
5. $(|\phi\rangle \otimes |\chi\rangle)^\dagger = |\phi\rangle^\dagger \otimes |\chi\rangle^\dagger$

Note: $|\phi\rangle \otimes |\chi\rangle = |\phi\rangle|\chi\rangle = |\phi\chi\rangle$

2.6 Partial Trace

Basic idea behind the partial trace is to obtain the density operator for one of the subsystem alone. If our system is made up of two or more individual systems,then the complete system is known as a composite system. Density operator plays a crucial role in the characterization of such system.

The density operator is an excellent tool for describing and manipulating the states of subsystems. Let us considered a composite system where Bob has one part of the system and Alice has other part of the system and they move in opposite direction. The complete state of the system carries information about both subsystems, but Alice who is very far away form Bob, can't know about Bob's state unless they contact each other. Let $\hat{\rho}$ be the density operator of composite system.

We need a way to take the density operator for the entire system and reduce it down to a density operator that just carries information of Alice's state. We can do this by calculating the partial trace of entire density operator with respect to Bob, which will give us Alice's density operator called reduced density operator.

$$\hat{\rho}_{Alice} = Tr_{Bob}\left[\hat{\rho}\right].$$

Similarly

$$\hat{\rho}_{Bob} = Tr_{Alice}\left[\hat{\rho}\right].$$

Example:

Let us call Alice as $A$and Bob as B for convenience.

$$|\beta_{10}\rangle = \frac{1}{\sqrt{2}}\left(|0_A\rangle|0_B\rangle - |1_A\rangle|1_B\rangle\right),$$

$$\hat{\rho} = |\beta_{10}\rangle\langle\beta_{10}|,$$

$$\hat{\rho} = \frac{1}{2}\left(|0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B| - |0_A\rangle|0_B\rangle\langle 1_A|\langle 1_B| - |1_A\rangle|1_B\rangle\langle 0_A|\langle 0_B| + |1_A\rangle|1_B\rangle\langle 1_A|\langle 1_B|\right).$$

Now we are calculating partial trace with respect to Bob, this will give us the state of Alice alone.

$$\hat{\rho}_A = Tr_B\left[\hat{\rho}\right],$$

$$\hat{\rho}_A = \langle 0_B|\hat{\rho}|0_B\rangle + \langle 1_B|\hat{\rho}|1_B\rangle,$$

$$\hat{\rho}_A = \frac{1}{2}\left(|0_A\rangle|\langle 0_A| + |1_A\rangle\langle 1_A|\right).$$

This $\hat{\rho}_A$ is the state of Alice alone, it carries information only about Alice.

Where

$$Tr\left[\hat{\rho}_A^2\right] = \frac{1}{2} < 1.$$

This shows that state of Alice is completely mixed state.

2.7 Measurements

In classical mechanics, we can consider ideal measurements that have no effect on system. However, in quantum mechanics, generic measurements have a non trivial effect on systems - destroying its state in an irreversible way. When we perform a quantum measurement, the state of quantum system collapses. It tells us what is the probability of finding any state and what will be the post measurement state of system. Consider a two state quantum system represented by

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle.$$

Measurement will push the quantum system either into the state $|0\rangle$ with probability $|\alpha|^2$ or state $|1\rangle$ with probability $|\beta|^2$. This shows that after the measurements, original state of system becomes lost permanently. These are what is known as projective, Strong or von Neumann measurements.

2.7.1 Projective Measurement

The basic idea behind the projective measurement is that the state of a quantum system is the superposition of mutually exclusive events (events which do not occur at the same time) or states. We can think of an atom, it may have ground state $|g\rangle$ or excited state $|e\rangle$ such that $|g\rangle$ and $|e\rangle$ are two mutually exclusive states. In this case, to know the state of the system we can use projective measurements. For projective measurement, first we need to construct operators called projectors.

We know, in quantum mechanics an observable is represented by Hermitian operator and any Hermitian operator can be written as a sum of outer product of eigenstates weighted with eigenvalues. This sum is known as spectral decomposition or eigenstate decomposition of the operator. Let the observable be $\hat{O}$:

$$\hat{O} = \sum_i \lambda_i \hat{P}_i,$$

where $\hat{P}_i = |i\rangle|\langle i|$ is the projector on ith state.

Properties of projectors:

Properties of projectors are as follows.

1. Projectors are Hermitian

$$\hat{P}_i^\dagger = \hat{P}_i.$$

2. Projectors are orthogonal

$$\hat{P}_i \hat{P}_j = \delta_{ij} \hat{P}_i.$$

3. Projectors are idempotent

$$\hat{P}_i^2 = \hat{P}_i.$$

4. Projectors obey completeness relation

$$\sum_i \hat{P}_i = \hat{I}.$$

- Sum of two projectors is projector if they are mutually orthogonal.

$$\hat{P} = \hat{P}_1 + \hat{P}_2.$$

P is projector if

$$\hat{P}_1\hat{P}_2 = \hat{P}_2\hat{P}_1 = 0.$$

This condition ensures that P is idempotent.

- Product of two projectors is a projector if two projectors commute.

$$\hat{P} = \hat{P}_1\hat{P}_2.$$

$\hat{P}$ is projector, if

$$\hat{P}_1\hat{P}_2 - \hat{P}_2\hat{P}_1 = 0.$$

This condition ensures that P is Hermitian.

Case 1

When state of quantum system is represented by a ket $|\psi\rangle$. Probability of finding any state $|m\rangle$ will be

$$p\,(m) = \langle\psi|\hat{P}_m|\psi\rangle,$$

$$p\,(m) = \langle\psi|m\rangle\langle m|\psi\rangle,$$

$$p\,(m) = |\langle m|\psi\rangle|^2.$$

Post measurement state will be

$$|\psi'\rangle = \frac{\hat{P}_m|\psi\rangle}{\sqrt{p\,(m)}}$$

Post measurement state is always normalized.

Example 1

Let $|\psi\rangle$ be the state of quantum system such that:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle,$$

here $\hat{P}_1$ and $\hat{P}_2$ are two projectors

$$\hat{P}_0 = |0\rangle\langle 0|,$$

$$\hat{P}_1 = |1\rangle\langle 1|.$$

Probability of finding a quantum system in state $|0\rangle$ can be calculated as

$$p\left(0\right) = \langle\psi|\hat{P}_0|\psi\rangle = |\alpha|^2.$$

Post measurement state is

$$|\psi'\rangle = \frac{\hat{P}_0|\psi\rangle}{\sqrt{p\left(0\right)}} = |0\rangle.$$

Example 2
Let us considered a composite system in state $|\beta_{10}\rangle$

$$|\beta_{10}\rangle = \frac{1}{\sqrt{2}}\left(|0_A\rangle|0_B\rangle - |1_A\rangle|1_B\rangle\right).$$

Here $\hat{P}_0^A$ and $\hat{P}_1^A$ are two projectors to project the state of system A such that:

$$\hat{P}_0^A = \hat{P}_0 \otimes \hat{I},$$

$$\hat{P}_1^A = \hat{P}_1 \otimes \hat{I}.$$

Similarly $\hat{P}_0^B$ and $\hat{P}_1^B$ are two projectors to project the state of system B such that:

$$\hat{P}_0^B = \hat{I} \otimes \hat{P}_0,$$

$$\hat{P}_1^B = \hat{I} \otimes \hat{P}_1,$$

The probability of finding system A in state $|0_A\rangle$ can be calculated as

$$p(0_A) = \langle\beta_{10}|\hat{P}_0^A|\beta_{10}\rangle,$$

$$p(0_A) = \langle\beta_{10}|\hat{P}_0 \otimes \hat{I}\left[\frac{1}{\sqrt{2}}\left(|0_A\rangle|0_B\rangle - |1_A\rangle|1_B\rangle\right)\right],$$

$$p(0_A) = \langle\beta_{10}|\frac{1}{\sqrt{2}}|0_A\rangle|0_B\rangle,$$

$$p(0_A) = \frac{1}{2}.$$

Post measurement state is

$$|\beta_{10}'\rangle = \frac{\hat{P}_0^A|\beta_{10}\rangle}{\sqrt{p(0_A)}} = |0_A\rangle|0_B\rangle.$$

Case 2

When state of quantum system is represented by density operator $\hat{\rho}$. Probability of finding any state $|m\rangle$ will be

$$p\left(m\right) = Tr\left[\hat{P}_m \hat{\rho} \hat{P}_m^\dagger\right].$$

Using cyclic property of trace

$$p\left(m\right) = Tr\left[\hat{P}_m^\dagger \hat{P}_m \hat{\rho}\right],$$

$$\hat{P}_m \hat{P}_m^\dagger = \hat{P}_m \hat{P}_m = \hat{P}_m,$$

$$p\left(m\right) = Tr\left[\hat{P}_m \hat{\rho}\right].$$

Post measurement state will be

$$\hat{\rho}' = \frac{\hat{P}_m \hat{\rho} \hat{P}_m^\dagger}{Tr\left[\hat{P}_m \hat{\rho}\right]}.$$

Post measurement state is always normalized.

Example 1

Let $|\psi\rangle$ be the state of quantum system such that:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle.$$

Density operator $\hat{\rho}$ can be written as

$$\hat{\rho} = |\psi\rangle\langle\psi|,$$

$$\hat{\rho} = |\alpha|^2|0\rangle\langle 0| + |\alpha^*\beta||1\rangle\langle 0| + |\alpha\beta^*||0\rangle\langle 1| + |\beta|^2|1\rangle\langle 1|,$$

$\hat{P}_1$ and $\hat{P}_2$ are two projectors

$$\hat{P}_0 = |0\rangle\langle 0|,$$

$$\hat{P}_1 = |1\rangle\langle 1|.$$

Probability of finding state $|0\rangle$ will be

$$p\left(0\right) = Tr\left[\hat{P}_0 \hat{\rho}\right],$$

$$p\left(0\right) = Tr\left[|0\rangle\langle 0|\left(|\alpha|^2|0\rangle\langle 0| + |\alpha^*\beta||1\rangle\langle 0| + |\alpha\beta^*||0\rangle\langle 1| + |\beta|^2|1\rangle\langle 1|\right)\right],$$

$$p(0) = Tr\left[|\alpha|^2|0\rangle\langle 0| + |\alpha\beta^*||0\rangle\langle 1|\right],$$

$$p(0) = \langle 0|\left[|\alpha|^2|0\rangle\langle 0| + |\alpha\beta^*||0\rangle\langle 1|\right]|0\rangle + \langle 1|\left[|\alpha|^2|0\rangle\langle 0| + |\alpha\beta^*||0\rangle\langle 1|\right]|1\rangle,$$

$$p(0) = |\alpha|^2,$$

Post measurement state is give by

$$\hat{\rho}' = \frac{\hat{P}_0\hat{\rho}\hat{P}_0^\dagger}{Tr\left[\hat{P}_m\hat{\rho}\right]}.$$

Post measurement state will be

$$\hat{\rho}' = \frac{|0\rangle\langle 0|\left(|\alpha|^2|0\rangle\langle 0| + |\alpha^*\beta||1\rangle\langle 0| + |\alpha\beta^*||0\rangle\langle 1| + |\beta|^2|1\rangle\langle 1|\right)|0\rangle\langle 0|}{|\alpha|^2},$$

$$\hat{\rho}' = \frac{|\alpha|^2|0\rangle\langle 0|}{|\alpha|^2},$$

$$\hat{\rho}' = |0\rangle\langle 0|,$$

Example 2

Let us considered a composite system $|\beta_{10}\rangle$

$$|\beta_{10}\rangle = \frac{1}{\sqrt{2}}\left(|0_A\rangle|0_B\rangle - |1_A\rangle|1_B\rangle\right).$$

Density operator $\hat{\rho}_{AB}$ can be written as

$$\hat{\rho}_{AB} = \frac{1}{2}\left(|0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B| - |0_A\rangle|0_B\rangle\langle 1_A|\langle 1_B| - |1_A\rangle|1_B\rangle\langle 0_A|\langle 0_B| + |1_A\rangle|1_B\rangle\langle 1_A|\langle 1_B|\right).$$

Here $\hat{P}_0^A$ and $\hat{P}_1^A$ are two projectors to project the state of system A such that:

$$\hat{P}_0^A = \hat{P}_0 \otimes \hat{I},$$

$$\hat{P}_1^A = \hat{P}_1 \otimes \hat{I}.$$

Similarly $\hat{P}_0^B$ and $\hat{P}_1^B$ are two projectors to project the state of system B such that:

$$\hat{P}_0^B = \hat{I} \otimes \hat{P}_0,$$

$$\hat{P}_1^B = \hat{I} \otimes \hat{P}_1.$$

Probability of finding state $|0_A\rangle$ will be

$$p\left(0_A\right) = Tr\left[\hat{P}_0^A \hat{\rho}_{AB}\right]$$

$$\Rightarrow p\left(0_A\right) = Tr\left[\frac{1}{2}\left(|0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B| - |0_A\rangle|0_B\rangle\langle 1_A|\langle 1_B|\right)\right]$$

$$\begin{aligned} p\left(0_A\right) =& \langle 0_A|\langle 0_B|\left[\frac{1}{2}\left(|0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B| - |0_A\rangle|0_B\rangle\langle 1_A|\langle 1_B|\right)\right]|0_A\rangle|0_B\rangle \\ &+\langle 0_A|\langle 1_B|\left[\frac{1}{2}\left(|0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B| - |0_A\rangle|0_B\rangle\langle 1_A|\langle 1_B|\right)\right]|0_A\rangle|1_B\rangle \\ &+\langle 1_A|\langle 0_B|\left[\frac{1}{2}\left(|0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B| - |0_A\rangle|0_B\rangle\langle 1_A|\langle 1_B|\right)\right]|1_A\rangle|0_B\rangle \\ &+\langle 1_A|\langle 1_B|\left[\frac{1}{2}\left(|0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B| - |0_A\rangle|0_B\rangle\langle 1_A|\langle 1_B|\right)\right]|1_A\rangle|1_B\rangle \end{aligned}$$

$$p\left(0_A\right) = \frac{1}{2}$$

Post measurement state will be

$$\hat{\rho}'_{AB} = \frac{\hat{P}_0^A \hat{\rho}_{AB} \hat{P}_0^{A\dagger}}{Tr\left[\hat{P}_0^A \hat{\rho}_{AB}\right]},$$

because

$$\hat{P}_0^{A\dagger} = \left(\hat{P}_0 \otimes \hat{I}\right)^\dagger = \hat{P}_0^\dagger \otimes \hat{I} = \hat{P}_0 \otimes \hat{I},$$

$$\Rightarrow \hat{P}_0^A \hat{\rho}_{AB} \hat{P}_0^{A\dagger} = \frac{1}{2}|0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B|,$$

so

$$\hat{\rho}'_{AB} = \frac{\frac{1}{2}|0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B|}{\frac{1}{2}},$$

$$\hat{\rho}'_{AB} = |0_A\rangle|0_B\rangle\langle 0_A|\langle 0_B|.$$

Other than projective/strong measurements, we can also perform weak measurements [30]. Weak measurements give more general results than projective measurements. In many practicals situations, state of quantum system may not be orthogonal. In such situation, we can use another technique of measurements known as generalized measurements. We will not discuss in detail these measurement techniques here.

2.8 Partition Function

The partition function, denoted by Z plays the role of generating function in statistical mechanics that provides a way to calculate thermodynamic properties of a system from its microscopic (particle-level) description. It is defined as the sum of the Boltzmann weights of all possible microstates of the system at a given temperature, and provides a bridge between the microscopic and macroscopic descriptions of the system. Mathematically, the partition function is defined as

$$Z = \sum_n e^{-\beta E_n},$$

where $\beta = {}^1/_{k_B T}$, E_n is the energy of the nth microstate, k_B is the Boltzmann constant, and T is the temperature. The sum is taken over all possible microstates of the system, and the Boltzmann weight for each microstate is given by the exponential term. The partition function is an important tool for calculating thermodynamic quantities such as the free energy, average energy, entropy, and heat capacity.

Using the partition function, thermodynamic quantities can be calculated without considering the details of each individual microstate. This is particularly useful in many-particle systems where the number of possible microstates can be very large, making a direct calculation of thermodynamic properties difficult.

2.9 Thermodynamical Quantities

2.9.1 Free Energy

Energy available in a system to perform some useful work is know as free energy. There are two common forms of free energy, Helmholtz free energy A and Gibbs free energy G.

Helmholtz free energy is defined as

$$A = U - TS,$$

where T is temperature, S is entropy and U is internal energy.

In term of partition function

$$A = -k_B T ln Z. \tag{2.12}$$

2.9.2 Average Energy

From Eq. (2.4), average energy can be calculated as

$$E_{avg} = \langle \hat{H} \rangle,$$

$$E_{avg} = Tr\left[\hat{\rho}\hat{H}\right].$$

If the system is in contact with a thermal bath,

$$\hat{\rho} = \frac{1}{Z}\sum_{n=0}^{\infty} e^{-\beta E_n}|\psi_n\rangle\langle\psi_n|,$$

therefore

$$E_{avg} = Tr\left[\frac{1}{Z}\sum_{n=0}^{\infty} e^{-\beta E_n}|\psi_n\rangle\langle\psi_n|\hat{H}\right].$$

Taking trace over the energy eigenstates $|\psi_m\rangle$

$$E_{avg} = \sum_{m=0}^{\infty} \langle\psi_m|\left(\frac{1}{Z}\sum_{n=0}^{\infty} e^{-\beta E_n}|\psi_n\rangle\langle\psi_n|\hat{H}\right)|\psi_m\rangle,$$

$$E_{avg} = \frac{1}{Z}\sum_{m,n=0}^{\infty} e^{-\beta E_n}\langle\psi_m|\psi_n\rangle\langle\psi_n|\hat{H}|\psi_m\rangle,$$

since

$$\hat{H}|\psi_m\rangle = E_m|\psi_m\rangle,$$

$$\Rightarrow E_{avg} = \frac{1}{Z}\sum_{m,n}^{\infty} e^{-\beta E_n}\langle\psi_m|\psi_n\rangle\langle\psi_n|E_m|\psi_m\rangle,$$

$$E_{avg} = \frac{1}{Z}\sum_{m,n}^{\infty} E_m e^{-\beta E_n}\langle\psi_m|\psi_n\rangle\langle\psi_n|\psi_m\rangle,$$

using orthonormality condition,

$$E_{avg} = \frac{1}{Z}\sum_{n}^{\infty} E_n e^{-\beta E_n}.$$

But we know

$$Z = \sum_{n}^{\infty} e^{-\beta E_n},$$

$$\frac{\partial}{\partial \beta} Z = -\sum_{n}^{\infty} E_n e^{-\beta E_n}.$$

So E_{avg} will be

$$E_{avg} = \frac{1}{Z}\left(-\frac{\partial}{\partial \beta} Z\right),$$

$$\Rightarrow E_{avg} = -\frac{\partial}{\partial \beta}\left(lnZ\right). \tag{2.13}$$

2.9.3 Entropy

Entropy is directly related to the number of ways to arrange the gas atoms (microstate) without changing the macrostate. If Ω are the number of microstates,

$$S = k_B \ln \Omega,$$

If we assume that all states are equally probable. Let p_i be the probability of an *ith* state then p_i

$$p_i = \frac{1}{\Omega},$$

$$S = k_B ln \frac{1}{p_i}.$$

So we can write the above equation as

$$S = k_B \sum_i p_i ln \frac{1}{p_i}$$

$$S = -k_B \sum_i p_i ln p_i \tag{2.14}$$

This is the formula for Gibbs entropy. In quantum mechanics, the counter part of Gibbs entropy is von Neumann entropy.

Let density operator $\hat{\rho}$ is diagonalized,

$$\hat{\rho} = \sum_{n=0}^{\infty} p_n |\psi_n\rangle\langle\psi_n|,$$

if $\hat{\rho}$ is diagonalized then $ln\left(\hat{\rho}\right)$ can be calculated as

$$ln\left(\hat{\rho}\right) = \sum_{n=0}^{\infty} ln p_n |\psi_n\rangle\langle\psi_n|,$$

we can write

$$\hat{\rho} ln\left(\hat{\rho}\right) = \sum_{n=0}^{\infty} p_n|\psi_n\rangle\langle\psi_n| \sum_{m=0}^{\infty} lnp_m|\psi_m\rangle\langle\psi_m|,$$

$$\hat{\rho} ln\left(\hat{\rho}\right) = \sum_{n,m=0}^{\infty} p_n lnp_m|\psi_n\rangle\langle\psi_n|\psi_m\rangle\langle\psi_m|,$$

using orthonormality condition

$$\hat{\rho} ln\left(\hat{\rho}\right) = \sum_{n=0}^{\infty} p_n lnp_n|\psi_n\rangle\langle\psi_n|.$$

Taking trace over the energy eigenstates $|\psi_m\rangle$,

$$Tr\left[\hat{\rho} ln\left(\hat{\rho}\right)\right] = \sum_{m=0}^{\infty} \langle\psi_m| \left(\sum_{n=0}^{\infty} p_n lnp_n|\psi_n\rangle\langle\psi_n|\right)|\psi_m\rangle,$$

$$Tr\left[\hat{\rho} ln\left(\hat{\rho}\right)\right] = \sum_{m,n=0}^{\infty} p_n lnp_n\langle\psi_m|\psi_n\rangle\langle\psi_n|\psi_m\rangle,$$

using orthonormality condition again

$$Tr\left[\hat{\rho} ln\left(\hat{\rho}\right)\right] = \sum_{n=0}^{\infty} p_n lnp_n.$$

Using above in Eq. (2.14)

$$\boldsymbol{S = -k_B Tr\left[\hat{\rho} ln \hat{\rho}\right]} \tag{2.15}$$

This is von Neumann entropy. If λ_i are the eigenvalues of density operator $\hat{\rho}$, then von Neumann can be written as

$$S = -k_B \sum_i \lambda_i ln \lambda_i$$

If our system is in contact with a thermal bath, then

$$\hat{\rho} = \frac{1}{Z}\sum_{n=0}^{\infty} e^{-\beta E_n}|\psi_n\rangle\langle\psi_n|,$$

$$\Rightarrow S = -k_B Tr\left[\frac{1}{Z}\sum_{n=0}^{\infty} e^{-\beta E_n}|\psi_n\rangle\langle\psi_n| ln\left(\frac{1}{Z}\sum_{m=0}^{\infty} e^{-\beta E_m}|\psi_m\rangle\langle\psi_m|\right)\right],$$

$$S = -k_B Tr\left[\frac{1}{Z}\sum_{n=0}^{\infty} e^{-\beta E_n} ln\left(\frac{1}{Z}\sum_{m=0}^{\infty} e^{-\beta E_m}\right)|\psi_n\rangle\langle\psi_n|\psi_m\rangle\langle\psi_m|\right],$$

using orthonormality condition

$$S=-k_BTr\left[\frac{1}{Z}\sum_{n=0}^{\infty}e^{-\beta E_n}ln\left(\frac{1}{Z}e^{-\beta E_n}\right)|\psi_n\rangle\langle\psi_n|\right],$$

$$S=-k_BTr\left[\frac{1}{Z}\sum_{n=0}^{\infty}e^{-\beta E_n}\left(lne^{-\beta E_n}\right)|\psi_n\rangle\langle\psi_n|-lnZ|\psi_n\rangle\langle\psi_n|\right],$$

$$S=-k_BTr\left[\frac{1}{Z}\sum_{n=0}^{\infty}e^{-\beta E_n}lne^{-\beta E_n}|\psi_n\rangle\langle\psi_n|-\frac{1}{Z}\sum_{n=0}^{\infty}e^{-\beta E_n}lnZ|\psi_n\rangle\langle\psi_n|\right],$$

$$S=-\beta k_BTr\left[\frac{1}{Z}\sum_{n}^{\infty}e^{-\beta E_n}\left(-E_n\right)|\psi_n\rangle\langle\psi_n|\right]+k_BTr\left[\frac{1}{Z}\sum_{n}^{\infty}e^{-\beta E_n}lnZ|\psi_n\rangle\langle\psi_n|\right],$$

$$S=-\beta k_BTr\left[\frac{1}{Z}\sum_{n=0}^{\infty}\frac{\partial}{\partial\beta}\left(e^{-\beta E_n}\right)|\psi_n\rangle\langle\psi_n|\right]+k_BTr\left[\frac{1}{Z}\sum_{n=0}^{\infty}e^{-\beta E_n}lnZ|\psi_n\rangle\langle\psi_n|\right],$$

$$S=\frac{-\beta k_B}{Z}\sum_{n=0}^{\infty}\frac{\partial}{\partial\beta}\left(e^{-\beta E_n}\right)+\frac{k_B}{Z}\sum_{n=0}^{\infty}e^{-\beta E_n}lnZ,$$

$$S=\frac{-\beta k_B}{Z}\frac{\partial}{\partial\beta}Z+\frac{k_B}{Z}ZlnZ,$$

$$S=-\beta k_B\frac{\partial}{\partial\beta}lnZ+k_BlnZ,$$

$$S=-\frac{1}{k_BT}k_B\frac{\partial}{\partial\left(1/k_BT\right)}lnZ+k_BlnZ,$$

$$S=\frac{T^2k_B}{T}\frac{\partial}{\partial T}lnZ+k_BlnZ,$$

$$S=k_BT\frac{\partial}{\partial T}lnZ+k_BlnZ.$$

Form Eq. (2.12)

$$A=-k_BTlnZ,$$

$$\frac{\partial A}{\partial T}=-k_BT\frac{\partial}{\partial T}lnZ-k_BlnZ.$$

Therefore, S will become

$$S=-\frac{\partial A}{\partial T}. \tag{2.16}$$

Chapter 3

Quantum Analysis of Harmonic Szilard Engine

The quantum Szilard engine is the extension of the classical version to quantum systems. A quantum version of Szilard's original atom-in-a-box model can be realized with 1-D non-relativistic quantum particle of mass m confined by a symmetric potential $V(q)$, q being the position of particle , to a finite region of space. The quantum dynamics can be describe by the Hamiltonian $\hat{H}$

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}),$$

where $V(\pm\infty) = \infty$.

Zurek studied quantum Szilard engine in detail for infinite square well potential [17]. By replacing the square well potential with harmonic oscillator potential, a more elegant model can be obtained that captures the same physical processes. The particle is taken to be in a thermal state bounded in the harmonic well. Then a thin barrier (modeled by a time dependent potential) is inserted quasi-statically at the center of the well and a strong projective measurement is performed on the particle to determine whether it is located to the right or left side of the partition. Demon can extract work from the setup with this information. We can consider the demon either as a quantum system itself with internal states that couples to the atom or as an external "observer". In both cases, the measurement collapses the wave function in a irreversible way.

For a particle having angular frequency ω trapped in harmonic well, Hamiltonian can be written as

$$\hat{H}_{in} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2, \tag{3.1}$$

where $V(\hat{q}) = \frac{1}{2}m\omega^2\hat{q}^2$.

For the quantum harmonic Szilard engine, we can determined exactly the partition function of the particle, and all the relevant thermodynamic quantities can be calculated analytically. In **Section-3.1**, an initial thermal state of particle is prepared bounded in a harmonic well. In **Section-3.2**, a Dirac delta potential barrier is inserted quasi-statically in the middle of the well, that modifies the quantum state of the particle. In **Secton-3.3**, demon localizes the particle to either left or the right side of the barrier by performing a quantum projective measurement [21] on the position of particle. In **Secton-3.4**, the demon extracts useful work from the system, when one particle quantum gas expands isothermally; second law of thermodynamics seems to violate. In **chapter 4,** we will treat the demon itself as a part of the system and explain why this is, in fact, not the case of the violation of the second law of thermodynamics.

3.1 Initial state

We have a particle of mass m bounded in a harmonic potential $V(q)$, hence the initial Hamiltonian from Eq. (3.1) can be written as

$$\hat{H}_{in} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2.$$

We want to calculate the energy eigenvalues and corresponding energy eigenstates of the above Hamiltonian.

There are many standard books which present the diagonalization of the above Hamiltonian, given in Eq. (3.1), so we can use those results directly.

Energy eigenvalues are

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{3.2}$$

Corresponding energy eigenstates in position space are

$$\psi_n(q) = \mathbb{H}_n(\alpha q)e^{-\alpha\frac{q^2}{2}}, \tag{3.3}$$

where $\alpha = \sqrt{\frac{m\omega}{\hbar}}$ and $\mathbb{H}_n(\alpha q)$ are Hermite polynomials.

3.1.1 Density Operator

As the initial state is mixed state (a thermal state) , the density operator for a mixed state from Eq. (2.1) can be written as

$$\hat{\rho}_{in} = \sum_{n=0}^{\infty} p_n|\psi_n\rangle\langle\psi_n|.$$

As our system is coupled to a thermal bath, so our system is in a canonical ensemble. The probability of *nth* state can be written as

$$p_n = \frac{e^{-\beta E_n}}{Z_{in}},$$

Initial State will be

$$\hat{\rho}_{in} = \frac{1}{Z_{in}} \sum_{n=0}^{\infty} e^{-\beta E_n} |\psi_n\rangle\langle\psi_n|.$$

From Eq. (3.2),

$$\hat{\rho}_{in} = \frac{1}{Z_{in}} \sum_{n=0}^{\infty} e^{-\beta(n+\frac{1}{2}\hbar\omega)} |\psi_n\rangle\langle\psi_n|. \tag{3.4}$$

Here p_n is the probability of nth pure state such that:

$$\sum_{n=0}^{\infty} p_n = 1.$$

3.1.2 Partition Function

For a valid density operator, trace of density operator must be equal to one.

$$Tr\left[\hat{\rho}_{in}\right] = 1,$$

$$Tr\left[\sum_{n=0}^{\infty} \frac{e^{-\beta E_n}}{Z_{in}} |\psi_n\rangle\langle\psi_n|\right] = 1,$$

$$\sum_{m=0}^{\infty} \langle\psi_m| \left(\sum_{n=0}^{\infty} \frac{e^{-\beta E_n}}{Z_{in}} |\psi_n\rangle\langle\psi_n|\right) |\psi_m\rangle = 1,$$

$$\frac{1}{Z_{in}} \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta E_n} \langle\psi_m|\psi_n\rangle\langle\psi_n|\psi_m\rangle = 1,$$

using orthonormality condition

$$\frac{1}{Z_{in}} \sum_{n=0}^{\infty} e^{-\beta E_n} = 1,$$

$$Z_{in} = \sum_{n=0}^{\infty} e^{-\beta E_n}.$$

From Eq. (3.2),

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega.$$

$$\Rightarrow Z_{in} = \sum_{n=0}^{\infty} e^{-\beta(n+\frac{1}{2})\hbar\omega}.$$

We can see this is the geometric series , with initial term a_1 and common ratio r :

$$a_1 = e^{-\frac{\beta\hbar\omega}{2}}, r = e^{-\beta\hbar\omega}.$$

Sum of geometric series can be written as

$$sum = a_1 \frac{(1-r^n)}{(1-r)},$$

when $|r| << 1$ then sum reduces to

$$sum = a_1 \frac{1}{(1-r)}$$

Now we can write the partition function utilizing sum of geometric series

$$Z_{in} = \frac{e^{-\frac{\beta\hbar\omega}{2}}}{1-e^{-\beta\hbar\omega}},$$

$$Z_{in} = \frac{1}{2} cosech(\frac{\beta\hbar\omega}{2}). \tag{3.5}$$

This is the partition function of our system in the initial state. Partition function acts as a generating function. All thermodynamical quantities can be determined using this function.

3.1.3 Thermodynamical Quantities

3.1.3.1 Helmholtz Free Energy

Let us denote the initial Helmholtz free energy by A_{in}. From Eq. (2.12),

$$A_{in} = -k_B T ln Z_{in},$$

using Eq. (3.5)

$$A_{in} = -k_B T ln \left[\frac{1}{2} cosech(\frac{\beta\hbar\omega}{2})\right],$$

$$A_{in} = k_B T ln \left[2 sinh(\frac{\beta\hbar\omega}{2})\right]. \tag{3.6}$$

3.1.3.2 Average Energy

Let us denote the initial average energy by E_{in}. From Eq. (2.13),

$$E_{in} = -\frac{\partial}{\partial\beta} lnZ_{in},$$

using Eq. (3.5)

$$E_{in} = -\frac{\partial}{\partial\beta} ln\left[\frac{1}{2}sinh(\frac{\beta\hbar\omega}{2})\right],$$

$$E_{in} = \frac{1}{2}\hbar\omega\left[coth\left(\frac{\beta\hbar\omega}{2}\right)\right]. \tag{3.7}$$

Low temperature Limit:
When $T \to 0 \Rightarrow \beta \to \infty$
then

$$\underset{T\to\infty}{E_{in}} = \lim_{\beta\to\infty}\left[\frac{1}{2}\hbar\omega coth\left(\frac{\beta\hbar\omega}{2}\right)\right],$$

$$\underset{T\to\infty}{E_{in}} = \frac{1}{2}\hbar\omega.$$

From the above equation we can see that as temperature approaches *zero* Kelvin, particle is in the ground state.

High Temperature Limit:
When $T \to \infty \Rightarrow \beta \to 0$
then

$$\underset{T\to\infty}{E_{in}} = \lim_{\beta\to 0}\frac{1}{2}\hbar\omega\left[coth\left(\frac{\beta\hbar\omega}{2}\right)\right],$$

here we can use the Taylor expansion of $coth\left(\frac{\beta\hbar\omega}{2}\right)$

$$coth\left(\frac{\beta\hbar\omega}{2}\right) = \frac{2}{\beta\hbar\omega} + \frac{\beta\hbar\omega}{6} + ...,$$

we will keep only the first term:

$$\underset{T\to\infty}{E_{in}} = \frac{1}{2}\hbar\omega\left(\frac{2}{\beta\hbar\omega} + ...\right),$$

$$\underset{T\to\infty}{E_{in}} = \frac{1}{2}\hbar\omega\frac{2}{\beta\hbar\omega},$$

$$\underset{T\to\infty}{E_{in}} = k_B T.$$

From the above equation we can see that this is consistent with equipartition energy theorem. This simply means that if we give energy to N numbers of gas particle, then each degree of freedom appearing quadratically in total energy has an equal contribution in total energy i.e. average energy of single quadratic degrees of freedom for each particle will be

$$\frac{1}{2}k_BT.$$

Here, we have a quantum system of a single particle in one dimension with two degrees of freedom i.e. position q and momentum p to describe the dynamics of the system. So,

$$E_n\left(q,p\right) = 2\left(\frac{1}{2}k_BT\right) = k_BT,$$

hence in our case, when we have two degrees of freedom,

$$E_{in} = k_BT.$$

3.1.3.3 Entropy

Since our system is in a mixed state, so we can represent it in terms of density operator and the entropy of such a system can be written from Eq. (2.15) as

$$S_{in} = -Tr\left(\hat{\rho}_{in} ln \hat{\rho}_{in}\right).$$

But from Eq. (2.16), above relation can also be written as

$$S_{in} = -\frac{d}{dT}A_{in}.$$

We can calculate the entropy using the relation of initial Helmholtz free energy from Eq. (3.6)

$$S_{in} = -\frac{d}{dT}\left\{k_BTln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right]\right\},$$

$$S_{in} = -\frac{d}{dT}\left\{k_BTln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right]\right\},$$

$$S_{in} = -k_Bln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right] - k_BT\frac{d}{dT}ln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right],$$

$$S_{in} = -k_Bln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right] - k_BT\frac{2cosh\left(\frac{\beta\hbar\omega}{2}\right)}{2sinh\left(\frac{\beta\hbar\omega}{2}\right)}\left(-\frac{\beta\hbar\omega}{2T}\right),$$

$$S_{in} = -k_Bln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right] + k_B\left[\frac{\beta\hbar\omega}{2}coth\left(\frac{\beta\hbar\omega}{2}\right)\right],$$

$$S_{in} = k_B\left\{\frac{\beta\hbar\omega}{2}coth\left(\frac{\beta\hbar\omega}{2}\right) - ln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right]\right\}. \tag{3.8}$$

High Temperature Limit:
$T \to \infty \Rightarrow \beta \to 0$,

$$\underset{T\to\infty}{S_{in}} = \lim_{T\to\infty} k_B \left\{ \frac{\beta\hbar\omega}{2} coth\left(\frac{\beta\hbar\omega}{2}\right) - ln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right]\right\},$$

$$\underset{T\to\infty}{S_{in}} = \lim_{T\to\infty} k_B \left[\frac{\beta\hbar\omega}{2}\frac{cosh\left(\frac{\beta\hbar\omega}{2}\right)}{sinh\left(\frac{\beta\hbar\omega}{2}\right)}\right] - \lim_{T\to\infty} k_B ln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right],$$

$$\underset{T\to\infty}{S_{in}} = k_B\left[1\right] - \lim_{T\to\infty} k_B ln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right],$$

$$\underset{T\to\infty}{S_{in}} = k_B\left\{1 - \lim_{T\to\infty} ln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right]\right\},$$

$$\underset{T\to\infty}{S_{in}} \approx -k_B\left\{\lim_{T\to\infty} ln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right]\right\},$$

As $\frac{\beta\hbar\omega}{2} \to 0$ when $T \to \infty$, we can use the Taylor expansion

$$\underset{T\to\infty}{S_{in}} = -k_B \lim_{T\to\infty} ln\left[2\left(\frac{\beta\hbar\omega}{2} + ...\right)\right],$$

$$\underset{T\to\infty}{S_{in}} = -k_B \lim_{T\to\infty} \left[ln\left(\beta\hbar\omega\right)\right],$$

$$\underset{T\to\infty}{S_{in}} = k_B \lim_{T\to\infty} \left[ln\left(\frac{1}{\beta\hbar\omega}\right)\right],$$

we can write the above expression for high temperature as

$$S_{in} = k_B ln\left(\frac{k_B T}{\hbar\omega}\right). \tag{3.9}$$

Low Temperature Limit:
$T \to 0 \Rightarrow \beta \to \infty$,

$$\underset{T\to 0}{S_{in}} = \lim_{T\to 0} k_B \left\{ \frac{\beta\hbar\omega}{2} coth\left(\frac{\beta\hbar\omega}{2}\right) - ln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right]\right\},$$

$$\underset{T\to 0}{S_{in}} = \lim_{T\to 0} k_B \left(\frac{\beta\hbar\omega}{2}\right)\left[coth\left(\frac{\beta\hbar\omega}{2}\right)\right] - k_B ln\left(2\frac{e^{\frac{\beta\hbar\omega}{2}} - e^{-\frac{\beta\hbar\omega}{2}}}{2}\right),$$

$$\underset{T\to 0}{S_{in}} = k_B\left(\lim_{T\to 0}\frac{\beta\hbar\omega}{2}\right)\left[\lim_{T\to 0} coth\left(\frac{\beta\hbar\omega}{2}\right)\right] - k_B \lim_{T\to 0}\left[ln\left(e^{\frac{\beta\hbar\omega}{2}} - e^{-\frac{\beta\hbar\omega}{2}}\right)\right].$$

Since

$$\lim_{T\to 0} coth\left(\frac{\beta\hbar\omega}{2}\right) = 1,$$

and

$$\lim_{T\to 0}\left[ln\left(e^{\frac{\beta\hbar\omega}{2}}-e^{-\frac{\beta\hbar\omega}{2}}\right)\right]=ln\left(\lim_{T\to 0} e^{\frac{\beta\hbar\omega}{2}}-\lim_{T\to 0} e^{-\frac{\beta\hbar\omega}{2}}\right),$$

$$\lim_{T\to 0}\left[ln\left(e^{\frac{\beta\hbar\omega}{2}}-e^{-\frac{\beta\hbar\omega}{2}}\right)\right]=ln\left(\lim_{T\to 0} e^{\frac{\beta\hbar\omega}{2}}\right),$$

$$\lim_{T\to 0}\left[ln\left(e^{\frac{\beta\hbar\omega}{2}}-e^{-\frac{\beta\hbar\omega}{2}}\right)\right]=\lim_{T\to 0}\left[ln\left(e^{\frac{\beta\hbar\omega}{2}}\right)\right].$$

So,

$$\underset{T\to 0}{S_{in}}=k_B\left(\lim_{T\to 0}\frac{\beta\hbar\omega}{2}\right)-k_B\lim_{T\to 0}\left[ln\left(e^{\frac{\beta\hbar\omega}{2}}\right)\right],$$

$$\underset{T\to 0}{S_{in}}=k_B\left(\lim_{T\to 0}\frac{\beta\hbar\omega}{2}\right)-k_B\lim_{T\to 0}\left(\frac{\beta\hbar\omega}{2}lne\right),$$

$$\underset{T\to 0}{S_{in}}=k_B\left(\lim_{T\to 0}\frac{\beta\hbar\omega}{2}\right)-k_B\lim_{T\to 0}\left(\frac{\beta\hbar\omega}{2}\right),$$

$$\underset{T\to 0}{S_{in}}=k_B\lim_{T\to 0}\left(\frac{\beta\hbar\omega}{2}-\frac{\beta\hbar\omega}{2}\right),$$

$$\underset{T\to 0}{S_{in}}=k_B\lim_{T\to 0}(0).$$

So, we can write the above expression in the low temperature limit as

$$S_{in}=0. \tag{3.10}$$

Eq. (3.10) is consistent with the **third law of thermodynamics** as expected. This law states that "for an isolated system entropy is always zero at absolute zero temperature, if there is a unique ground state".

3.2 Barrier Insertion

An infinite but thin potential barrier at $q=0$ is inserted quasi-statically in order to localize the particle to the right or left side of the harmonic potential. Hence, Hamiltonian will change to $\hat{H}_{\perp}$

$$\hat{H}_{\perp}=\frac{\hat{p}^2}{2m}+\frac{1}{2}m\omega^2\hat{q}^2+\hat{V}_{\perp}(q). \tag{3.11}$$

3.2.1 Shape of Barrier

Now we have to determine $\hat{V}_{\perp}(q)$ by keeping in mind that it is zero everywhere except at $q = 0$. Also we must construct $\hat{V}_{\perp}(q)$ in such a way that its strength increases with time.

We choose ε to be a small number, and α is a parameter which may or may not be time dependent in general. But we will take this as a time dependent parameter as we need $\hat{V}_{\perp}$ to be time dependent. Although $\hat{V}_{\perp}$ is infinite at $q = 0$ but its integral from $-\infty$ to ∞ must be finite.

$$\int_{-\infty}^{\infty} \hat{V}_{\perp}(q)dq = \int_{-\infty}^{-\varepsilon} \hat{V}_{\perp}(q)dq + \int_{-\varepsilon}^{+\varepsilon} \hat{V}_{\perp}(q)dq + \int_{+\varepsilon}^{-\infty} \hat{V}_{\perp}(q)dq,$$

$$\int_{-\infty}^{\infty} \hat{V}_{\perp}(q)dq = \cancelto{0}{\int_{-\infty}^{-\varepsilon} \hat{V}_{\perp}(q)dq} + \int_{-\varepsilon}^{+\varepsilon} \hat{V}_{\perp}(q)dq + \cancelto{0}{\int_{+\varepsilon}^{-\infty} \hat{V}_{\perp}(q)dq},$$

$$\int_{-\infty}^{\infty} \hat{V}_{\perp}(q)dq = \int_{-\varepsilon}^{+\varepsilon} \frac{\alpha(t)}{\varepsilon}dq,$$

$$\int_{-\infty}^{\infty} \hat{V}_{\perp}(q)dq = \frac{\alpha(t)}{\varepsilon}\left[\int_{-\varepsilon}^{+\varepsilon} dq\right],$$

$$\int_{-\infty}^{\infty} \hat{V}_{\perp}(q)dq = \frac{\alpha(t)}{\varepsilon}\left[2\varepsilon\right],$$

$$\int_{-\infty}^{\infty} \hat{V}_{\perp}(q)dq = 2\alpha(t).$$

By virtue of Dirac delta function , we can write $\hat{V}_{\perp}$ as

$$\hat{V}_{\perp} = 2\alpha(t)\delta(q-0),$$

at $q = 0$, above equation becomes

$$\int_{-\infty}^{\infty} \hat{V}_{\perp}(q)dq = 2\alpha(t).$$

We can ignore the factor of 2 as it has no physical significance, so we can take $\hat{V}_{\perp}$ finally in the form given below:

$$\hat{V}_{\perp} = \alpha(t)\delta(q-0).$$

Hence, the Hamiltonian after barrier insertion at $q = 0$, we have called $\hat{H}_{\perp}$ can be written as

$$\hat{H}_{\perp} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 + \alpha(t)\delta(q-0).$$

We want to prevent the particle to tunnel through the barrier at later times, hence

$$\begin{cases} \alpha(t) = 0 & t \to -\infty \\ \alpha(t) = \infty & t \to +\infty \end{cases}.$$

We want to insert the barrier adiabatically, the slowness condition can be imposed as

$$|\frac{\dot{\alpha}}{\alpha}| << \omega,$$

where ω is the frequency of particle's oscillations in harmonic potential while$|\frac{\dot{\alpha}}{\alpha}|$ is the rate at which barrier is inserted.

This condition allows us to evaluate the wave function adiabatically, ensuring that system is consistently in thermal equilibrium with the bath at temperature T.

3.2.2 Effect of Barrier Insertion

Let the eigenstates of $\hat{H}_{\perp}$ be $|\psi_n^{\alpha}\rangle$, α in superscript represents that eigenstates are instantaneous. With the passage of time eignestates changes and their corresponding eigenvalues E_n^{α} also change. We are not interested in the instantaneous values, our main focus is when the barrier is fully inserted i.e $t \to +\infty$

To compute the instantaneous eigenstates $|\psi_n^{\alpha}\rangle$ and instantaneous eigenvalues E_n^{α}, Schrodinger wave equation can be written as

$$\hat{H}_{\perp}\psi_n^{\alpha}(q) = E_n^{\alpha}\psi_n^{\alpha}(q),$$

$$\left[\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 + \alpha(t)\delta(q-0)\right]\psi_n^{\alpha}(q) = E_n^{\alpha}\psi_n^{\alpha}(q). \tag{3.12}$$

Before the barrier insertion, some of the wave functions were odd and some were even.

$\psi_0, \psi_2, \psi_4, \psi_6, \psi_8$... were even eigenstates.

$\psi_1, \psi_3, \psi_5, \psi_7, \psi_9$... were odd eigenstates.

Let us check whether the barrier insertion affects the wave functions or not. Later we will do analytical calculation if it is required.

For odd wave functions

We will integrate Eq. (3.12) from -ε to +ε to check the behavior of odd wave functions near the barrier.

Note that ε is a small number such that $\varepsilon \to 0$

$$\int_{-\varepsilon}^{+\varepsilon} \left[\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 + \alpha(t)\delta(q-0)\right]\psi^{\alpha}_{2n+1}(q)dq = \int_{-\varepsilon}^{+\varepsilon} E^{\alpha}_{2n+1}\psi^{\alpha}_{2n+1}(q)dq,$$

$$\int_{-\varepsilon}^{+\varepsilon} \left[-\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{1}{2}m\omega^2 q^2 + \alpha(t)\delta(q-0)\right]\psi^{\alpha}_{2n+1}(q)dq = \int_{-\varepsilon}^{+\varepsilon} E^{\alpha}_{2n+1}\psi^{\alpha}_{2n+1}(q)dq.$$

We know that if $\psi^{\alpha}_{2n+1}(q)$ is odd, then

$$\int_{-\varepsilon}^{+\varepsilon} \psi^{\alpha}_{2n+1}(q) = 0,$$

and

$$\int_{-\varepsilon}^{+\varepsilon} \frac{1}{2}m\omega^2 q^2\psi^{\alpha}_{2n+1}(q)dq = 0,$$

$$\Rightarrow -\frac{\hbar^2}{2m}\int_{-\varepsilon}^{+\varepsilon} \frac{d^2}{dq^2}\psi^{\alpha}_{2n+1}(q)dq + \int_{-\varepsilon}^{+\varepsilon} \alpha(t)\delta(q-0)\psi^{\alpha}_{2n+1}(q)dq = 0. \tag{3.13}$$

Using the property of delta function

$$\int_{-\varepsilon}^{+\varepsilon} \alpha(t)\delta(q-0)\psi^{\alpha}_{2n+1}(q)dq = \alpha(t)\psi^{\alpha}_{2n+1}(0).$$

So we can write Eq. (3.13) as

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{+\varepsilon} \frac{d^2}{dq^2}\psi^{\alpha}_{2n+1}(q)dq + \alpha(t)\psi^{\alpha}_{2n+1}(0) = 0,$$

$$-\frac{\hbar^2}{2m}\frac{d}{dq}\psi^{\alpha}_{2n+1}(q)\Big|_{-\varepsilon}^{+\varepsilon} + \alpha(t)\psi^{\alpha}_{2n+1}(0) = 0,$$

$$-\frac{\hbar^2}{2m}\left[\frac{d}{dq}\psi^{\alpha}_{2n+1}(+\varepsilon) - \frac{d}{dq}\psi^{\alpha}(-\epsilon)\right] + \alpha(t)\psi^{\alpha}_{2n+1}(0) = 0. \tag{3.14}$$

But we know from the property that derivative of odd function is even function i.e.

$$\frac{d}{dq}\psi^{\alpha}_{2n+1}(-\varepsilon) = \frac{d}{dq}\psi^{\alpha}_{2n+1}(+\varepsilon).$$

So Eq. (3.14) becomes

$$\alpha(t)\psi^{\alpha}_{2n+1}(0) = 0,$$

$$\Rightarrow \psi^{\alpha}_{2n+1}(0) = 0. \tag{3.15}$$

We can see that odd wave functions are not affected by barrier. They vanished before barrier insertion and continue to do so after barrier insertion.

Even wave functions

Now we will do the same for even wave functions .

$$\int_{-\varepsilon}^{+\varepsilon} \left[\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 + \alpha(t)\delta(q-0)\right] \psi^{\alpha}_{2n}(q)dq = \int_{-\varepsilon}^{+\varepsilon} E^{\alpha}_{2n}\psi^{\alpha}_{2n}(q)dq,$$

$$\int_{-\varepsilon}^{+\varepsilon} \left[-\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{1}{2}m\omega^2 q^2 + \alpha(t)\delta(q-0)\right] \psi^{\alpha}_{2n}(q)dq = \int_{-\varepsilon}^{+\varepsilon} E^{\alpha}_{2n}\psi^{\alpha}_{2n}(q)dq,$$

$$-\int_{-\varepsilon}^{+\varepsilon} \frac{\hbar^2}{2m}\frac{d^2}{dq^2}\psi^{\alpha}_{2n}(q)dq + \int_{-\varepsilon}^{+\varepsilon} \frac{1}{2}m\omega^2 q^2\psi^{\alpha}_{2n}(q)dq + \int_{-\varepsilon}^{+\varepsilon} \alpha(t)\delta(q-0)\psi^{\alpha}_{2n}(q)dq = \int_{-\varepsilon}^{+\varepsilon} E^{\alpha}_{2n}\psi^{\alpha}_{2n}(q)dq. \tag{3.16}$$

One of the necessary condition for the wave function is that it must be continuous everywhere. This means that if we approach the even wave function form left, it would give the same result as if we approach it form right.

$$\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon} \psi^{\alpha}_{2n}(q)dq = 0,$$

and $\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon} q^2\psi^{\alpha}_{2n}(q)dq$ goes to zero as

$$\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon} q^2\psi^{\alpha}_{2n}(q)dq = \lim_{\varepsilon\to 0} q^2 \underbrace{\int_{-\varepsilon}^{+\varepsilon} \psi^{\alpha}_{2n}(q)dq}_{\to 0} - \lim_{\varepsilon\to 0} q^2 \int_{-\varepsilon}^{+\varepsilon}\int_{-\varepsilon}^{+\varepsilon} \psi^{\alpha}_{2n}(q).2qdq,$$

$$\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon} q^2\psi^{\alpha}_{2n}(q)dq = \lim_{\varepsilon\to 0}\left[-q^2\int_{-\varepsilon}^{+\varepsilon}\int_{-\varepsilon}^{+\varepsilon} \psi^{\alpha}_{2n}(q).2qdq\right],$$

$$\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon} q^2\psi^{\alpha}_{2n}(q)dq = -2\lim_{\varepsilon\to 0} q \underbrace{\int_{-\varepsilon}^{+\varepsilon}\int_{-\varepsilon}^{+\varepsilon} \psi^{\alpha}_{2n}(q).dq}_{\to 0} + 2\lim_{\varepsilon\to 0} \underbrace{\int_{-\varepsilon}^{+\varepsilon}\int_{-\varepsilon}^{+\varepsilon}\int_{-\varepsilon}^{+\varepsilon}\int_{-\varepsilon}^{+\varepsilon} \psi^{\alpha}_{2n}(q).dq}_{\to 0}.$$

Eq. (3.16) will become

$$-\frac{\hbar^2}{2m}\int\limits_{-\varepsilon}^{+\varepsilon}\frac{d^2}{dq^2}\psi_{2n}^{\alpha}(q)+\alpha(t)\int\limits_{-\varepsilon}^{+\varepsilon}\delta(q-0)\psi_{2n}^{\alpha}(q)dq=0,$$

$$-\frac{\hbar^2}{2m}\lim_{\varepsilon\to 0}\frac{d}{dq}\psi_{2n}^{\alpha}(q)\Big|_{-\varepsilon}^{+\varepsilon}+\alpha(t))\psi_{2n}^{\alpha}(0)=0,$$

$$-\frac{\hbar^2}{2m}\lim_{\varepsilon\to 0}\left[\frac{d}{dq}\psi_{2n}^{\alpha}(q)\Big|_{+\varepsilon}-\frac{d}{dq}\psi^{\alpha}(q)\Big|_{-\varepsilon}\right]+\alpha(t))\psi_{2n}^{\alpha}(0)=0.$$

As $\frac{d}{dq}\psi_{2n}^{\alpha}(q)$ is odd

$$\frac{d}{dq}\psi_{2n}^{\alpha}(q)\Big|_{-\varepsilon}=-\frac{d}{dq}\psi_{2n}^{\alpha}(q)\Big|_{+\varepsilon}.$$

So,

$$-\frac{\hbar^2}{2m}\lim_{\varepsilon\to 0}\left[\frac{d}{dq}\psi_{2n}^{\alpha}(q)\Big|_{+\varepsilon}+\frac{d}{dq}\psi^{\alpha}(q)\Big|_{+\varepsilon}\right]+\alpha(t))\psi_{2n}^{\alpha}(0)=0,$$

$$-\frac{\hbar^2}{2m}\lim_{\varepsilon\to 0}\left[2\frac{d}{dq}\psi_{2n}^{\alpha}(q)\Big|_{+\varepsilon}\right]+\alpha(t))\psi_{2n}^{\alpha}(0)=0,$$

$$\Rightarrow\frac{d}{dq}\psi_{2n}^{\alpha}(q)\Big|_{q=0}=\frac{m}{\hbar^2}\alpha(t)\psi_{2n}^{\alpha}(0). \tag{3.17}$$

This equation shows that, even function at $q=0$ is affected by the presence of barrier. This equation will give the **quantization condition** later. Hence we have to calculate only even wave functions.

3.2.3 Eigenstates of Even Modes after the Barrier Insertion

For the even wave function we will considered only the right side ($q>0$) because of symmetry. For ($q>0$) delta function does not take part and Eq. (3.12) becomes Weber differential equation.

Eq. (3.12) for $q>0$

$$\left(\frac{\hat{p}^2}{2m}+\frac{1}{2}m\omega^2\hat{q}^2\right)\psi_{2n}^{\alpha}(q)=E_{2n}^{\alpha}\psi_{2n}^{\alpha}(q), \tag{3.18}$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dq^2}\psi_{2n}^{\alpha}(q)+\frac{1}{2}m\omega^2q^2\psi_{2n}^{\alpha}(q)=E_{2n}^{\alpha}\psi_{2n}^{\alpha}(q)$$

dividing both sides by $\hbar\omega$

$$-\frac{\hbar^2}{2m\hbar\omega}\frac{d^2}{dq^2}\psi_{2n}^{\alpha}(q)+\frac{1}{2}\frac{m\omega^2q^2}{\hbar\omega}\psi_{2n}^{\alpha}(q)=\frac{E_{2n}^{\alpha}}{\hbar\omega}\psi_{2n}^{\alpha}(q),$$

$$-\frac{\hbar}{2m\omega}\frac{d^2}{dq^2}\psi_{2n}^{\alpha}(q)+\frac{1}{4}\frac{2m\omega q^2}{\hbar}\psi_{2n}^{\alpha}(q)=\frac{E_{2n}^{\alpha}}{\hbar\omega}\psi_{2n}^{\alpha}(q).$$

Let

$z^2{=}\dfrac{2m\omega q^2}{\hbar}\Rightarrow q^2=\dfrac{\hbar z^2}{2m\omega}$ and $v=-\dfrac{E_{2n}^{\alpha}}{\hbar\omega}$, so

$$-\frac{\hbar}{2m\omega}\frac{d^2}{d\left(\dfrac{\hbar z^2}{2m\omega}\right)}\psi_{2n}^{\alpha}(q)+\frac{1}{4}z^2\psi_{2n}^{\alpha}(q)=-v\psi_{2n}^{\alpha}(q),$$

$$\frac{d^2}{dz^2}\psi_{2n}^{\alpha}(q)-\frac{1}{4}z^2\psi_{2n}^{\alpha}(q)=v\psi_{2n}^{\alpha}(q),$$

$$\frac{d^2}{dz^2}\psi_{2n}^{\alpha}(q)-\left(\frac{1}{4}z^2+v\right)\psi_{2n}^{\alpha}(q)=0. \tag{3.19}$$

This Eq. (3.19) is known as Weber [30] differential equation and its solutions are

$$\psi_{2n}^{\alpha}(q)=Ae^{-\left(\frac{z^2}{4}+v\right)}+Be^{\left(\frac{z^2}{4}+v\right)},$$

$$\psi_{2n}^{\alpha}(q)=Ae^{-\left(\frac{z^2}{4}+v\right)}+Be^{\left(\frac{z^2}{4}+v\right)}.$$

The second term diverges when $z\to\pm\infty$ so we keep only the first term

$$\psi_{2n}^{\alpha}(q)=Ae^{-\left(\frac{z^2}{4}+v\right)},$$

$$\psi_{2n}^{\alpha}(q)=Ce^{-\frac{z^2}{4}}. \tag{3.20}$$

C may have z dependence, so we can also write the above equation as

$$\psi_{2n}^{\alpha}(q)=f\left(z\right)e^{-\frac{z^2}{4}}. \tag{3.21}$$

To determine $f\left(z\right)$, we take the derivatives and substitute the result in Eq. (3.19):

$$\frac{d}{dz}\psi_{2n}^{\alpha}(q)=\frac{d}{dz}\left(f\left(z\right)e^{-\frac{z^2}{4}}\right),$$

$$\frac{d}{dz}\psi_{2n}^{\alpha}(q)=\left[f\left(z\right)'e^{-\frac{z^2}{4}}-\frac{1}{2}zf\left(z\right)e^{-\frac{z^2}{4}}\right]. \tag{3.22}$$

$$\frac{d^2}{dz^2}\psi_{2n}^{\alpha}(q)=\left[f''\left(z\right)e^{-\frac{z^2}{4}}-\frac{1}{2}zf'\left(z\right)e^{-\frac{z^2}{4}}-\frac{1}{2}f\left(z\right)e^{-\frac{z^2}{4}}-\frac{1}{2}zf'\left(z\right)e^{-\frac{z^2}{4}}+\frac{1}{4}z^2f\left(z\right)e^{-\frac{z^2}{4}}\right],$$

$$\frac{d^2}{dz^2}\psi_{2n}^{\alpha}(q) = \left[f''(z)\,e^{-\frac{z^2}{4}} - zf'(z)\,e^{-\frac{z^2}{4}} - \frac{1}{2}f(z)\,e^{-\frac{z^2}{4}} + \frac{1}{4}z^2 f(z)\,e^{-\frac{z^2}{4}}\right],$$

$$\frac{d^2}{dz^2}\psi_{2n}^{\alpha}(q) = \left[f''(z)\,e^{-\frac{z^2}{4}} - zf'(z)\,e^{-\frac{z^2}{4}} - \frac{1}{2}f(z)\,e^{-\frac{z^2}{4}} + \frac{1}{4}z^2 f(z)\,e^{-\frac{z^2}{4}}\right]. \tag{3.23}$$

Substituting Eq. (3.21) and (3.23) in Eq. (3.19) we obtain

$$\left[f''(z)\,e^{-\frac{z^2}{4}} - zf'(z)\,e^{-\frac{z^2}{4}} - \frac{1}{2}f(z)\,e^{-\frac{z^2}{4}} + \frac{1}{4}z^2 f(z)\,e^{-\frac{z^2}{4}}\right] - \left(\frac{1}{4}z^2 + v^2\right) f(z)\,e^{-\frac{z^2}{4}} = 0,$$

$$\left[f''(z) - zf'(z) - \frac{1}{2}f(z) + \frac{1}{4}z^2 f(z) - \left(\frac{1}{4}z^2 + v^2\right) f(z)\right] = 0,$$

$$\left[f''(z) - zf'(z) - \frac{1}{2}f(z) - vf(z)\right] = 0,$$

$$\left[f''(z) - zf'(z) - \left(v + \frac{1}{2}\right) f(z)\right] = 0. \tag{3.24}$$

Let us define a parameter a for convenience

$$a = -\left(v + \frac{1}{2}\right), \tag{3.25}$$

where $v = -\frac{E_{2n}^{\alpha}}{\hbar\omega}$.
As $z = 0$ is an ordinary point, so we can solve Eq. (3.24) by power series method. Let the solution of Eq. (3.24) be

$$f(z) = \sum_{n=0}^{\infty} c_n z^n,$$

$$f(z)' = \sum_{n=1}^{\infty} n c_n z^{n-1},$$

$$f(z)'' = \sum_{n=2}^{\infty} n(n-1)\, c_n z^{n-2}.$$

Then Eq. (3.24) will become

$$\left[\sum_{n=2}^{\infty} n(n-1)\, c_n z^{n-2} - z\sum_{n=1}^{\infty} n c_n z^{n-1} + a\sum_{n=0}^{\infty} c_n z^n\right] = 0,$$

$$\left[\sum_{n=0}^{\infty} (n+2)(n+1)\, c_{n+2} z^n - \sum_{n=0}^{\infty} n c_n z^n + a\sum_{n=0}^{\infty} c_n z^n\right] = 0,$$

$$\sum_{n=0}^{\infty}\left[(n+2)(n+1)c_{n+2}-nc_n+ac_n\right]z^n=0.$$

Comparing the coefficients:

$$(n+2)(n+1)c_{n+2}-nc_n+ac_n=0,$$

we obtain

$$c_{n+2}=\frac{(n-a)}{(n+2)(n+1)}c_n.$$

Using the above recurrence relation, we can write the solution of Eq. (3.24) as

$$\begin{aligned}f(z)=&c_o\left[1+\frac{-a}{2!}z^2+\frac{-a(2-a)}{4!}z^4+\frac{-a(2-a)(4-a)}{6!}z^6+...\right]\\&+c_1z\left[1+\frac{(1-a)}{3!}z^2+\frac{(1-a)(3-a)}{5!}z^4+\frac{(1-a)(3-a)(5-a)}{7!}z^6+...\right],\end{aligned}\quad(3.26)$$

$$f(z)=c_oF_1\left(-\frac{a}{2},\frac{1}{2},\frac{z^2}{2}\right)+c_1zF_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{z^2}{2}\right),$$

where$z^2=\dfrac{2m\omega q^2}{\hbar}$
and $F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right)$ and $F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right)$ are confluent hypergeometric function [20] of the first kind. Hence Eq. (3.25) will become

$$\psi_{2n}^{\alpha}(q)=c_oe^{-\frac{m\omega}{2\hbar}q^2}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right)+c_1\sqrt{\frac{2m\omega}{\hbar}}qe^{-\frac{m\omega}{2\hbar}q^2}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right).$$

Using boundary conditions i.e.

$$\psi_{2n}^{\alpha}(\pm\infty)=0$$

and

$$\psi_{2n}^{\alpha}(0^+)=\psi_{2n}^{\alpha}(0^-)=0$$

Hence

$$\psi^{\alpha}_{2n}(q) = \frac{\sqrt{\pi}2^{a/2}}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)} e^{-\frac{m\omega}{2\hbar}q^2} F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right)$$
$$-\frac{\sqrt{\pi}2^{(a+1)/2}}{\mathit{\Gamma}\left(-\frac{a}{2}\right)} e^{-\frac{m\omega}{2\hbar}q^2}\sqrt{\frac{2m\omega}{\hbar}} qF_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right),$$

normalized wave function can be written as

$$\psi^{\alpha}_{2n}(q) = ND_a\left(q\sqrt{\frac{2m\omega}{\hbar}}\right), \tag{3.27}$$

where $D_a\left(q\sqrt{\frac{2m\omega}{\hbar}}\right)$ [19, 18] is a parabolic cylinder function and N is the normalization constant

$$N = \left[\sqrt{\frac{\pi\hbar}{4m\omega}}\frac{\phi\left(\frac{1-a}{2}\right)-\phi\left(\frac{-a}{2}\right)}{\Gamma\left(-a\right)}\right]^{\frac{1}{2}},$$

$$D_a\left(q\sqrt{\frac{2m\omega}{\hbar}}\right) = \frac{\sqrt{\pi}2^{a/2}}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)} e^{-\frac{m\omega}{2\hbar}q^2} F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right), \tag{3.28}$$
$$-\frac{\sqrt{\pi}2^{(a+1)/2}}{\mathit{\Gamma}\left(-\frac{a}{2}\right)} e^{-\frac{m\omega}{2\hbar}q^2} q\sqrt{\frac{2m\omega}{\hbar}} F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right),$$

$\Gamma(x)$ is Gama function [22] and $\phi(x)$ is Digamma function [23].
Recall Eq. (3.17):

$$\frac{d}{dq}\psi^{\alpha}_{2n}(q)\underset{q=0}{|} = \frac{m}{\hbar^2}\alpha(t)\psi^{\alpha}_{2n}(0).$$

We substitute $\psi^{\alpha}_{2n}(q)$ from Eq. (3.27) to obtain

$$\frac{d}{dq}ND_a\left(q\sqrt{\frac{2m\omega}{\hbar}}\right)\underset{q=0}{|} = \frac{m}{\hbar^2}\alpha(t)ND_a(0),$$

$$\frac{d}{dq}D_a\left(q\sqrt{\frac{2m\omega}{\hbar}}\right)\underset{q=0}{|} = \frac{m}{\hbar^2}\alpha(t)D_a(0),$$

$$D'_a(0)\sqrt{\frac{2m\omega}{\hbar}} = \frac{m}{\hbar^2}\alpha(t))D_a(0),$$

$$\alpha D_a(0) = \sqrt{\frac{2\hbar^3\omega}{m}} D'_a(0),$$

$$\alpha\sqrt{\frac{m}{2\hbar^3\omega}} = \frac{D'_a(0)}{D_a(0)}, \tag{3.29}$$

Let us calculate $D'_a(0)$ and $D_a(0)$ [24] using Eq. (3.28)

$$\begin{aligned} D_a(0) = & \frac{\sqrt{\pi}2^{a/2}}{\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)} e^{-\frac{m\omega}{2\hbar}0^2} F_1\left(-\frac{a}{2},\frac{1}{2},\frac{0^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right), \\ & -\frac{\sqrt{\pi}2^{(a+1)/2}}{\Gamma\left(-\frac{a}{2}\right)} e^{-\frac{m\omega}{2\hbar}0^2}(0)\sqrt{\frac{2m\omega}{\hbar}} F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{0^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right). \end{aligned}$$

Since (we can check these values directly from the series expansion (Eq. (3.26))

$$F_1\left(-\frac{a}{2},\frac{1}{2},\frac{0^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right) = 1,$$

$$F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{0^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right) = 1.$$

Therefore

$$D_a(0) = \frac{\sqrt{\pi}2^{a/2}}{\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}.$$

Using a from Eq. (3.25) we obtain

$$D_a(0) = \frac{\sqrt{\pi}2^{(2E^{\alpha}_{2n}-\hbar\omega)/4\hbar\omega}}{\Gamma\left[\frac{1}{2}-\frac{2E^{\alpha}_{2n}-\hbar\omega}{4\hbar\omega}\right]}. \tag{3.30}$$

Now $D'_a(0)$ using Eq. (3.28)

$$D'_a\left(q\sqrt{\frac{2m\omega}{\hbar}}\right) = \frac{d}{dq}\left[D_a\left(q\sqrt{\frac{2m\omega}{\hbar}}\right)\right],$$

$$
\begin{aligned}
D'_a\left(q\sqrt{\frac{2m\omega}{\hbar}}\right) =& \frac{\sqrt{\pi}2^{a/2}}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}\left(-\frac{m\omega}{\hbar}qe^{-\frac{m\omega}{2\hbar}q^2}\right)F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right)\\
&+\frac{\sqrt{\pi}2^{a/2}}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}\left(e^{-\frac{m\omega}{2\hbar}q^2}\right)\frac{d}{dq}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right)\\
&-\frac{\sqrt{\pi}2^{(a+1)/2}}{\mathit{\Gamma}\left(-\frac{a}{2}\right)}\left(-\frac{m\omega}{\hbar}e^{-\frac{m\omega}{2\hbar}q^2}\right)q\sqrt{\frac{2m\omega}{\hbar}}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right)\\
&-\frac{\sqrt{\pi}2^{(a+1)/2}}{\mathit{\Gamma}\left(-\frac{a}{2}\right)}\left(e^{-\frac{m\omega}{2\hbar}q^2}\right)\sqrt{\frac{2m\omega}{\hbar}}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right)\\
&-\frac{\sqrt{\pi}2^{(a+1)/2}}{\mathit{\Gamma}\left(-\frac{a}{2}\right)}\left(e^{-\frac{m\omega}{2\hbar}q^2}\right)q\sqrt{\frac{2m\omega}{\hbar}}\frac{d}{dq}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right).
\end{aligned}
$$

Since (we can check these values directly from the series expansion (Eq. 3.26))

$$F_1\left(-\frac{a}{2},\frac{1}{2},\frac{0^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right)=1,$$

$$F_1\left(-\frac{a}{2},\frac{1}{2},\frac{0q}{2}\left(\frac{2m\omega}{\hbar}\right)\right)=1.$$

and

$$\frac{d}{dq}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{0^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right)=0,$$

$$\frac{d}{dq}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{0^2}{2}\left(\frac{2m\omega}{\hbar}\right)\right)=0.$$

Therefore at $q=0$, $D'_a\left(q\sqrt{\frac{2m\omega}{\hbar}}\right)$ becomes

$$D'_a(0)=\frac{\sqrt{\pi}2^{(a+1)/2}}{\mathit{\Gamma}\left(-\frac{a}{2}\right)},$$

$$D'_a(0)=-\frac{\sqrt{\pi}2^{(2E^{\alpha}_{2n}+\hbar\omega)/4\hbar\omega}}{\Gamma\left[-\frac{2E^{\alpha}_{2n}-\hbar\omega}{4\hbar\omega}\right]}. \tag{3.31}$$

Eq. (3.29) will become

$$\alpha\sqrt{\frac{m}{2\hbar^3\omega}} = \frac{-\dfrac{2^{(2E^{\alpha}_{2n}+\hbar\omega)/4\hbar\omega}}{\Gamma\left[-\frac{2E^{\alpha}_{2n}-\hbar\omega}{4\hbar\omega}\right]}}{\dfrac{2^{(2E^{\alpha}_{2n}-\hbar\omega)/4\hbar\omega}}{\Gamma\left[\frac{1}{2}-\frac{2E^{\alpha}_{2n}-\hbar\omega}{4\hbar\omega}\right]}},$$

$$\alpha\sqrt{\frac{m}{2\hbar^3\omega}} = -\frac{\Gamma\left[\frac{1}{2}-\frac{2E^{\alpha}_{2n}-\hbar\omega}{4\hbar\omega}\right]}{\Gamma\left[-\frac{2E^{\alpha}_{2n}-\hbar\omega}{4\hbar\omega}\right]} \times \frac{2^{(2E^{\alpha}_{2n}+\hbar\omega)/4\hbar\omega}}{2^{(2E^{\alpha}_{2n}-\hbar\omega)/4\hbar\omega}},$$

$$\alpha\sqrt{\frac{m}{2\hbar^3\omega}} = -2^{1/2}\frac{\Gamma\left[\frac{1}{2}-\frac{2E^{\alpha}_{2n}-\hbar\omega}{4\hbar\omega}\right]}{\Gamma\left[-\frac{2E^{\alpha}_{2n}-\hbar\omega}{4\hbar\omega}\right]},$$

$$\alpha\sqrt{\frac{m}{\hbar^3\omega}} = -2\frac{\Gamma\left[\frac{3}{4}-\frac{E^{\alpha}_{2n}}{2\hbar\omega}\right]}{\Gamma\left[\frac{1}{4}-\frac{E^{\alpha}_{2n}}{2\hbar\omega}\right]}. \tag{3.32}$$

This implicit equation cannot be solve analytically. However, we can solve this Eq. (3.32) graphically (see Figure 3.1), noticing that α varies from 0 to ∞. When there is no barrier $\alpha = 0$, with increasing barrier strength α increases and at some later time when the height of barrier becomes maximum then $\alpha \to \infty$. Graph of this implicit equation is shown in Figure 3.1.

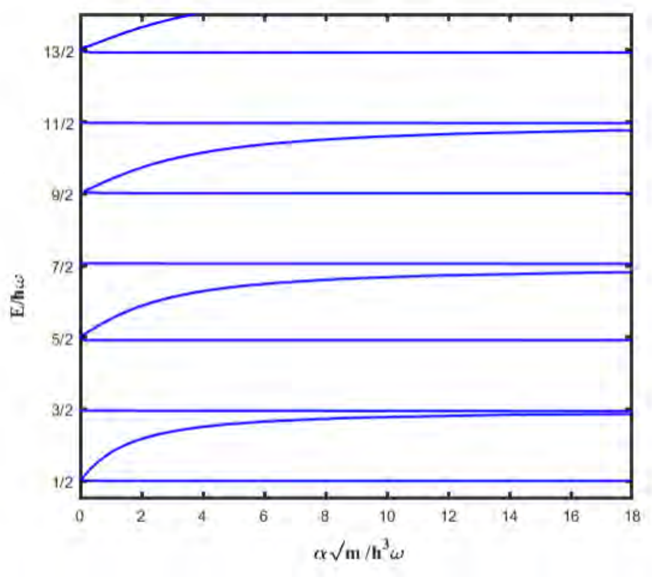

Figure 3.1: Graphical solution to the implicit equation (3.32) relating E and α; energy levels of the even modes are represent by the solid blue curves for a given value of α. While the energy levels of the odd modes are represented by solid blue lines(alternative lines).

For even eigenstates, we can see from Figure 3.1

At $\alpha = 0$

$$E_{2n} = \left(2n + \frac{1}{2}\right)\hbar\omega, \tag{3.33}$$

where $n = 0, 1, 2, 3...$.

When α (strength of barrier) increases, E_{2n}(energy eigenvalues of even modes) also increase and shifted to the E_{2n+1}(energy eigenvalues of odd modes) when $\alpha \to \infty$(barrier is fully inserted).

At $\alpha \to \infty$

$$E_{2n} \to \left(2n + \frac{1}{2}\right)\hbar\omega + \hbar\omega$$

$$\Rightarrow E_{2n} \to \left(2n + \frac{3}{2}\right)\hbar\omega. \tag{3.34}$$

or

$$E_{2n} \to \left[(2n+1) + \frac{1}{2}\hbar\omega\right],$$

$$E_{2n} \to E_{2n+1}.$$

From Eq. (3.34) we notice that energy eigenvalues of even modes are as same as energy eigenvalues of odd modes (odd modes have same energy eigenvalues before and after barrier insertion). Hence each energy eigenstate is now degenerate. These states produce the energy spectrum similar to the harmonic oscillator with energy gap $2\hbar\omega$, if bottom of well is shifted upward by $\hbar\omega/2$ as shown in Figure 3.2.

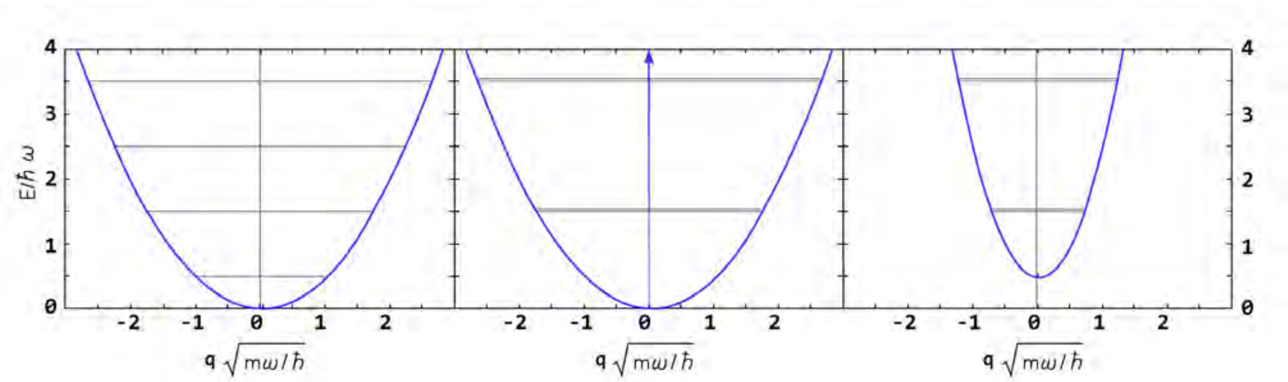

Figure 3.2: Left: Energy levels of the simple harmonic oscillator potential. Center: Energy levels of the simple harmonic oscillator potential plus the delta function potential in the limit $\alpha \to \infty$. Double horizontal lines represent the energy levels with twofold degeneracy. Right: The harmonic oscillator plus delta function potential has energy levels similar to the harmonic oscillator with frequency 2ω, with two-fold degeneracy at each energy level and shifted up by an energy $\hbar\omega/2$.

3.2.4 Density Operator

Now, we can construct $\hat{\rho}_{\perp}$ which represents the state of system after complete barrier insertion. From Eq. (2.1)

$$\hat{\rho}_{\perp} = \sum_{n=0}^{\infty} p_n |\psi_n^{\infty}\rangle\langle\psi_n^{\infty}|.$$

Note that each eigenstate of harmonic oscillator is now degenerate (see Fig. 3.2) with two-fold degeneracy, so we can write the density operator $\hat{\rho}_{\perp}$as

$$\hat{\rho}_{\perp} = \sum_{n=0}^{\infty} p_n \left(|\psi_{2n}^{\infty}\rangle\langle\psi_{2n}^{\infty}| + |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}|\right). \tag{3.35}$$

As our system is coupled to a thermal bath, we can consider our whole system as a canonical ensemble. The probability of nth state can be written as

$$p_n = \frac{e^{-\beta E_n}}{Z_{\perp}}.$$

Energy eigenvalues of two consecutive even and odd modes are same (see Fig. 3.2), such that:

$$E_n = E_{2n} = E_{2n+1} = \left(2n + \frac{3}{2}\right)\hbar\omega,$$

where $n = 0, 1, 2, 3, 4...$,

$$\Rightarrow p_n = \frac{e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega}}{Z_{\perp}}.$$

Eq. (3.35) well become

$$\hat{\rho}_{\perp} = \frac{1}{Z_{\perp}} \sum_{n=}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega} \left(|\psi_{2n}^{\infty}\rangle\langle\psi_{2n}^{\infty}| + |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}|\right). \tag{3.36}$$

3.2.5 Partition Function

To find the partition function, we use the following condition on the density operator.

For a valid density operator, trace of density operator must be equal to one:

$$Tr\left[\hat{\rho}_{\perp}\right] = 1,$$

$$Tr\left[\frac{1}{Z_{\perp}} \sum_{n=0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega} \left(|\psi_{2n}^{\infty}\rangle\langle\psi_{2n}^{\infty}| + |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}|\right)\right] = 1,$$

$$\sum_{m=0}^{\infty} \langle\psi_{2m}| \left[\frac{1}{Z_\perp}\sum_{0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega}\left(|\psi_{2n}^{\infty}\rangle\langle\psi_{2n}^{\infty}| + |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}|\right)\right]|\psi_{2m}\rangle$$
$$+\sum_{m=0}^{\infty} \langle\psi_{2m+1}| \left[\frac{1}{Z_\perp}\sum_{n=0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega}\left(|\psi_{2n}^{\infty}\rangle\langle\psi_{2n}^{\infty}| + |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}|\right)\right]|\psi_{2m+1}\rangle = 1,$$

$$\frac{1}{Z_\perp}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega}\langle\psi_{2m}|\psi_{2n}\rangle\langle\psi_{2n}|\psi_{2m}\rangle$$
$$+\frac{1}{Z_\perp}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega}\langle\psi_{2m}|\psi_{2n+1}\rangle\langle\psi_{2n+1}|\psi_{2m}\rangle$$
$$+\frac{1}{Z_\perp}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega}\langle\psi_{2m+1}|\psi_{2n}\rangle\langle\psi_{2n}|\psi_{2m+1}\rangle$$
$$+\frac{1}{Z_\perp}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega}\langle\psi_{2m+1}|\psi_{2n+1}\rangle\langle\psi_{2n+1}|\psi_{2m+1}\rangle = 1$$

using orthonormality condition

$$\langle\psi_{2n}|\psi_{2m}\rangle = \delta_{mn}, \quad \langle\psi_{2n+1}|\psi_{2m+1}\rangle = \delta_{mn},$$
$$\langle\psi_{2n+1}|\psi_{2m}\rangle = 0, \qquad \langle\psi_{2n}|\psi_{2m+1}\rangle = 0.$$

So

$$\frac{1}{Z_\perp}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega}\delta_{mn} + \frac{1}{Z_\perp}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega}\delta_{mn} = 1.$$

For $m = n$

$$\frac{1}{Z_\perp}\sum_{n=0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega} + \frac{1}{Z_\perp}\sum_{n=0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega} = 1.$$

Therefore, we obtain

$$Z_\perp = 2\sum_{n=0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega}.$$

This is a geometric series , with the initial term a_1 and common ratio r:

$$a_1 = e^{-\frac{3}{2}\beta\hbar\omega}, r = e^{-2\beta\hbar\omega}.$$

$$\Rightarrow Z_\perp = \frac{2e^{-\frac{3}{2}\beta\hbar\omega}}{1 - e^{-2\beta\hbar\omega}},$$

$$Z_{\perp} = \frac{e^{-\frac{1}{2}\beta\hbar\omega}}{\left(\frac{e^{-\beta\hbar\omega} - e^{-\beta\hbar\omega}}{2}\right)},$$

$$Z_{\perp} = \frac{e^{-\frac{1}{2}\beta\hbar\omega}}{sinh\left(\beta\hbar\omega\right)},$$

$$Z_{\perp} = e^{-\frac{1}{2}\beta\hbar\omega} cosech\left(\beta\hbar\omega\right). \tag{3.37}$$

This is the partition function of our system when the barrier is fully inserted. Partition function plays the role of generating function and it can be used to determine all thermodynamical quantities.

3.2.6 Thermodynamical Quantities

3.2.6.1 Helmholtz Free Energy

Let us denote the Helmholtz free energy after the barrier insertion by $A_{\perp}$

$$A_{\perp} = -k_B T ln Z_{\perp}.$$

From Eq. (3.37)

$$A_{\perp} = -k_B T ln\left[e^{-\frac{1}{2}\beta\hbar\omega} cosech\left(\beta\hbar\omega\right)\right],$$

$$A_{\perp} = -\frac{1}{\beta} ln\left(e^{-\frac{1}{2}\beta\hbar\omega}\right) + ln\left[sinh\left(\beta\hbar\omega\right)\right],$$

$$A_{\perp} = \frac{1}{2}\hbar\omega + \frac{1}{\beta} ln\left[sinh\left(\beta\hbar\omega\right)\right],$$

$$A_{\perp} = \frac{1}{\beta} ln\left[sinh\left(\beta\hbar\omega\right)\right] + \frac{1}{2}\hbar\omega. \tag{3.38}$$

From Eq. (3.6) and (3.38), we can determine the difference in Helmholtz free energy between the initial state and the state after barrier insertion:

$$A_{\perp} - A_{in} = \frac{1}{\beta} ln\left[sinh\left(\beta\hbar\omega\right)\right] + \frac{1}{2}\hbar\omega - k_B T ln\left[2 sinh(\frac{\beta\hbar\omega}{2})\right],$$

$$A_{\perp} - A_{in} = \frac{1}{\beta} ln\left[2 sinh\left(\frac{\beta\hbar\omega}{2}\right) cosh\left(\frac{\beta\hbar\omega}{2}\right)\right] + \frac{1}{2}\hbar\omega - k_B T ln\left[2 sinh(\frac{\beta\hbar\omega}{2})\right],$$

$$A_\perp - A_{in} = \frac{1}{\beta}ln\left[2sinh\left(\frac{\beta\hbar\omega}{2}\right)\right] + \frac{1}{\beta}ln\left[cosh\left(\frac{\beta\hbar\omega}{2}\right)\right] + \frac{1}{2}\hbar\omega - \frac{1}{\beta}ln\left[2sinh(\frac{\beta\hbar\omega}{2})\right],$$

$$A_\perp - A_{in} = \frac{1}{\beta}ln\left[cosh\left(\frac{\beta\hbar\omega}{2}\right)\right] + \frac{1}{2}\hbar\omega. \tag{3.39}$$

High Temperature Limit:

$T \to \infty \Rightarrow \beta \to 0$,

$$\lim_{T\to 0}(A_\perp - A_{in}) = \lim_{T\to\infty}\left[\frac{1}{\beta}ln\left[cosh\left(\frac{\beta\hbar\omega}{2}\right)\right] + \frac{1}{2}\hbar\omega\right],$$

we can also write

$$\lim_{T\to 0}(A_\perp - A_{in}) = \lim_{\beta\to 0}\left[\frac{1}{\beta}ln\left[cosh\left(\frac{\beta\hbar\omega}{2}\right)\right] + \frac{1}{2}\hbar\omega\right],$$

$$\lim_{T\to 0}(A_\perp - A_{in}) = \lim_{\beta\to 0}\frac{ln\left[cosh\left(\frac{\beta\hbar\omega}{2}\right)\right]}{\beta} + \frac{1}{2}\hbar\omega,$$

since $\lim_{\beta\to 0}\frac{ln\left[cosh\left(\frac{\beta\hbar\omega}{2}\right)\right]}{\beta}$ is $\frac{0}{0}$ form , so we can apply L'Hopital's rule

$$\lim_{T\to 0}(A_\perp - A_{in}) = \lim_{\beta\to 0}\left[tanh\left(\frac{\beta\hbar\omega}{2}\right)\frac{1}{2}\hbar\omega\right] + \frac{1}{2}\hbar\omega,$$

because $\lim_{\beta\to 0}\left[tanh\left(\frac{\beta\hbar\omega}{2}\right)\frac{1}{2}\hbar\omega\right] = 0$,therefore

$$\lim_{T\to 0}(A_\perp - A_{in}) = \frac{1}{2}\hbar\omega, \tag{3.40}$$

Low Temperature Limit:

$T \to 0 \Rightarrow \beta \to \infty$,

$$\lim_{T\to 0}(A_\perp - A_{in}) = \lim_{T\to\infty}\left\{\frac{1}{\beta}ln\left[cosh\left(\frac{\beta\hbar\omega}{2}\right)\right] + \frac{1}{2}\hbar\omega\right\},$$

$$\lim_{T\to 0}(A_\perp - A_{in}) = \lim_{T\to 0}\frac{1}{\beta}ln\left[\lim_{T\to 0}\left(\frac{e^{\frac{\beta\hbar\omega}{2}} + e^{-\frac{\beta\hbar\omega}{2}}}{2}\right)\right] + \frac{1}{2}\hbar\omega,$$

since $\lim_{T\to 0}\frac{e^{\frac{\beta\hbar\omega}{2}} + e^{-\frac{\beta\hbar\omega}{2}}}{2} = \lim_{T\to 0}\frac{1}{2}e^{\frac{\beta\hbar\omega}{2}}$, therefore

$$\lim_{T\to 0}(A_\perp - A_{in}) = \lim_{T\to 0}\frac{1}{\beta}ln\left[\frac{1}{2}\lim_{T\to 0}e^{\frac{\beta\hbar\omega}{2}}\right] + \frac{1}{2}\hbar\omega,$$

$$\lim_{T\to 0}(A_\perp - A_{in}) = \lim_{T\to 0}\left[\frac{1}{\beta}ln\left(\frac{1}{2}e^{\frac{\beta\hbar\omega}{2}}\right)\right] + \frac{1}{2}\hbar\omega,$$

$$\lim_{T\to 0}(A_\perp - A_{in}) = \lim_{T\to 0}\left[\frac{1}{\beta}\left(\frac{\beta\hbar\omega}{2} - ln2\right)\right] + \frac{1}{2}\hbar\omega,$$

$$\lim_{T\to 0}(A_\perp - A_{in}) = \lim_{T\to 0}\left(\frac{\hbar\omega}{2} - \frac{ln2}{\beta}\right) + \frac{1}{2}\hbar\omega,$$

$$\lim_{T\to 0}(A_\perp - A_{in}) = \lim_{T\to 0}\left(\frac{\hbar\omega}{2} - k_B T ln2\right) + \frac{1}{2}\hbar\omega,$$

$$\lim_{T\to 0}(A_\perp - A_{in}) = \frac{1}{2}\hbar\omega + \frac{1}{2}\hbar\omega = \hbar\omega, \tag{3.41}$$

Hence from eq (3.40) and (3.41) we can write in general as

$$(A_\perp - A_{in}) \simeq \hbar\omega \tag{3.42}$$

This implies that demon has to do work on the system during barrier insertion.

3.2.6.2 Average Energy:

Let us denote the average energy after the barrier insertion by $E_\perp$

$$E_\perp = -\frac{\partial}{\partial\beta}lnZ_\perp.$$

From Eq. (3.37)

$$E_\perp = -\frac{\partial}{\partial\beta}ln\left[e^{-\frac{1}{2}\beta\hbar\omega}cosech\left(\beta\hbar\omega\right)\right],$$

$$E_\perp = -\frac{1}{e^{-\frac{1}{2}\beta\hbar\omega}cosech\left(\beta\hbar\omega\right)}\frac{\partial}{\partial\beta}\left[e^{-\frac{1}{2}\beta\hbar\omega}cosech\left(\beta\hbar\omega\right)\right],$$

$$E_\perp = -\frac{1}{e^{-\frac{1}{2}\beta\hbar\omega}cosech\left(\beta\hbar\omega\right)}e^{-\frac{1}{2}\beta\hbar\omega}\left[-cosech\left(\beta\hbar\omega\right)coth\left(\beta\hbar\omega\right)\right]\hbar\omega$$
$$-\frac{1}{e^{-\frac{1}{2}\beta\hbar\omega}cosech\left(\beta\hbar\omega\right)}e^{-\frac{1}{2}\beta\hbar\omega}\left(-\frac{1}{2}\hbar\omega\right)cosech\left(\beta\hbar\omega\right),$$

$$E_\perp = \frac{e^{-\frac{1}{2}\beta\hbar\omega}coth(\beta\hbar\omega)cosech\left(\beta\hbar\omega\right)}{e^{-\frac{1}{2}\beta\hbar\omega}cosech\left(\beta\hbar\omega\right)}\hbar\omega + \frac{e^{-\frac{1}{2}\beta\hbar\omega}cosech\left(\beta\hbar\omega\right)}{2e^{-\frac{1}{2}\beta\hbar\omega}cosech\left(\beta\hbar\omega\right)}\hbar\omega,$$

$$E_\perp = \hbar\omega\left[coth\left(\beta\hbar\omega\right)\right] + \frac{1}{2}\hbar\omega. \tag{3.43}$$

From the classical analysis of Szilard engine [4], we can assume that barrier insertion can be done at the cost of zero energy. However, quantum mechanically the situation is not the same.

From Eq. (3.7) and (3.43), we can determine the difference in average energy between the initial state and the state after barrier insertion:

$$E_{\perp} - E_{in} = \hbar\omega \left[coth\left(\beta\hbar\omega\right)\right] + \frac{1}{2}\hbar\omega - \frac{1}{2}\hbar\omega\left[coth\left(\frac{\beta\hbar\omega}{2}\right)\right],$$

$$E_{\perp} - E_{in} = \hbar\omega \left[coth\left(\beta\hbar\omega\right)\right] + \frac{1}{2}\hbar\omega - \frac{1}{2}\hbar\omega\left[coth\left(\frac{\beta\hbar\omega}{2}\right)\right],$$

$$E_{\perp} - E_{in} = \frac{1}{2}\hbar\omega\left\{\left[2coth\left(\beta\hbar\omega\right)\right] + 1 - \frac{1}{2}\hbar\omega\left[coth\left(\frac{\beta\hbar\omega}{2}\right)\right]\right\},$$

$$\Rightarrow E_{\perp} - E_{in} \neq 0.$$

This implies that average energy of system increases after barrier insertion. Now the question arises, from where does this energy come? The only source of energy increase is the demon action (barrier insertion).

3.2.6.3 Entropy

When our quantum system is in a mixed state then it is represented in terms of a density operator and the entropy of a such system can be written (from Eq. (2.15)) as

$$S_{\perp} = -Tr\left[\hat{\rho}_{\perp} ln \hat{\rho}_{\perp}\right].$$

But from Eq. (2.16), above relation can also be written as;

$$S_{\perp} = -\frac{d}{dT}A_{\perp},$$

from Eq. (3.38)

$$S_{\perp} = -\frac{d}{dT}\left[\frac{1}{\beta}ln\left\{sinh\left(\beta\hbar\omega\right)\right\} + \frac{1}{2}\hbar\omega\right],$$

$$S_{\perp} = -\frac{d}{dT}\left\{k_B T ln\left[sinh\left(\frac{\hbar\omega}{k_B T}\right)\right] + \frac{1}{2}\hbar\omega\right\},$$

$$S_{\perp} = -k_B ln\left[sinh\left(\frac{\hbar\omega}{k_B T}\right)\right] - k_B T\frac{cosh\left(\frac{\hbar\omega}{k_B T}\right)}{sinh\left(\frac{\hbar\omega}{k_B T}\right)}\left(-\frac{\hbar\omega}{k_B T^2}\right),$$

$$S_{\perp} = -k_B ln\left[sinh\left(\beta\hbar\omega\right)\right] + k_B\beta\left[coth\left(\beta\hbar\omega\right)\right]\hbar\omega,$$

$$S_{\perp} = k_B \left\{ \beta\hbar\omega \left[coth\left(\beta\hbar\omega\right)\right] - ln\left[sinh\left(\beta\hbar\omega\right)\right]\right\}. \tag{3.44}$$

High Temperature Limit:
$T \to \infty \Rightarrow \beta \to 0$**,**

$$\underset{T\to\infty}{S_{\perp}} = \lim_{T\to\infty} S_{\perp} = k_B \left\{ \beta\hbar\omega \left[coth\left(\beta\hbar\omega\right)\right] - ln\left[sinh\left(\beta\hbar\omega\right)\right]\right\},$$

$$\underset{T\to\infty}{S_{\perp}} = \lim_{T\to\infty} k_B \left[\beta\hbar\omega . coth\left(\beta\hbar\omega\right)\right] - \lim_{T\to\infty} k_B ln\left[sinh\left(\beta\hbar\omega\right)\right],$$

$$\underset{T\to\infty}{S_{\perp}} = k_B \left[1\right] - \lim_{T\to\infty} k_B ln\left[sinh\left(\beta\hbar\omega\right)\right],$$

$$\underset{T\to\infty}{S_{\perp}} = k_B \left\{1 - \lim_{T\to\infty} ln\left[sinh\left(\beta\hbar\omega\right)\right]\right\}$$

$$\underset{T\to\infty}{S_{\perp}} \approx -k_B \left\{\lim_{T\to\infty} ln\left[sinh\left(\beta\hbar\omega\right)\right]\right\}$$

As $\beta \to 0$ when $T \to \infty$, we can use the Taylor expansion

$$\underset{T\to\infty}{S_{\perp}} = -k_B \lim_{T\to\infty} \left[ln\left(\beta\hbar\omega + ...\right)\right],$$

$$\underset{T\to\infty}{S_{\perp}} = -k_B \lim_{T\to\infty} ln\left(\beta\hbar\omega\right),$$

$$\underset{T\to\infty}{S_{\perp}} = k_B \lim_{T\to\infty} ln\left(\frac{1}{\beta\hbar\omega}\right).$$

We can write the above expression for $T \to \infty$as

$$S_{\perp} = k_B ln\left(\frac{k_B T}{\hbar\omega}\right). \tag{3.45}$$

From Eq. (3.9)

$$S_{\perp} = S_{in}. \tag{3.46}$$

In high temperature limit we can see that entropy of the system before (S_{in}) and after barrier insertion ($S_{\perp}$) is same. Hence the effect of barrier insertion is considered negligible in this limit.

Low Temperature Limit:
$T \to 0 \Rightarrow \beta \to \infty$**,**

$$\underset{T\to 0}{S_{\perp}} = \lim_{T\to 0} k_B \left\{ \beta\hbar\omega \left[coth\left(\beta\hbar\omega\right)\right] - ln\left[sinh\left(\beta\hbar\omega\right)\right]\right\},$$

$$\underset{T\to 0}{S_{\perp}} = k_B \left(\underset{T\to 0}{lim}\beta\hbar\omega\right)\left[\underset{T\to 0}{lim}coth\left(\beta\hbar\omega\right)\right] - k_B ln\left(\frac{e^{\beta\hbar\omega}-e^{-\beta\hbar\omega}}{2}\right),$$

$$\underset{T\to 0}{S_{\perp}} = k_B \left(\underset{T\to 0}{lim}\beta\hbar\omega\right)\left[\underset{T\to 0}{lim}coth\left(\beta\hbar\omega\right)\right] - k_B \underset{T\to 0}{lim}\left[ln\left(e^{\beta\hbar\omega}-e^{-\beta\hbar\omega}\right)+kln2\right].$$

Since

$$\underset{T\to 0}{lim}coth(\beta\hbar\omega) = 1,$$

and

$$\underset{T\to 0}{lim}ln\left(e^{\beta\hbar\omega}-e^{-\beta\hbar\omega}\right) = ln\left(\underset{T\to 0}{lim}e^{\beta\hbar\omega} - \underset{T\to 0}{lim}e^{-\beta\hbar\omega}\right),$$

$$\underset{T\to 0}{lim}ln\left(e^{\beta\hbar\omega}-e^{-\beta\hbar\omega}\right) = ln\left(\underset{T\to 0}{lim}e^{\beta\hbar\omega}\right),$$

$$\underset{T\to 0}{lim}ln\left(e^{\beta\hbar\omega}-e^{-\beta\hbar\omega}\right) = \underset{T\to 0}{lim}ln\left(e^{\beta\hbar\omega}\right).$$

So,

$$\underset{T\to 0}{S_{\perp}} = k_B \left(\underset{T\to 0}{lim}\beta\hbar\omega\right) - k_B \underset{T\to 0}{lim}\left[ln\left(e^{\beta\hbar\omega}\right)+k_B ln2\right],$$

$$\underset{T\to 0}{S_{\perp}} = k_B \left(\underset{T\to 0}{lim}\beta\hbar\omega\right) - k_B \underset{T\to 0}{lim}\left(\beta\hbar\omega\right) + k_B ln2,$$

$$\underset{T\to 0}{S_{\perp}} = k_B \left(\underset{T\to 0}{lim}\beta\hbar\omega\right) - k_B \underset{T\to 0}{lim}\left(\beta\hbar\omega\right) + k_B ln2,$$

$$\underset{T\to 0}{S_{\perp}} = k_B \underset{T\to 0}{lim}\left(\beta\hbar\omega - \beta\hbar\omega\right) + k_B ln2.$$

$$\underset{T\to 0}{S_{\perp}} = k_B \underset{T\to 0}{lim}\left(0\right) + k_B ln2,$$

so we can write the above relation in low temperature limit as

$$\underset{T\to 0}{S_{\perp}} = k_B ln2. \tag{3.47}$$

Eq. (3.47) shows that particle occupies a doubly degenerate ground state at absolute zero temperature.

3.3 Quantum Measurement

In this section we are interested in projective(strong) measurements. We will use the state of system that we have prepared in the previous section. Before the quantum measurements on the system [25], we will define Left and Right eigenstates. We can write the "Left" and "Right" eigenstates as linear combination of even ($|\psi_{2n}^{\infty}\rangle$) and odd ($|\psi_{2n+1}^{\infty}\rangle$) eigenstates.

Left eigenstate can be written as

$$|L\rangle = \frac{1}{\sqrt{2}}\left(|\psi_{2n}^{\infty}\rangle - |\psi_{2n+1}^{\infty}\rangle\right). \tag{3.48}$$

Right eigenstate can be written as

$$|R\rangle = \frac{1}{\sqrt{2}}\left(|\psi_{2n}^{\infty}\rangle + |\psi_{2n+1}^{\infty}\rangle\right). \tag{3.49}$$

Here we can see that

$$\begin{aligned}\langle L_n|L_n\rangle = 1, \quad \langle R_n|R_n\rangle = 1,\\ \langle L_n|R_n\rangle = 0, \quad \langle R_n|L_n\rangle = 0.\end{aligned}$$

3.3.1 Density Operator

Now let us try to write $\hat{\rho}_{\perp}$in term of $|L_n\rangle$ and $|R_n\rangle$

$$\hat{\rho}_{\perp} = \frac{1}{Z_{\perp}} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)} \left(|\psi_{2n}^{\infty}\rangle\langle\psi_{2n}^{\infty}| + |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}|\right).$$

As

$$|L_n\rangle\langle L_n| = \frac{1}{\sqrt{2}}\left(|\psi_{2n}^{\infty}\rangle - |\psi_{2n+1}^{\infty}\rangle\right)\frac{1}{\sqrt{2}}\left(\langle\psi_{2n}^{\infty}| - \langle\psi_{2n+1}^{\infty}|\right),$$

$$|L_n\rangle\langle L_n| = \frac{1}{2}\left(|\psi_{2n}^{\infty}\rangle\langle\psi_{2n}^{\infty}| - |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n}^{\infty}| - |\psi_{2n}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}| + |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}|\right).$$

Similarly

$$|R_n\rangle\langle R_n| = \frac{1}{\sqrt{2}}\left(|\psi_{2n}^{\infty}\rangle + |\psi_{2n+1}^{\infty}\rangle\right)\frac{1}{\sqrt{2}}\left(\langle\psi_{2n}^{\infty}| + \langle\psi_{2n+1}^{\infty}|\right),$$

$$|R_n\rangle\langle R_n| = \frac{1}{2}\left(|\psi_{2n}^{\infty}\rangle\langle\psi_{2n}^{\infty}| + |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n}^{\infty}| + |\psi_{2n}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}| + |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}|\right).$$

Then $|L_n\rangle\langle L_n| + |R_n\rangle\langle R_n|$ will be

$$
\begin{aligned}
|L_n\rangle\langle L_n| + |R_n\rangle\langle R_n| =& \frac{1}{2}\left(|\psi_{2n}^{\infty}\rangle\langle\psi_{2n}^{\infty}| - |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n}^{\infty}| - |\psi_{2n}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}| + |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}|\right) \\
&+ \frac{1}{2}\left(|\psi_{2n}^{\infty}\rangle\langle\psi_{2n}^{\infty}| + |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n}^{\infty}| + |\psi_{2n}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}| + |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}|\right),
\end{aligned}
$$

$$
|L_n\rangle\langle L_n| + |R_n\rangle\langle R_n| = \frac{1}{2}\left(2|\psi_{2n}^{\infty}\rangle\langle\psi_{2n}^{\infty}| + 2|\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}|\right),
$$

$$
|L_n\rangle\langle L_n| + |R_n\rangle\langle R_n| = |\psi_{2n}^{\infty}\rangle\langle\psi_{2n}^{\infty}| + |\psi_{2n+1}^{\infty}\rangle\langle\psi_{2n+1}^{\infty}|.
$$

Using this relation we can write $\hat{\rho}_\perp$ as

$$
\hat{\rho}_\perp = \frac{1}{Z_\perp}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+\frac{3}{2})}\left(|L_n\rangle\langle L_n| + |R_n\rangle\langle R_n|\right). \tag{3.50}
$$

$|L_n\rangle$: Describes the state of quantum particle when it is located on the left side of partition.

$|R_n\rangle$: Describes the state of quantum particle when it is located on the right side of partition.

3.3.2 Projectors

By quantum measurements we can find whether the particle is located on the right or left side of the barrier. Since we are doing projective measurements so we need to construct the corresponding projection operators [17].

The associated projection operators are

$$
\hat{P}_L = \sum_{n=0}^{\infty} |L_n\rangle\langle L_n|, \tag{3.51}
$$

$$
\hat{P}_R = \sum_{n=0}^{\infty} |R_n\rangle\langle R_n|. \tag{3.52}
$$

Let us define the left and right density operators.

$\hat{\rho}_L$: Left density operator represent the state of particle when it is located on the left side of partition.

$\hat{\rho}_R$: Right density operator represent the state of particle when it is located on the right side of partition.

3.3.3 Projective Measurements

When we do projective measurements, one of the eigenstate is projected with some probability. Let us first determined the left eigenstate associated with $\hat{P}_L$.

For this we have to evaluate

$$\hat{\rho}_L = \frac{\hat{P}_L\left(\hat{\rho}_\perp\right)\hat{P}_L^\dagger}{Tr\left[\hat{P}_L\hat{\rho}_\perp\right]}.$$

Consider $\hat{P}_L\left(\hat{\rho}_\perp\right)\hat{P}_L^\dagger$

$$\hat{P}_L\left(\hat{\rho}_\perp\right)\hat{P}_L^\dagger = \sum_{k=0}^{\infty}|L_k\rangle\langle L_k|\left(\frac{1}{Z_\perp}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|L_n\rangle\langle L_n| + |R_n\rangle\langle R_n|\right)\right)\sum_{k'=0}^{\infty}|L_{k'}\rangle\langle L_{k'}|,$$

$$\begin{aligned}\hat{P}_L\left(\hat{\rho}_\perp\right)\hat{P}_L^\dagger =& \frac{1}{Z_\perp}\sum_{k=0}^{\infty}|L_k\rangle\langle L_k|\left[\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_n\rangle\langle L_n|\right]\sum_{k'=0}^{\infty}|L_{k'}\rangle\langle L_{k'}| \\ &+\frac{1}{Z_\perp}\sum_{k=0}^{\infty}|L_k\rangle\langle L_k|\left[\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|R_n\rangle\langle R_n|\right]\sum_{k'=0}^{\infty}|L_{k'}\rangle\langle L_{k'}|,\end{aligned}$$

$$\begin{aligned}\hat{P}_L\left(\hat{\rho}_\perp\right)\hat{P}_L^\dagger =& \frac{1}{Z_\perp}\sum_{k=0}^{\infty}\sum_{k'=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_k\rangle\langle L_k|\left(|L_n\rangle\langle L_n|\right)|L_{k'}\rangle\langle L_{k'}| \\ &+\sum_{k=0}^{\infty}\sum_{k'=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_k\rangle\langle L_k|\left(|R_n\rangle\langle R_n|\right)|L_{k'}\rangle\langle L_{k'}|,\end{aligned}$$

$$\begin{aligned}\hat{P}_L\left(\hat{\rho}_\perp\right)\hat{P}_L^\dagger =& \frac{1}{Z_\perp}\left[\sum_{k=0}^{\infty}\sum_{k'=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_k\rangle\left(\langle L_k|L_n\rangle\right)\left(\langle L_n|L_{k'}\rangle\right)\langle L_{k'}|\right] \\ &+\frac{1}{Z_\perp}\left[\sum_{k=0}^{\infty}\sum_{k'=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_k\rangle\left(\langle L_k|R_n\rangle\right)\left(\langle R_n|L_{k'}\rangle\right)\langle L_{k'}|\right].\end{aligned}$$

From the orthonormality condition of quantum states:

$$\begin{aligned}\langle L_k|R_n\rangle = 0, \qquad \langle R_n|L_{k'}\rangle = 0, \\ \langle L_k|L_n\rangle = \delta_{k,n}, \quad \langle L_n|L_{k'}\rangle = \delta_{n,k'},\end{aligned}$$

we obtain

$$\begin{aligned}\hat{P}_L\left(\hat{\rho}_\perp\right)\hat{P}_L^\dagger =& \frac{1}{Z_\perp}\left[\sum_{k=0}^{\infty}\sum_{k'=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_k\rangle\delta_{k,n}\delta_{n,k'}\langle L_{k'}|\right] \\ &+\frac{1}{Z_\perp}\left[\sum_{k=0}^{\infty}\sum_{k'=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_k\rangle\left(0\right)\langle L_{k'}|\right],\end{aligned}$$

for $n=k$ and $n=k'$

$$\hat{P}_L\left(\hat{\rho}_\perp\right)\hat{P}_L^\dagger=\frac{1}{Z_\perp}\left[\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_n\rangle\langle L_n|\right].$$

Now consider $Tr\left[\hat{P}_L\hat{\rho}_\perp\right]$

$$Tr\left[\hat{P}_L\hat{\rho}_\perp\right]=Tr\left[\sum_{k=0}^{\infty}|L_k\rangle\langle L_k|\frac{1}{Z_\perp}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|L_n\rangle\langle L_n|+|R_n\rangle\langle R_n|\right)\right],$$

$$Tr\left[\hat{P}_L\hat{\rho}_\perp\right]=Tr\left[\frac{1}{Z_\perp}\sum_{k=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|L_k\rangle\langle L_k|L_n\rangle\langle L_n|+|L_k\rangle\langle L_k|R_n\rangle\langle R_n|\right)\right],$$

$$Tr\left[\hat{P}_L\hat{\rho}_\perp\right]=Tr\left[\frac{1}{Z_\perp}\sum_{k=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|L_k\rangle\delta_{k,n}\langle L_n|+|L_k\rangle\left(0\right)\langle R_n|\right)\right],$$

for $k=n$

$$Tr\left[\hat{P}_L\hat{\rho}_\perp\right]=Tr\left[\frac{1}{Z_\perp}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|L_n\rangle\langle L_n|\right)\right],$$

$$\begin{aligned}Tr\left[\hat{P}_L\hat{\rho}_\perp\right]=&\frac{1}{Z_\perp}\sum_{k=0}^{\infty}\langle L_k|\left[\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|L_n\rangle\rangle\langle L_n|\right)\right]|L_k\rangle\\&+\frac{1}{Z_\perp}\sum_{k=0}^{\infty}\langle R_k|\left[\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|L_n\rangle\langle L_n|\right)\right]|R_k\rangle,\end{aligned}$$

$$\begin{aligned}Tr\left[\hat{P}_L\hat{\rho}_\perp\right]=&\frac{1}{Z_\perp}\sum_{k=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\langle L_k|\left(|L_n\rangle\langle L_n|\right)|L_k\rangle\\&+\frac{1}{Z_\perp}\sum_{k=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\langle R_k|\left(|L_n\rangle\langle L_n|\right)|R_k\rangle,\end{aligned}$$

$$\begin{aligned}Tr\left[\hat{P}_L\hat{\rho}_\perp\right]=&\frac{1}{Z_\perp}\sum_{k=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\langle L_k|L_n\rangle\langle L_n|L_k\rangle\\&+\frac{1}{Z_\perp}\sum_{k=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\langle R_k|L_n\rangle\langle L_n|R_k\rangle,\end{aligned}$$

using the orthonormality conditions

$$Tr\left[\hat{P}_L\hat{\rho}_\perp\right] = \frac{1}{Z_\perp}\sum_{k=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\delta_{k,n}\delta_{n,k} + \frac{1}{Z_\perp}\sum_{k=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(0\right),$$

for $k = n$

$$Tr\left[\hat{P}_L\hat{\rho}_\perp\right] = \frac{1}{Z_\perp}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}.$$

Since (from Eq. (3.37))

$$Z_\perp = e^{-\frac{\beta\hbar\omega}{2}} cosech\left(\beta\hbar\omega\right),$$

and $\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}$ is a geometric series:

$$\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)} = \frac{e^{-\frac{\beta\hbar\omega}{2}} cosech\left(\beta\hbar\omega\right)}{2}.$$

So,

$$Tr\left[\hat{P}_L\hat{\rho}_\perp\right] = \frac{1}{e^{-\frac{\beta\hbar\omega}{2}} cosech\left(\beta\hbar\omega\right)}\frac{e^{-\frac{\beta\hbar\omega}{2}} cosech\left(\beta\hbar\omega\right)}{2},$$

which yields

$$Tr\left(\hat{P}_L\hat{\rho}_\perp\right) = \frac{1}{2}.$$

$\hat{\rho}_L$ finally will become

$$\hat{\rho}_L = \frac{\frac{1}{Z_\perp}\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_n\rangle\langle L_n|\right]}{\frac{1}{2}},$$

$$\hat{\rho}_L = \frac{2}{Z_\perp}\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_n\rangle\langle L_n|\right]. \tag{3.53}$$

Here we define $\frac{Z_\perp}{2} = Z_L$ (we will calculate it later in a proper way)

$$\hat{\rho}_L = \frac{1}{Z_L}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_n\rangle\langle L_n| \tag{3.54}$$

Similarly $\hat{\rho}_R$ can be determined

$$\hat{\rho}_R = \frac{\hat{P}_L\left(\hat{\rho}_\perp\right)\hat{P}_L^\dagger}{Tr\left[\hat{P}_L\hat{\rho}_\perp\right]}.$$

First we consider $\hat{P}_R\left(\hat{\rho}_\perp\right)\hat{P}_R^\dagger$

$$\hat{P}_R\left(\hat{\rho}_\perp\right)\hat{P}_R^\dagger = \sum_{k=0}^{\infty}|R_k\rangle\langle R_k|\left[\frac{1}{Z_\perp}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|L_n\rangle\langle L_n|+|R_n\rangle\langle R_n|\right)\right]\sum_{k'=0}^{\infty}|R_{k'}\rangle\langle R_{k'}|,$$

$$\begin{aligned}\hat{P}_R\left(\hat{\rho}_\perp\right)\hat{P}_R^\dagger =& \frac{1}{Z_\perp}\sum_{k=0}^{\infty}|R_k\rangle\langle R_k|\left(\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_n\rangle\langle L_n|\right)\sum_{k'=0}^{\infty}|R_{k'}\rangle\langle R_{k'}|\\ &+\frac{1}{Z_\perp}\sum_{k=0}^{\infty}|R_k\rangle\langle R_k|\left(\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|R_n\rangle\langle R_n|\right)\sum_{k'=0}^{\infty}|R_{k'}\rangle\langle R_{k'}|,\end{aligned}$$

$$\begin{aligned}\hat{P}_R\left(\hat{\rho}_\perp\right)\hat{P}_R^\dagger =& \frac{1}{Z_\perp}\sum_{k=0}^{\infty}\sum_{k'=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|R_k\rangle\langle R_k|\left(|L_n\rangle\langle L_n|\right)|R_{k'}\rangle\langle R_{k'}|\\ &+\sum_{k=0}^{\infty}\sum_{k'=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|R_k\rangle\langle R_k|\left(|R_n\rangle\langle R_n|\right)|R_{k'}\rangle\langle R_{k'}|,\end{aligned}$$

$$\begin{aligned}\hat{P}_R\left(\hat{\rho}_\perp\right)\hat{P}_R^\dagger =& \frac{1}{Z_\perp}\left[\sum_{k=0}^{\infty}\sum_{k'=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|R_k\rangle\left(\langle R_k|L_n\rangle\right)\left(\langle L_n|R_{k'}\rangle\right)\langle R_{k'}|\right]\\ &+\frac{1}{Z_\perp}\left[\sum_{k=0}^{\infty}\sum_{k'=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|R_k\rangle\left(\langle R_k|R_n\rangle\right)\left(\langle R_n|R_{k'}\rangle\right)\langle R_{k'}|\right],\end{aligned}$$

from the orthonormality condition of quantum states, we obtain

$$\begin{aligned}\hat{P}_R\left(\hat{\rho}_\perp\right)\hat{P}_R^\dagger =& \frac{1}{Z_\perp}\left[\sum_{k=0}^{\infty}\sum_{k'=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|R_k\rangle\left(0\right)\langle R_{k'}|\right]\\ &+\frac{1}{Z_\perp}\left[\sum_{k=0}^{\infty}\sum_{k'=0}^{\infty}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|R_k\rangle\delta_{k,n}\delta_{n,k'}\rangle\langle R_{k'}|\right],\end{aligned}$$

for $k=n$ and $k=n'$

$$\hat{P}_R\left(\hat{\rho}_\perp\right)\hat{P}_R^\dagger = \frac{1}{Z_\perp}\left[\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|R_n\rangle\langle R_n|\right]. \tag{3.55}$$

Now consider $Tr\left[\hat{P}_R\hat{\rho}_\perp\right]$

$$Tr\left[\hat{P}_R\hat{\rho}_\perp\right] = Tr\left[\sum_{k=0}^{\infty}|R_k\rangle\langle R_k|\frac{1}{Z_\perp}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|L_n\rangle\langle L_n|+|R_n\rangle\langle R_n|\right)\right],$$

$$Tr\left[\hat{P}_L\hat{\rho}_\perp\right] = Tr\left[\frac{1}{Z_\perp}\sum_{k=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|R_k\rangle\langle R_k|L_n\rangle\langle L_n| + |R_k\rangle\langle R_k|R_n\rangle\langle R_n|\right)\right],$$

for $k = n$, using orthonormality condition of quantum states:

$$Tr\left[\hat{P}_R\hat{\rho}_\perp\right] = Tr\left[\frac{1}{Z_\perp}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|R_n\rangle\langle R_n|\right)\right],$$

$$\begin{aligned} Tr\left[\hat{P}_R\hat{\rho}_\perp\right] =& \frac{1}{Z_\perp}\sum_{k=0}^{\infty}\langle L_k|\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|R_n\rangle\langle R_n|\right)\right]|L_k\rangle \\ &+ \frac{1}{Z_\perp}\sum_{k=0}^{\infty}\langle R_k|\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|R_n\rangle\langle R_n|\right)\right]|R_k\rangle, \end{aligned}$$

$$\begin{aligned} Tr\left[\hat{P}_R\hat{\rho}_\perp\right] =& \frac{1}{Z_\perp}\sum_{k=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\langle L_k|\left(|R_n\rangle\langle R_n|\right)|L_k\rangle \\ &+ \frac{1}{Z_\perp}\sum_{k=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\langle R_k|\left(|R_n\rangle\langle R_n|\right)|R_k\rangle. \end{aligned}$$

using the orthonormality condition of quantum states:

$$Tr\left[\hat{P}_R\hat{\rho}_\perp\right] = \frac{1}{Z_\perp}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}.$$

Since (from Eq. (3.37))

$$Z_\perp = e^{-\frac{\beta\hbar\omega}{2}} cosech\left(\beta\hbar\omega\right)$$

and $\sum\limits_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}$ is a geometric series:

$$\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)} = \frac{e^{-\frac{\beta\hbar\omega}{2}} cosech\left(\beta\hbar\omega\right)}{2}.$$

So,

$$Tr\left[\hat{P}_R\hat{\rho}_\perp\right] = \frac{1}{e^{-\frac{\beta\hbar\omega}{2}} cosech\left(\beta\hbar\omega\right)}\frac{e^{-\frac{\beta\hbar\omega}{2}} cosech\left(\beta\hbar\omega\right)}{2},$$

which yields

$$Tr\left(\hat{P}_R\hat{\rho}_\perp\right) = \frac{1}{2}.$$

$\hat{\rho}_R$ finally will become

$$\hat{\rho}_R = \frac{\frac{1}{Z_\perp}\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|R_n\rangle\langle R_n|\right]}{\frac{1}{2}},$$

$$\hat{\rho}_R = \frac{2}{Z_\perp}\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|R_n\rangle\langle R_n|\right]. \tag{3.56}$$

Here, we define $\frac{Z_\perp}{2} = Z_R$ (we will calculate it later in a proper way)

$$\hat{\rho}_R = \frac{1}{Z_R}\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|R_n\rangle\langle R_n|\right]. \tag{3.57}$$

From Eq. (3.54) and (3.57), complete density matrix after barrier insertion can be written as

$$\hat{\rho}_\perp = \frac{1}{2}\left(\hat{\rho}_L + \hat{\rho}_R\right) \tag{3.58}$$

3.3.4 Partition Function

Partition function plays the role of generating function in statistical mechanics. Here we have two partition functions Z_L and Z_R.

Left Partition Function

Z_L is defined as partial trace over the Hilbert space spanned by the left eigenstates. It can be obtained from

$$Tr\left[\hat{\rho}_L\right] = 1.$$

From Eq. (3.54)

$$Tr\left[\frac{1}{Z_L}\left(\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_n\rangle\langle L_n|\right)\right] = 1,$$

$$\frac{1}{Z_L}Tr\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_n\rangle\langle L_n|\right] = 1.$$

Carrying out the trace:

$$Z_L = \sum_{k=0}^{\infty}\langle L_k|\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_n\rangle\langle L_n|\right]|L_k\rangle$$
$$+\sum_{k=0}^{\infty}\langle R_k|\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}|L_n\rangle\langle L_n|\right]|R_k\rangle,$$

$$
\begin{aligned}
Z_L = & \sum_{k=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+\frac{3}{2})}\langle L_k|L_n\rangle\langle L_n|L_k\rangle \\
& + \sum_{k=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+\frac{3}{2})}\langle R_k|L_n\rangle\langle L_n|R_k\rangle,
\end{aligned}
$$

using the orthonormality conditions

$$
Z_L = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+\frac{3}{2})}. \tag{3.59}
$$

$\sum\limits_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+\frac{3}{2})}$ is a geometric series, we can evaluate the sum:

$$
Z_L = \frac{e^{-\frac{\beta\hbar\omega}{2}} cosech\,(\beta\hbar\omega)}{2} \tag{3.60}
$$

but $Z_{\perp} = e^{-\frac{\beta\hbar\omega}{2}} cosech\,(\beta\hbar\omega)$

$$
\Rightarrow Z_L = \frac{Z_{\perp}}{2} \tag{3.61}
$$

Right Partition Function

Z_R is defined as partial trace over the Hilbert space spanned by the right eigenstates. It can be obtained from

$$
Tr\,[\hat{\rho}_R] = 1.
$$

From Eq. (3.57)

$$
\begin{aligned}
Tr\left[\frac{1}{Z_R}\left(\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+\frac{3}{2})}|R_n\rangle\langle R_n|\right)\right] &= 1, \\
\frac{1}{Z_R} Tr\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+\frac{3}{2})}|R_n\rangle\langle R_n|\right] &= 1.
\end{aligned}
$$

Carrying out the trace:

$$
\begin{aligned}
Z_R = & \sum_{k=0}^{\infty} \langle L_k|\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+\frac{3}{2})}|R_n\rangle\langle R_n|\right]|L_k\rangle \\
& + \sum_{k=0}^{\infty} \langle R_k|\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+\frac{3}{2})}|R_n\rangle\langle R_n|\right]|R_k\rangle,
\end{aligned}
$$

$$Z_R = \sum_{k=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+\frac{3}{2})}\langle L_k|R_n\rangle\langle R_n|L_k\rangle$$
$$+ \sum_{k=0}^{\infty}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+\frac{3}{2})}\langle R_k|R_n\rangle\langle R_n|R_k\rangle,$$

using the orthonormality condition

$$Z_R = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+\frac{3}{2})}. \tag{3.62}$$

$\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(2n+\frac{3}{2})}$ is a geometric series, we can evaluate the sum:

$$Z_R = \frac{e^{-\frac{\beta\hbar\omega}{2}} cosech\,(\beta\hbar\omega)}{2}, \tag{3.63}$$

but $Z_\perp = e^{-\frac{\beta\hbar\omega}{2}} cosech\,(\beta\hbar\omega)$

$$Z_R = \frac{Z_\perp}{2}. \tag{3.64}$$

From Eq. (3.61) and (3.64), we can see that the partition function of complete system can be obtained by adding left and right partition function.

$$Z_\perp = Z_L + Z_R$$

3.3.5 Thermodynamical Quantities

We have partition function for both left and right states so we can calculate thermodynamical quantities using the partition functions.

3.3.5.1 Helmholtz Free Energy

Let us denote the Helmholtz free energy after the projective measurement by A_R and A_L when the particle is projected to right and left side of the barrier respectively.

Using Z_L, Helmholtz free energy can be calculated as

$$A_L = -\frac{1}{\beta} ln Z_L.$$

From Eq. (3.60)

$$A_L = -\frac{1}{\beta} ln \left[\frac{e^{-\frac{\beta\hbar\omega}{2}} cosech\,(\beta\hbar\omega)}{2}\right],$$

$$A_L = -\frac{1}{\beta}\left(-\frac{\beta\hbar\omega}{2}\right) + \frac{1}{\beta}ln2 - \frac{1}{\beta}ln\left[cosech\left(\beta\hbar\omega\right)\right],$$

$$A_L = \frac{\hbar\omega}{2} + \frac{1}{\beta}ln2 + \frac{1}{\beta}ln\left[sinh\left(\beta\hbar\omega\right)\right].$$

Similarly from Z_R

$$A_R = -\frac{1}{\beta}lnZ_R.$$

From Eq. (3.63)

$$A_R = -\frac{1}{\beta}ln\left[\frac{e^{-\frac{\beta\hbar\omega}{2}}cosech\left(\beta\hbar\omega\right)}{2}\right],$$

$$A_R = -\frac{1}{\beta}\left(-\frac{\beta\hbar\omega}{2}\right) + \frac{1}{\beta}ln2 - \frac{1}{\beta}ln\left[cosech\left(\beta\hbar\omega\right)\right],$$

$$A_R = \frac{\hbar\omega}{2} + \frac{1}{\beta}ln2 + \frac{1}{\beta}ln\left[sinh\left(\beta\hbar\omega\right)\right].$$

Here we found

$$A_L = A_R = \frac{\hbar\omega}{2} + \frac{1}{\beta}ln2 + \frac{1}{\beta}ln\left[sinh\left(\beta\hbar\omega\right)\right]. \tag{3.65}$$

3.3.5.2 Average Energy

Let us denote the average energy after the projective measurement by E_R and E_L when the particle is projected to right and left side of the barrier respectively.

Using Z_L, average energy can be calculated as

$$E_L = -\frac{1}{Z_L}\frac{d}{d\beta}Z_L.$$

From Eq. (3.60)

$$E_L = -\frac{1}{Z_L}\frac{d}{d\beta}\left[\frac{e^{-\frac{\beta\hbar\omega}{2}}cosech\left(\beta\hbar\omega\right)}{2}\right],$$

$$E_L = -\frac{1}{2Z_L}\left\{-\frac{\hbar\omega}{2}e^{-\frac{\beta\hbar\omega}{2}}cosech\left(\beta\hbar\omega\right) + e^{-\frac{\beta\hbar\omega}{2}}\hbar\omega\left[-cosech\left(\beta\hbar\omega\right)\right]coth\left(\beta\hbar\omega\right)\right\},$$

$$E_L = -\frac{1}{2Z_L}\left\{-\frac{\hbar\omega}{2}e^{-\frac{\beta\hbar\omega}{2}}cosech\left(\beta\hbar\omega\right) - e^{-\frac{\beta\hbar\omega}{2}}\hbar\omega\left[cosech\left(\beta\hbar\omega\right)\right]coth\left(\beta\hbar\omega\right)\right\}$$

Since $Z_L = e^{-\frac{\beta\hbar\omega}{2}} cosech\left(\beta\hbar\omega\right)$, we can write

$$E_L = -\frac{1}{Z_L}\left[-\frac{\hbar\omega}{2}Z_L - \hbar\omega.coth\left(\beta\hbar\omega\right)Z_L\right],$$

$$E_L = \hbar\omega\left[coth\left(\beta\hbar\omega\right)\right] + \frac{1}{2}\hbar\omega.$$

Similarly from Z_R

$$E_R = -\frac{1}{Z_R}\frac{d}{d\beta}Z_R.$$

From Eq. (3.63)

$$E_L = -\frac{1}{Z_R}\frac{d}{d\beta}\left[\frac{e^{-\frac{\beta\hbar\omega}{2}} cosech\left(\beta\hbar\omega\right)}{2}\right],$$

$$E_R = -\frac{1}{2Z_R}\left\{-\frac{\hbar\omega}{2}e^{-\frac{\beta\hbar\omega}{2}} cosech\left(\beta\hbar\omega\right) + e^{-\frac{\beta\hbar\omega}{2}}\hbar\omega\left[-cosech\left(\beta\hbar\omega\right)\right]coth\left(\beta\hbar\omega\right)\right\},$$

$$E_R = -\frac{1}{2Z_R}\left\{-\frac{\hbar\omega}{2}e^{-\frac{\beta\hbar\omega}{2}} cosech\left(\beta\hbar\omega\right) - e^{-\frac{\beta\hbar\omega}{2}}\hbar\omega cosech\left(\beta\hbar\omega\right)coth\left(\beta\hbar\omega\right)\right\}.$$

Since $Z_R = e^{-\frac{\beta\hbar\omega}{2}} cosech\left(\beta\hbar\omega\right)$, we can write

$$E_R = -\frac{1}{Z_R}\left[-\frac{\hbar\omega}{2}Z_R - \hbar\omega coth\left(\beta\hbar\omega\right)Z_R\right],$$

$$E_R = \hbar\omega\left[coth\left(\beta\hbar\omega\right)\right] + \frac{1}{2}\hbar\omega,$$

Here we found

$$E_L = E_R = \hbar\omega\left[coth\left(\beta\hbar\omega\right)\right] + \frac{1}{2}\hbar\omega. \tag{3.66}$$

3.3.5.3 Entropy

Let us denote the entropy after the projective measurement by S_R and S_L when the particle is projected to right and left side of the barrier respectively.

If the particle is found on left side of the barrier, $\hat{\rho}_L$ is the state of particle. Using this density operator, we can calculate S_L which is the entropy of particle if it is located on the left side of barrier.

$$S_L = -k_B Tr\left[\hat{\rho}_L ln\hat{\rho}_L\right].$$

But we know from Eq. (2.16)

$$S_L = -\frac{d}{dT}\left(A_L\right),$$

$$S_L = -\frac{d}{dT}\left(-\frac{1}{\beta}lnZ_L\right),$$

$$S_L = -\frac{d}{dT}\left\{-\frac{1}{\beta}ln\left[\frac{e^{-\frac{\beta\hbar\omega}{2}}cosech\left(\beta\hbar\omega\right)}{2}\right]\right\},$$

$$S_L = -\frac{d}{dT}\left[-\frac{1}{\beta}\left(-\frac{\beta\hbar\omega}{2}\right)+\frac{1}{\beta}ln2-\frac{1}{\beta}cosech\left(\beta\hbar\omega\right)\right],$$

$$S_L = -\frac{d}{dT}\left\{\frac{\hbar\omega}{2}+k_BTln2+k_BTln\left[sinh\left(\beta\hbar\omega\right)\right]\right\},$$

$$S_L = -k_Bln2 - k_Bln\left[sinh\left(\beta\hbar\omega\right)\right] + k_Bcoth\left(\beta\hbar\omega\right)\beta\hbar\omega,$$

$$S_L = k_B\left\{\beta\hbar\omega\left[coth\left(\beta\hbar\omega\right)\right] - ln\left[sinh\left(\beta\hbar\omega\right)\right]\right\} - k_Bln2.$$

Similarly, if particle is located on the right side, the entropy will be

$$S_R = -k_BTr\left(\hat{\rho}_Rln\hat{\rho}_R\right).$$

But we know from Eq. (2.16)

$$S_R = -\frac{d}{dT}\left(-\frac{1}{\beta}lnZ_R\right),$$

$$S_R = -\frac{d}{dT}\left\{-\frac{1}{\beta}ln\left[\frac{e^{-\frac{\beta\hbar\omega}{2}}cosech\left(\beta\hbar\omega\right)}{2}\right]\right\},$$

$$S_R = -\frac{d}{dT}\left[-\frac{1}{\beta}\left(-\frac{\beta\hbar\omega}{2}\right)+\frac{1}{\beta}ln2-\frac{1}{\beta}cosech\left(\beta\hbar\omega\right)\right],$$

$$S_R = -\frac{d}{dT}\left\{\frac{\hbar\omega}{2}+k_BTln2+k_BTln\left[sinh\left(\beta\hbar\omega\right)\right]\right\},$$

$$S_R = -k_Bln2 - k_Bln\left[sinh\left(\beta\hbar\omega\right)\right] + k_Bcoth\left(\beta\hbar\omega\right)\beta\hbar\omega,$$

$$S_R = k_B\left\{\beta\hbar\omega\left[coth\left(\beta\hbar\omega\right)\right] - ln\left[sinh\left(\beta\hbar\omega\right)\right]\right\} - k_Bln2.$$

Here we found

$$S_L = S_R = k_B \left\{ \beta\hbar\omega \left[coth \left(\beta\hbar\omega \right) \right] - ln \left[sinh \left(\beta\hbar\omega \right) \right] \right\} - k_B ln2. \tag{3.67}$$

3.3.6 Comparison of Thermodynamical Quantities

From the above calculations, we can see that measurements alter many quantities such as density operator, partition function and some thermodynamical quantities. In this section we will do a comparison of some of the thermodynamical quantities.

3.3.6.1 Average Energy

From Eq. (3.66) and (3.43)

$$\triangle E = E_{L,R} - E_{\perp},$$

$$\triangle E = \left\{ \hbar\omega \left[coth \left(\beta\hbar\omega \right) \right] + \frac{1}{2}\hbar\omega \right\} - \left\{ \hbar\omega \left[coth \left(\beta\hbar\omega \right) \right] + \frac{1}{2}\hbar\omega \right\},$$

$$\boldsymbol{\triangle E = 0}. \tag{3.68}$$

Here we found that measurements leave the average energy of quantum system unchanged.

3.3.6.2 Helmholtz Free Energy

We have seen that measurements cast some effects on Helmholtz free energy. From Eq. (3.38) Helmholtz free energy of the system before measurements is

$$A_{\perp} = \frac{1}{\beta} ln \left[sinh \left(\beta\hbar\omega \right) \right] + \frac{\hbar\omega}{2}.$$

As a results of quantum measurement the Helmholtz free energy becomes (from Eq. (3.65))

$$A_{L,R} = \frac{\hbar\omega}{2} + \frac{1}{\beta} ln2 + \frac{1}{\beta} ln \left[sinh \left(\beta\hbar\omega \right) \right].$$

Change in Helmholtz free energy can be calculate as

$$\triangle A = A_{L,R} - A_{\perp},$$

$$\triangle A = \left\{ \frac{\hbar\omega}{2} + \frac{1}{\beta} ln2 + \frac{1}{\beta} ln \left[sinh \left(\beta\hbar\omega \right) \right] \right\} - \left\{ \frac{1}{\beta} ln \left[sinh \left(\beta\hbar\omega \right) \right] + \frac{\hbar\omega}{2} \right\},$$

$$\triangle A = \frac{1}{\beta} ln2,$$

$$\triangle \boldsymbol{A} = \boldsymbol{k_B T ln2}. \tag{3.69}$$

This equation shows that free energy of the particle increases by an amount of $k_B T ln2$. So we conclude that particle has some energy available to perform a useful work.

3.3.6.3 Entropy

From the above calculations we have seen that entropy also changes after the quantum measurements. Here we will see it quantitatively. Entropy of the particle before the quantum measurement is (from Eq. (3.44))

$$S_{\perp} = k_B \left\{\beta\hbar \left[coth\left(\beta\hbar\omega\right)\right]\right\} - ln\left[sinh\left(\beta\hbar\omega\right)\right].$$

As a result of quantum measurements entropy of particle becomes (from Eq. (3.67))

$$S_{L,R} = k_B \left\{\beta\hbar\omega \left[coth\left(\beta\hbar\omega\right)\right] - ln\left[sinh\left(\beta\hbar\omega\right)\right]\right\} - k_B ln2.$$

Change can be calculated as

$$\triangle S = S_{L,R} - S_{\perp},$$

$$\triangle \boldsymbol{S} = -\boldsymbol{k_B ln2}. \tag{3.70}$$

This equation shows that entropy of particle decreases by an amount of $-k_B ln2$, which leads to the apparent violation of the second law of thermodynamics.

3.4 Quantum Isothermal Expansion

Once the measurement is performed, the particle is projected onto one side of the partition either left or right side. Let us say that particle is located on the right side of the barrier. The density operator of the particle is $\hat{\rho}_R$ (from Eq. (3.57)) and can be written as

$$\hat{\rho}_R = \frac{1}{Z_R}\left[\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)} |R_n\rangle\langle R_n|\right].$$

Once the particle location is ensured, it pushes the barrier towards left with some force F. Initially when barrier is at origin, then the delta function is $\delta\left(q-0\right)$. When particle pushes the barrier towards left then delta function is displaced and it becomes the function of $q_o\left(t\right)$ such that:

$$\delta\left(q\right) \longrightarrow \delta\left(q - q_o(t)\right),$$

where

$$q_0(t) = \begin{cases} 0 & t \longrightarrow 0 \\ -\infty & t \longrightarrow \infty \end{cases}.$$

But during the expansion the barrier is moved slowly such that adiabatic condition for expansion is satisfied i.e.

$$\mid \frac{\dot{q}_o}{q_o} \mid \leqslant \omega$$

3.4.1 Energy Eigenstates

As the barrier is pushed towards left, instantaneous Hamiltonian will be

$$\hat{H}_{\leftarrow}(t) = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 + \alpha\delta\left(\hat{q} - q_o(t)\right). \tag{3.71}$$

Similarly if the particle is located on the left side of barrier, then it pushes the barrier towards left with some force F. Density matrix will be $\hat{\rho}_L$;

$\hat{H}_{\leftarrow}(t)$ changes with the barrier position $q_o(t)$, so our wave function will also change with changing $q_o(t)$.

$$\hat{H}_{\leftarrow}(t)\left(\psi^{q_o}(q)\right) = E^{q_o}\psi^{q_o}(q),$$

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{1}{2}m\omega^2\hat{q}^2 + \alpha\delta\left(\hat{q} - q_o(t)\right)\right]\psi^{q_o}(q) = E^{q_o}\psi^{q_o}(q). \tag{3.72}$$

Recall $\alpha(t) = \infty$, therefore wave function $\psi^{q_o}(q)$ exists on the right side of the barrier only and it satisfies the boundary condition:

$$\psi^{q_o}(q_o) = 0. \tag{3.73}$$

For the right side of barrier, Dirac delta function does not take part and Eq. (3.72) will become

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{1}{2}m\omega^2\hat{q}^2\right]\psi^{q_o}(q) = E^{q_o}\psi^{q_o}(q.)$$

This equation is solved in the same way as we have solved Eq. (3.18) in the section **Barrier Insertion**, from Eq. (3.27) the solution of the above equation can be written as for varying q_o

$$\psi^{q_o}(q) = ND_a\left(q\sqrt{\frac{2m\omega}{\hbar}}\right).$$

Where N is the normalization constant and can be found by orthonormality condition.

3.4.2 Energy Eigenvalues

When particle becomes localized to the right side of barrier, its wave function vanishes near the barrier. Using the boundary condition (Eq. (3.73))

$$\psi^{q_o}(q_o) = 0.$$

This equation gives the energy eigenvalues for all values of $q_o : 0 \to -\infty$

$$D_a\left(q\sqrt{\frac{2m\omega}{\hbar}}\right)|_{q=q_o} = 0,$$

$$\frac{\sqrt{\pi}2^{a/2}}{\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right) - \frac{\sqrt{\pi}2^{(a+1)/2}}{\Gamma\left(-\frac{a}{2}\right)}q_o\sqrt{\frac{2m\omega}{\hbar}}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right) = 0,$$

$$\frac{2^{a/2}}{\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right) - \frac{2^{(a+1)/2}}{\Gamma\left(-\frac{a}{2}\right)}q_o\sqrt{\frac{2m\omega}{\hbar}}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right) = 0.$$

Rearranging

$$\frac{\Gamma\left(-\frac{a}{2}\right)}{\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)} = \frac{F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q^2}{2}\frac{2m\omega}{\hbar}\right)\sqrt{\frac{m\omega}{\hbar}}}{F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q^2}{2}\frac{2m\omega}{\hbar}\right)}2q_o. \tag{3.74}$$

This implicit equation cannot be solved analytically for each value of q. However, we can solve this equation (Eq. (3.74)) graphically (see Figure 3.3), noticing that q_o varies from 0 to $-\infty$.

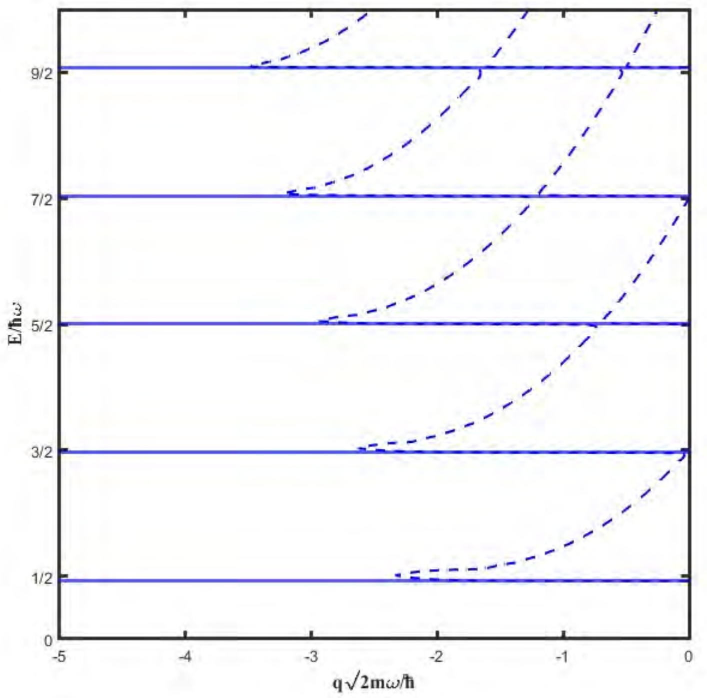

Figure 3.3: Graphical solution to the implicit equation (Eq. 3.74): Energy levels of the right modes $|R_n\rangle$ are represented by dashed blue curve for a given value of q_o. Energy levels of the harmonic oscillator without the barrier are represented by solid blue lines.

From the Figure (3.3)

At $q_o = 0$ (barrier is not displaced)

$$E_n = \left(2n + \frac{3}{2}\right)\hbar\omega. \tag{3.75}$$

$E_o = \frac{3}{2}\hbar\omega$, $E_1 = \frac{7}{2}\hbar\omega$, $E_2 = \frac{11}{2}\hbar\omega$, $E_3 = \frac{15}{2}\hbar\omega...$,

This is the energy eigenvalue of particle when particle is on the right side and barrier is fully inserted at $q_o = 0$. Gap between two consecutive energy levels is $2\hbar\omega$. This is the energy eigenvalue of particle when particle is on the right side and barrier is fully inserted at $q_o = 0$.

When barrier is displaced towards $-\infty$, q_o varies and E_n is shifted to lower value.

At $q_o = \infty$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{3.76}$$

These are the energy eigenvalues of particle when the particle is on the right side and barrier is fully inserted at $q = \infty$, Infact this is the case of no barrier insertion.

Figure 3.3 also shows that when q_o varies from 0 to $-\infty$, the states $|R_n\rangle$ shift towards the eigenstates $|\psi_n\rangle$ of the simple harmonic oscillator. As a result in this isothermal expansion, system finally returns back to its initial state $\hat{\rho}_{in}$.

As system is returned to it initial state, let us check the net change in free energy in a complete cycle. From Eq. (3.65) and (3.6)

$$A_R - A_{in} = \left\{ \frac{\hbar\omega}{2} + \frac{1}{\beta} ln2 + \frac{1}{\beta} ln \left[sinh \left(\beta\hbar\omega \right) \right] \right\} - \left\{ k_B T ln \left[2 sinh \left(\frac{\beta\hbar\omega}{2} \right) \right] \right\},$$

$$A_R - A_{in} = \frac{\hbar\omega}{2} + \frac{1}{\beta} ln2 + \frac{1}{\beta} ln \left[2 sinh \left(\frac{\beta\hbar\omega}{2} \right) cosh \left(\frac{\beta\hbar\omega}{2} \right) \right] - k_B T ln \left[2 sinh \left(\frac{\beta\hbar\omega}{2} \right) \right],$$

$$\begin{aligned} A_R - A_{in} =& \frac{\hbar\omega}{2} + k_B T ln2 + k_B T ln \left[2 sinh \left(\frac{\beta\hbar\omega}{2} \right) \right] + k_B T ln \left[cosh \left(\frac{\beta\hbar\omega}{2} \right) \right] \\ & - k_B T ln \left[2 sinh \left(\frac{\beta\hbar\omega}{2} \right) \right], \end{aligned}$$

$$A_R - A_{in} = \frac{\hbar\omega}{2} + k_B T n \left[cosh \left(\frac{\beta\hbar\omega}{2} \right) \right] + k_B T ln2. \tag{3.77}$$

Eq. (3.77) above shows the amount of free energy available in a system to perform useful mechanical work. The first two terms arise due to the work done by the demon during barrier insertion (from Eq. (3.39)). However, the last term quantifies the amount of energy (this term is responsible for the violation of second law) that can be extracted from thermal bath. This is the net available energy during each cycle[26] .

3.4.3 Force Exerted on the Barrier

Now, using semi-classical methods, the force applied to the barrier may be calculated from the infinitesimal variation of the system's free energy under an infinitesimal movement of the barrier. The first law of thermodynamics states that the mechanical work performed by the system must be opposite to the change in free energy for an isothermal process.

$$F = -\frac{dA}{dq_o}.$$

As our particle is projected to the right side of the barrier so we will use A_R

$$F = -\frac{dA_R}{dq_o},$$

where

$$A_R = -\frac{1}{\beta} ln Z_R.$$

This is the same result that we obtained in the quantum measurement section, however we are expressing A_R here in term of E_n.The reason is that we want to see the change of free energy with varying q_o.

$$A_R = -\frac{1}{\beta} ln \sum_{n=0}^{\infty} e^{-\beta E_n},$$

so

$$F = -\frac{d}{dq_o}\left(-\frac{1}{\beta} lnZ_R\right),$$

$$F = \frac{1}{\beta}\frac{d}{dq_o}\left(lnZ_R\right),$$

$$F = \frac{1}{\beta Z_R}\frac{d}{dq_o}Z_R,$$

$$F = \frac{1}{\beta Z_R}\frac{d}{dq_o}\left(\sum_{n=0}^{\infty} e^{-\beta E_n}\right),$$

$$F = \frac{1}{Z_R}\sum_{n=0}^{\infty} e^{-\beta E_n}\frac{dE_n}{dq_o}. \tag{3.78}$$

Now, we have to calculate $\frac{dE_n}{dq_o}$.

The force might theoretically be calculated at each point during the expansion, but this would necessitate a more comprehensive numerical calculations. Let us calculate this force analytically just at the beginning of expansion to see its behavior.

From Eq. (3.73)

$$\psi^{q_o}(q_o) = 0,$$

$$D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right) = 0.$$

We expand this function about $q_o = 0$ by Taylor series (Taylor series for two dependent variable)

$$D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{qo=0} + \frac{d}{dq_o}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{q_o=0}\,\delta q_o$$
$$+\frac{d}{da}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{q_o=0}\,\frac{da}{dq_o}\delta q_o + (O)\,\delta q_0^2 = 0$$

$$D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{qo=0} + \frac{d}{dq_o}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{q_o=0}\,\delta q_o \tag{3.79}$$

$$+\frac{d}{da}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{q_o=0}\,\frac{da}{dq_o}\delta q_o = 0. \tag{3.80}$$

Term-1
From Eq. (3.73)

$$D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{qo=0} = 0.$$

Term-2

$$\frac{d}{dq_o}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right) = \frac{d}{dq_o}\left[\frac{\sqrt{\pi}2^{a/2}}{\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q_0^2}{2}\frac{2m\omega}{\hbar}\right)\right] - \frac{d}{dq_o}\left[\frac{\sqrt{\pi}2^{(a+1)/2}}{\Gamma\left(-\frac{a}{2}\right)}q_o\sqrt{\frac{2m\omega}{\hbar}}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right)\right],$$

$$\frac{d}{dq_o}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right) = \frac{\sqrt{\pi}2^{a/2}}{\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}\frac{d}{dq_o}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right) - \frac{\sqrt{\pi}2^{(a+1)/2}}{\Gamma\left(-\frac{a}{2}\right)}\frac{d}{dq_o}\left[q_o\sqrt{\frac{2m\omega}{\hbar}}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right)\right],$$

$$\begin{aligned}\frac{d}{dq_o}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right) = {} & \frac{\sqrt{\pi}2^{a/2}}{\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}\frac{d}{dq_o}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right)\\ & - \frac{\sqrt{\pi}2^{(a+1)/2}}{\Gamma\left(-\frac{a}{2}\right)}q_o\sqrt{\frac{2m\omega}{\hbar}}\frac{d}{dq_o}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right)\\ & - \frac{\sqrt{\pi}2^{(a+1)/2}}{\Gamma\left(-\frac{a}{2}\right)}\sqrt{\frac{2m\omega}{\hbar}}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right).\end{aligned}$$

At $q_o = 0$

$$F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right)|_{q_o=0} = 1,$$

$$\frac{d}{dq_o}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q_o^2}{2}(\frac{2m\omega}{\hbar}\right)|_{q_o=0}=0,$$

$$F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right)|_{q_o=0}=1,$$

$$\frac{d}{dq_o}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right)|_{q_o=0}=0.$$

Therefore

$$\frac{d}{dq_o}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{q_o=0}=-\frac{2^{(a+1)/2}\sqrt{\pi}}{\Gamma\left(-\frac{a}{2}\right)}\sqrt{\frac{2m\omega}{\hbar}}.$$

Term-3

$$\frac{d}{da}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{q_o=0}=\frac{d}{da}\left[\frac{2^{a/2}\sqrt{\pi}}{\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q_0^2}{2}\frac{2m\omega}{\hbar}\right)\right]$$
$$-\frac{d}{da}\left[\frac{2^{(a+1)/2}\sqrt{\pi}}{\Gamma\left(-\frac{a}{2}\right)}q_o\sqrt{\frac{2m\omega}{\hbar}}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right)\right],$$

$$\frac{d}{da}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{q_o=0}=\frac{2^{a/2}\frac{1}{2}ln2\sqrt{\pi}}{\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q_0^2}{2}\frac{2m\omega}{\hbar}\right)$$
$$-2^{a/2}\sqrt{\pi}\frac{\frac{-1}{2}\frac{d}{da}\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}{\left[\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)\right]^2}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q_0^2}{2}\frac{2m\omega}{\hbar}\right)$$
$$+2^{a/2}\sqrt{\pi}\frac{2^{a/2}\sqrt{\pi}}{\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}\frac{d}{da}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q_0^2}{2}\frac{2m\omega}{\hbar}\right)$$
$$-\frac{2^{1/2}2^{a/2}\frac{1}{2}ln2\sqrt{\pi}}{\Gamma\left(-\frac{a}{2}\right)}q_o\sqrt{\frac{2m\omega}{\hbar}}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right)$$
$$-2^{(a+1)/2}\sqrt{\pi}\left\{\frac{-\frac{d}{da}\Gamma\left(-\frac{a}{2}\right)}{\left[\Gamma\left(-\frac{a}{2}\right)\right]^2}\right\}q_o\sqrt{\frac{2m\omega}{\hbar}}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right)$$
$$-\frac{2^{(a+1)/2}\sqrt{\pi}}{\Gamma\left(-\frac{a}{2}\right)}q_o\sqrt{\frac{2m\omega}{\hbar}}\frac{d}{da}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right).$$

At $q_o = 0$

$$F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q_0^2}{2}\frac{2m\omega}{\hbar}\right)=1,$$

$$F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right)=1,$$

$$\frac{d}{da}F_1\left(-\frac{a}{2},\frac{1}{2},\frac{q_0^2}{2}\frac{2m\omega}{\hbar})\right)=0,$$

$$\frac{d}{da}F_1\left(-\frac{a-1}{2},\frac{3}{2},\frac{q_o^2}{2}\frac{2m\omega}{\hbar}\right)=0.$$

Therefore

$$\frac{d}{da}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{q_o=0}=\frac{2^{a/2}\frac{1}{2}ln2\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}+2^{a/2}\sqrt{\pi}\left\{-\frac{\frac{-1}{2}\frac{d}{da}\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}{\left[\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)\right]^2}\right\},$$

$$\frac{d}{da}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{q_o=0}=\frac{2^{(a-2)/2}ln2\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}+\frac{2^{(a-2)/2}\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}\left[\frac{\frac{d}{da}\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}\right],$$

$$\frac{d}{da}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{q_o=0}=\frac{2^{(a-2)/2}\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}\left[ln2+\frac{\frac{d}{da}\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}\right].$$

We know the Digamma[23] function is

$$\Psi\left(-\frac{a}{2}+\frac{1}{2}\right)=\frac{\frac{d}{da}\Gamma\left(-\frac{a}{2}+\frac{1}{2}\right)}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}.$$

Therefore

$$\frac{d}{da}D_a\left(q_o\sqrt{\frac{2m\omega}{\hbar}}\right)|_{q_o=0}=\frac{2^{(a-2)/2}\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}\left[ln2+\Psi\left(-\frac{a}{2}+\frac{1}{2}\right)\right].$$

2^{nd} part of **Term-3**

$$\frac{da}{dq_o} = \frac{d}{dq_o}\left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right)$$

$$\frac{da}{dq_o} = \frac{1}{\hbar\omega}\frac{dE}{dq_o}$$

Using all these terms in Eq. (3.79) we obtain

$$-\frac{2^{(a+1)/2}\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}\right)}\sqrt{\frac{2m\omega}{\hbar}}\delta q_o + \frac{2^{(a-2)/2}\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}\left[ln2 + \Psi\left(-\frac{a}{2}+\frac{1}{2}\right)\right]\frac{1}{\hbar\omega}\frac{dE}{dq_o}\delta q_o = 0,$$

$$\left\{-\frac{2^{(a+1)/2}\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}\right)}\sqrt{\frac{2m\omega}{\hbar}} + \frac{2^{(a-2)/2}\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}\left[ln2 + \Psi\left(-\frac{a}{2}+\frac{1}{2}\right)\right]\frac{1}{\hbar\omega}\frac{dE}{dq_o}\right\}\delta q_o = 0,$$

$$\Rightarrow -\frac{2^{(a+1)/2}\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}\right)}\sqrt{\frac{2m\omega}{\hbar}} + \frac{2^{(a-2)/2}\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}\left[ln2 + \Psi\left(-\frac{a}{2}+\frac{1}{2}\right)\right]\frac{1}{\hbar\omega}\frac{dE}{dq_o} = 0,$$

$$\frac{2^{(a-2)/2}\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}\left[ln2 + \Psi\left(-\frac{a}{2}+\frac{1}{2}\right)\right]\frac{1}{\hbar\omega}\frac{dE}{dq_o} = \frac{2^{(a+1)/2}\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}\right)}\sqrt{\frac{2m\omega}{\hbar}},$$

$$\Rightarrow \frac{dE}{dq_o} = \frac{\frac{2^{(a+1)/2}\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}\right)}\sqrt{\frac{2m\omega}{\hbar}}\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)\hbar\omega}{2^{(a-2)/2}\sqrt{\pi}\left[ln2 + \Psi\left(-\frac{a}{2}+\frac{1}{2}\right)\right]},$$

$$\frac{dE}{dq_o} = \frac{\frac{2^{(a+1)/2}\sqrt{\pi}}{\mathit{\Gamma}\left(-\frac{a}{2}\right)}\sqrt{\frac{2m\omega}{\hbar}}\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)\hbar\omega}{2^{(a-2)/2}\sqrt{\pi}\left[ln2 + \Psi\left(-\frac{a}{2}+\frac{1}{2}\right)\right]},$$

$$\frac{dE}{dq_o} = \frac{2^2\sqrt{m\omega^3\hbar}\mathit{\Gamma}\left(-\frac{a}{2}+\frac{1}{2}\right)}{\mathit{\Gamma}\left(-\frac{a}{2}\right)\left[ln2 + \Psi\left(-\frac{a}{2}+\frac{1}{2}\right)\right]},$$

from Eq. (3.25)

$$a = \frac{E_n}{\hbar\omega} - \frac{1}{2},$$

$$\frac{dE}{dq_o} = \frac{4\sqrt{m\omega^3\hbar}\Gamma\left(-\frac{1}{2}\left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right) + \frac{1}{2}\right)}{\Gamma\left(-\frac{1}{2}\left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right)\right)\left(ln2 + \Psi\left(-\frac{1}{2}\left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right) + \frac{1}{2}\right)\right)},$$

$$\frac{dE}{dq_o} = \frac{4\sqrt{m\omega^3\hbar}\Gamma\left(\frac{3\hbar\omega - 2E_n}{4\hbar\omega}\right)}{\Gamma\left(\frac{\hbar\omega - 2E_n}{4\hbar\omega}\right)\left[ln2 + \Psi\left(\frac{3\hbar\omega - 2E_n}{4\hbar\omega} - \frac{1}{2}\right)\right]}.$$

Now we replace (assuming particle to be on the right side of partition when barrier is at $q_o = 0$)

$$E_n \to \left(2n + \frac{3}{2}\right)\hbar\omega.$$

Then the denominator and numerator diverge in the above equation, so we have to consider the limiting value.

$$E_n \to \left(2n + \frac{3}{2}\right)\hbar\omega + \sigma.$$

where $\sigma \to 0$, In this limit our desired equation reduces to

$$\frac{dE}{dq_o} = \frac{\sqrt{\frac{m\omega^3\hbar}{\pi}}(2n+2)!}{4^n n!\,(n+1)!}.$$

Using this relation in Eq. (3.78)

$$F = -\frac{1}{Z_R}\sum_{n=0}^{\infty} e^{-\beta E_n}\frac{\sqrt{\frac{m\omega^3\hbar}{\pi}}(2n+2)!}{4^n n!\,(n+1)!},$$

$$F = -\sqrt{\frac{m\omega^3\hbar}{\pi}}\frac{1}{Z_R}\sum_{n=0}^{\infty}\frac{(2n+2)!}{4^n n!\,(n+1)!}e^{-\beta E_n}.$$

At $q = q_o = 0$ and $E_n = \left(2n + \frac{3}{2}\right)\hbar\omega$, we obtain

$$F = -\sqrt{\frac{m\omega^3\hbar}{\pi}}\frac{1}{Z_R}\sum_{n=0}^{\infty}\frac{(2n+2)!}{4^n n!\,(n+1)!}e^{-\beta(2n+\frac{3}{2})\hbar\omega},$$

$$F = -\sqrt{\frac{m\omega^3\hbar}{\pi}}\frac{1}{Z_R}\sum_{n=0}^{\infty}\frac{(2n+2)!}{4^n n!\,(n+1)!}e^{-2\beta n\hbar\omega}e^{-\frac{3}{2}\beta\hbar\omega},$$

$$F = -\sqrt{\frac{m\omega^3\hbar}{\pi}}\frac{e^{-\frac{3}{2}\beta\hbar\omega}}{Z_R}\sum_{n=0}^{\infty}\frac{(2n+2)!}{4^n n!\,(n+1)!}\left(e^{-2\beta\hbar\omega}\right)^n. \tag{3.81}$$

Here

$$\sum_{n=0}^{\infty}\frac{(2n+2)!}{4^n n!\,(n+1)!}\left(e^{-2\beta\hbar\omega}\right)^n = 2+\frac{4!}{4.2!}e^{-2\beta\hbar\omega}+\frac{6!}{4^2.3!.2!}\left(e^{-2\beta\hbar\omega}\right)^2+\frac{8!}{4^3.3!.4!}\left(e^{-2\beta\hbar\omega}\right)^3...,$$

$$\sum_{n=0}^{\infty}\frac{(2n+2)!}{4^n n!\,(n+1)!}\left(e^{-2\beta\hbar\omega}\right)^n = 2+3e^{-2\beta\hbar\omega}+\frac{15}{2.2!}\left(e^{-2\beta\hbar\omega}\right)^2+\frac{105}{4.3!}\left(e^{-2\beta\hbar\omega}\right)^3....,$$

$$\sum_{n=0}^{\infty}\frac{(2n+2)!}{4^n n!\,(n+1)!}\left(e^{-2\beta\hbar\omega}\right)^n = 2\left[1+\frac{3}{2}e^{-2\beta\hbar\omega}+\frac{15}{4.2!}\left(e^{-2\beta\hbar\omega}\right)^2+\frac{105}{8.3!}\left(e^{-2\beta\hbar\omega}\right)^3...\right]. \tag{3.82}$$

From binomial series

$$\frac{1}{(1-x)^{3/2}} = 1+\frac{3}{2}x+\frac{15}{4.2!}x^2+\frac{105}{8.3!}x^3....,$$

for $x = e^{-2\beta\hbar\omega}$

$$\frac{1}{\left(1-e^{-2\beta\hbar\omega}\right)^{3/2}} = 1+\frac{3}{4.2!}e^{-2\beta\hbar\omega}+\frac{15}{4^2.3!.2!}\left(e^{-2\beta\hbar\omega}\right)^2+...,$$

so (3.82)

$$\sum_{n=0}^{\infty}\frac{(2n+2)!}{4^n n!\,(n+1)!}\left(e^{-2\beta\hbar\omega}\right)^n = \frac{2}{\left(1-e^{-2\beta\hbar\omega}\right)^{3/2}}.$$

Using this in Eq. (3.81)

$$F = -\sqrt{\frac{m\omega^3\hbar}{\pi}}\frac{e^{-\frac{3}{2}\beta\hbar\omega}}{Z_R}\frac{2}{\left(1-e^{-2\beta\hbar\omega}\right)^{3/2}},$$

where

$$Z_R=\sum_{n=0}^{\infty} e^{-\beta E_n},$$

from Eq. (3.75)

$$Z_R =\sum_{n=0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)\hbar\omega}.$$

$\sum_{n=0}^{\infty} e^{-\beta\left(2n+\frac{3}{2}\right)}$ is a geometric series with initial term $a_1 = \frac{3}{2}$ and common ratio $r = 2\hbar\omega$, we can evaluate the sum:

$$Z_R = \frac{e^{-\frac{3}{2}\beta\hbar\omega}}{1 - e^{-2\beta\hbar\omega}}.$$

Finally,

$$F = -\sqrt{\frac{m\omega^3\hbar}{\pi}} \frac{e^{-\frac{3}{2}\beta\hbar\omega}}{\frac{e^{-\frac{3}{2}\beta\hbar\omega}}{1 - e^{-2\beta\hbar\omega}}} \frac{2}{\left(1 - e^{-2\beta\hbar\omega}\right)^{3/2}},$$

$$F = -2\sqrt{\frac{m\omega^3\hbar}{\pi}} \left(1 - e^{-2\beta\hbar\omega}\right)^{-1/2}.$$

This is the force that pushes the barrier towards left when barrier is at $q = q_o = 0$.

Chapter 4

Full Quantum Analysis

In the previous chapter , we have seen that **Second law of thermodynamics is apparently violated**. Now we will see that in fact it is not violated when demon is treated dynamically during the quantum analysis.

4.1 Ready State of Demon

Let us consider the demon to be a two state quantum pointer variable.

$|\mathscr{D}_L\rangle$: This state corresponds to demon when he is present on the left side of the partition.

$|\mathscr{D}_R\rangle$: This state corresponds to demon when he is present on the right side of the partition.

Neutral or Ready state of Demon(pointer variable) can be written as:

$$|\mathscr{D}_o\rangle = \frac{1}{\sqrt{2}}\left(|\mathscr{D}_L\rangle + |\mathscr{D}_R\rangle\right).$$

Density operator of the ready state of demon will be

$$\hat{\rho}_D = |\mathscr{D}_o\rangle\langle\mathscr{D}_o|,$$

$$\hat{\rho}_D = \frac{1}{\sqrt{2}}\left(|\mathscr{D}_L\rangle + |\mathscr{D}_R\rangle\right)\frac{1}{\sqrt{2}}\left(\langle\mathscr{D}_L| + \langle\mathscr{D}_R|\right),$$

$$\hat{\rho}_D = \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R|\right). \tag{4.1}$$

Here we can see that the initially state of the demon is a pure state:

$$Tr\left(\hat{\rho}_D^2\right) = 1. \tag{4.2}$$

4.2 Initial Composite State of System

At this stage, we can write the composite state [27] of demon and particle.

$$\hat{\rho}_{in,s} = \hat{\rho}_{in} \otimes \hat{\rho}_D, \tag{4.3}$$

where $\hat{\rho}_{in}$ is calculated already given in Eq. (3.4).

4.3 Composite State of System after Barrier Insertion

Now, if we insert the barrier quasi-statically at $q = q_o$ neglecting the dynamical effects of pointer variable i.e. the demon state, full Hamiltonian will be

$$\hat{H}_{\alpha,s} = \hat{H}_\alpha \otimes \hat{I}_D.$$

α represents the strength or height of the barrier.

$\hat{H}_\alpha$ represents the Hamiltonian acting on the particle after barrier insertion.

$\hat{I}_D$ represents the identity operator acting on the demon's Hilbert space [28] after barrier insertion.

Now, we will construct the time evolution unitary operator $\hat{U}$ for the above Hamiltonian $\hat{H}_{\alpha,s}$.

$$\hat{U} = e^{-i\hat{H}_{\alpha,s}\delta t},$$

$$\hat{U} = e^{-i\left(\hat{H}_\alpha \otimes \hat{I}_D\right)\delta t},$$

$$\hat{U} = \hat{I}_\alpha \otimes \hat{I}_D - i\left(\hat{H}_\alpha \otimes \hat{I}_D\right)\delta t - \left(\hat{H}_\alpha \otimes \hat{I}_D\right)^2 \delta t^2 + ...$$

$$\because \left(\hat{H}_\alpha \otimes \hat{I}_D\right)^2 = \hat{H}_\alpha^2 \otimes \hat{I}_D^2.$$

$$\Rightarrow \hat{U} = \left(\hat{I}_\alpha - i\hat{H}_\alpha\delta t - \hat{H}_\alpha^2\delta t^2 + ...\right) \otimes \hat{I}_D,$$

$$\hat{U} = e^{-i\hat{H}_\alpha\delta t} \otimes \hat{I}_D,$$

and

$$\hat{U}^\dagger = e^{i\hat{H}_\alpha\delta t} \otimes \hat{I}_D.$$

Applying this unitary operator on the composite state given in Eq. (4.3)

$$\hat{\rho}_{\perp,s} = \hat{U}\left(\hat{\rho}_{in} \otimes \hat{\rho}_D\right)\hat{U}^{\dagger},$$

$$\hat{\rho}_{\perp,s} = e^{-i\hat{H}_\alpha \delta t} \otimes \hat{I}_D \left(\hat{\rho}_{in} \otimes \hat{\rho}_D\right) e^{i\hat{H}_\alpha \delta t} \otimes \hat{I}_D,$$

$$\hat{\rho}_{\perp,s} = e^{-i\hat{H}_\alpha \delta t}\hat{\rho}_{in} e^{i\hat{H}_\alpha \delta t} \otimes \hat{I}_D \hat{\rho}_D \hat{I}_D,$$

$$\hat{\rho}_{\perp,s} = e^{-i\hat{H}_\alpha \delta t}\hat{\rho}_{in} e^{i\hat{H}_\alpha \delta t} \otimes \hat{\rho}_D.$$

From Eq. (2.11)

$$\hat{\rho}(t) = \hat{\rho}_{\perp} = e^{-i\hat{H}_\alpha \delta t}\hat{\rho}_{in} e^{i\hat{H}_\alpha \delta t}$$

Therefore

$$\hat{\rho}_{\perp,s} = \hat{\rho}_{\perp} \otimes \hat{\rho}_D. \tag{4.4}$$

This is the composite state of system after the barrier insertion, where $\hat{\rho}_{\perp}$is already calculated given in Eq (3.50).

4.4 Composite State of System After Measurements

For measurements, we need to introduce interaction between demon (Pointer variable) and particle. We can now construct the interaction Hamiltonian.

Recall Eq. (3.51) and (3.52)

$$\hat{P}_L = \sum_{n=0}^{\infty} |L_n\rangle\langle L_n|,$$

$$\hat{P}_R = \sum_{n=0}^{\infty} |R\rangle\langle R_n|.$$

We define

$$\hat{\Pi} = \hat{P}_L - \hat{P}_R,$$

$$\hat{\Pi} = \sum_{n=0}^{\infty} \left(|L_n\rangle\langle L_n| - |R_n\rangle\langle R_n|\right).$$

For the demon contribution

$$|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|.$$

Note:

We can also choose $(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| - |\mathscr{D}_R\rangle\langle\mathscr{D}_R|)$, it will give the same results.

Finally, we can write the interaction Hamiltonian as

$$\hat{H}_{int} = i\lambda\hat{\Pi} \otimes (|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|)\,.$$

λ represent the interaction strength between particle and demon. Interaction is introduced for a very short interval of time δt. As the interaction Hamiltonian is independent of time, so the evolution operator can simply be written as;

$$\hat{U}_{int} = e^{-i\hat{H}_{int}\delta t},$$

$$\hat{U}_{int} = e^{-i\left(i\lambda\hat{\Pi}\otimes(|\mathscr{D}_L\rangle\langle\mathscr{D}_R|-|\mathscr{D}_R\rangle\langle\mathscr{D}_L|)\right)\delta t},$$

$$\hat{U}_{int} = e^{\lambda\hat{\Pi}\otimes(|\mathscr{D}_L\rangle\langle\mathscr{D}_R|-|\mathscr{D}_R\rangle\langle\mathscr{D}_L|)\delta t},$$

$$\begin{aligned}\hat{U}_{int} =& \hat{I}_P \otimes \hat{I}_D + \hat{\Pi} \otimes (|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|)\,\lambda\delta t \\ &+ \frac{\left(\hat{\Pi} \otimes (|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|)\right)^2}{2!}(\lambda\delta t)^3 \\ &+ \frac{\left(\hat{\Pi} \otimes (|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|)\right)^3}{3!}(\lambda\delta t)^3 + ...,\end{aligned}$$

where

$\hat{I}_P$ is the identity operator on particle Hilbert space.

$\hat{I}_D$ is the identity operator on demon Hilbert space.

$$\begin{aligned}\hat{U}_{int} =& \hat{I}_P \otimes \hat{I}_D + \hat{\Pi} \otimes (|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|)\,\lambda\delta t \\ &+ \frac{\hat{\Pi}^2 \otimes (|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|)^2}{2!}(\lambda\delta t)^2 \\ &+ \frac{\hat{\Pi}^3 \otimes (|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|)^3}{3!}(\lambda\delta t)^3 + ...\end{aligned}$$

but

$$\hat{\Pi}^2 = \sum_{n=0}^{\infty}(|L_n\rangle\langle L_n| - |R_n\rangle\langle R_n|)\sum_{m=0}^{\infty}(|L_m\rangle\langle L_m| - |R_m\rangle\langle R_m|)\,,$$

$$\hat{\Pi}^2 = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \left(|L_n\rangle\langle L_n| - |R_n\rangle\langle R_n|\right)\left(|L_m\rangle\langle L_m| - |R_m\rangle\langle R_m|\right),$$

$$\begin{aligned}\hat{\Pi}^2 + &\sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \left(|L_n\rangle\langle L_n|L_m\rangle\langle L_m| - |R_n\rangle\cancelto{0}{\langle R_n|L_m\rangle\langle L_m|}\right) \\ &+ \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \left(|R_n\rangle\langle R_n|R_m\rangle\langle R_m| - |L_n\rangle\cancelto{0}{\langle L_n|R_m\rangle\langle R_m|}\right),\end{aligned}$$

for $m = n$

$$\hat{\Pi}^2 = \sum_{n=0}^{\infty} \left(|L_n\rangle\langle L_n| + R_n\rangle\langle R_n|\right) = \hat{I}_P,$$

$$\Rightarrow \hat{\Pi}^2 = \hat{I}_P.$$

Furthermore,

$$\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)^2 = \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right),$$

$$\begin{aligned}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)^2 = &\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\right) \\ &+ \left(|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\mathscr{D}_R\rangle\langle\mathscr{D}_L| - |\mathscr{D}_L\rangle\langle\mathscr{D}_R|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right),\end{aligned}$$

$$\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)^2 = -\left(|\mathscr{D}_L\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right).$$

$$\because |\mathscr{D}_L\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R| = \hat{I}_D.$$

Therefore

$$\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)^2 = -\hat{I}_D.$$

Hence

$$\begin{aligned}\hat{U}_{int} = &\hat{I}_P \otimes \hat{I}_D + \hat{\Pi} \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\lambda\delta t - \frac{\hat{I}_P \otimes \hat{I}_D}{2!}(\lambda\delta t)^2 \\ &- \frac{\hat{\Pi} \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)}{3!}(\lambda\delta t)^3 + ...\end{aligned}$$

We know that projective measurement is a special case of generalized measurements. For projective measurement, we can take

$$\delta t = \frac{\pi\hbar}{4\lambda}, \Rightarrow \lambda\delta t = \frac{\pi}{4}.$$

$$\begin{aligned}\Rightarrow \hat{U}_{int} =& \hat{I}_P \otimes \hat{I}_D + \hat{\Pi} \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\frac{\pi}{4} - \frac{\hat{I}_P \otimes \hat{I}_D}{2!}\left(\frac{\pi}{4}\right)^2 \\ &- \frac{\hat{\Pi} \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)}{3!}\left(\frac{\pi}{4}\right)^3 + ...,\end{aligned}$$

$$\begin{aligned}\hat{U}_{int} =& \hat{I}_P \otimes \hat{I}_D \left[1 - \frac{1}{2!}\left(\frac{\pi}{4}\right)^2 + \frac{1}{4!}\left(\frac{\pi}{4}\right)^4 + ...\right] \\ &+ \hat{\Pi} \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\left[\frac{\pi}{4} - \frac{1}{3!}\left(\frac{\pi}{4}\right)^3 + ...\right].\end{aligned}$$

But we know

$$cos\left(\frac{\pi}{4}\right) = 1 - \frac{1}{2!}\left(\frac{\pi}{4}\right)^2 + \frac{1}{4!}\left(\frac{\pi}{4}\right)^4 + ... = \frac{1}{\sqrt{2}},$$

$$sin\left(\frac{\pi}{4}\right) = \frac{\pi}{4} - \frac{1}{3!}\left(\frac{\pi}{4}\right)^3 + \frac{1}{5!}\left(\frac{\pi}{4}\right)^5 ... = \frac{1}{\sqrt{2}}.$$

So,

$$\hat{U}_{int} = \frac{1}{\sqrt{2}}\hat{I}_P \otimes \hat{I}_D + \frac{1}{\sqrt{2}}\hat{\Pi} \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right),$$

$$\hat{U}_{int} = \frac{1}{\sqrt{2}}\left(\hat{I}_P \otimes \hat{I}_D + \hat{\Pi} \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\right), \tag{4.5}$$

$$\hat{U}^{\dagger}_{int} = \frac{1}{\sqrt{2}}\left[\hat{I}_P \otimes \hat{I}_D - \hat{\Pi} \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\right].$$

Now, we can calculate the time evolve state $\hat{\rho}_{evolved,s}$ of composite system using this unitary operator. From Eq. (4.4) and (4.5), composite state of system after time evolution can be obtained as

$$\hat{\rho}_{evolved,s} = \hat{U}_{int}\hat{\rho}_{\perp,s}\hat{U}^{\dagger}_{int},$$

$$\hat{\rho}_{evolved,s} = \hat{U}_{int}\left(\hat{\rho}_{\perp} \otimes \hat{\rho}_D\right)\hat{U}^{\dagger}_{int},$$

$$\hat{\rho}_{evolved,s} = \frac{1}{\sqrt{2}}\left[\hat{I}_P \otimes \hat{I}_D + \hat{\Pi} \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\right]\hat{\rho}_\perp$$
$$\otimes\hat{\rho}_D \frac{1}{\sqrt{2}}\left[\hat{I}_P \otimes \hat{I}_D - \hat{\Pi} \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\right],$$

$$\begin{aligned}\hat{\rho}_{evolved,s} =& \frac{1}{2}\left[\hat{I}_P\hat{\rho}_\perp\hat{I}_P \otimes \hat{I}_D\hat{\rho}_D\hat{I}_D\right]\\ &+\frac{1}{2}\left[\hat{\Pi}\hat{\rho}_\perp\hat{I}_P \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\hat{\rho}_D\hat{I}_D\right]\\ &-\frac{1}{2}\left[\hat{I}_P\hat{\rho}_\perp\hat{\Pi} \otimes \hat{I}_D\hat{\rho}_D\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\right]\\ &-\frac{1}{2}\left[\hat{\Pi}\hat{\rho}_\perp\hat{\Pi} \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\hat{\rho}_D\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\right],\end{aligned} \tag{4.6}$$

Now, we will solve each term of Eq. (4.6) separately,

Term-1

$$\left(\hat{I}_P\hat{\rho}_\perp\hat{I}_P \otimes \hat{I}_D\hat{\rho}_D\hat{I}_D\right) = \hat{\rho}_\perp \otimes \hat{\rho}_D,$$

$$\hat{I}_P\hat{\rho}_\perp\hat{I}_P \otimes \hat{I}_D\hat{\rho}_D\hat{I}_D = \hat{\rho}_\perp \otimes \hat{\rho}_D. \tag{4.7}$$

Using Eq. (4.1) and (3.58)

$$\hat{I}_P\hat{\rho}_\perp\hat{I}_P \otimes \hat{I}_D\hat{\rho}_D\hat{I}_D = \frac{1}{2}\left(\hat{\rho}_L + \hat{\rho}_R\right) \otimes \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right). \tag{4.8}$$

Term-2

$$\lambda\left[\hat{\Pi}\hat{\rho}_\perp\hat{I}_P \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\hat{\rho}_D\hat{I}_D\right].$$

Considered $\hat{\Pi}\hat{\rho}_\perp\hat{I}_P$

$$\hat{\Pi}\hat{\rho}_\perp\hat{I}_P = \sum_{n=0}^{\infty}\left(|L_n\rangle\langle L_n| - |R_n\rangle\langle R_n|\right)\hat{\rho}_\perp\sum_{k=0}^{\infty}\left(|L_k\rangle\langle L_k| + |R_k\rangle\langle R_k|\right).$$

Form Eq. (3.51) and (3.52)

$$\hat{\Pi}\hat{\rho}_\perp\hat{I}_P = \left(\hat{P}_L - \hat{P}_R\right)\hat{\rho}_\perp\left(\hat{P}_L + \hat{P}_R\right),$$

$$\hat{\Pi}\hat{\rho}_\perp\hat{I}_P = \left(\hat{P}_L\hat{\rho}_\perp\hat{P}_L - \hat{P}_R\hat{\rho}_\perp\hat{P}_L + \hat{P}_L\hat{\rho}_\perp\hat{P}_R - \hat{P}_R\hat{\rho}_\perp\hat{P}_R\right).$$

But from Eq. (3.53) and (3.56)

$$\hat{P}_L\hat{\rho}_\perp\hat{P}_L = \frac{\hat{\rho}_R}{2},$$

$$\hat{P}_R\hat{\rho}_\perp\hat{P}_R = \frac{\hat{\rho}_L}{2}.$$

Where as

$$\hat{P}_L\hat{\rho}_\perp\hat{P}_R = 0,$$

$$\hat{P}_R\hat{\rho}_\perp\hat{P}_L = 0.$$

Hence

$$\hat{\Pi}\hat{\rho}_\perp\hat{I}_P = \frac{1}{2}\left(\hat{\rho}_L - \hat{\rho}_R\right).$$

Now we consider $\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\hat{\rho}_D\hat{I}_D$:

$$\begin{aligned}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\hat{\rho}_D\hat{I}_D =& |\mathscr{D}_L\rangle\langle\mathscr{D}_R|\frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\\ &- |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right),\end{aligned}$$

$$\begin{aligned}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\hat{\rho}_D\hat{I}_D =& \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\mathscr{D}_R\rangle\langle\mathscr{D}_L| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R|\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\\ &- \frac{1}{2}\left(|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\right),\end{aligned}$$

$$\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\hat{\rho}_D\hat{I}_D = \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| - |\mathscr{D}_R\rangle\langle\mathscr{D}_R| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right),$$

Term-2 becomes

$$\begin{aligned}\left(\hat{\Pi}\hat{\rho}_\perp\hat{I}_P \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\hat{\rho}_D\hat{I}_D\right) =& \frac{1}{2}\left(\hat{\rho}_L - \hat{\rho}_R\right) \otimes \frac{1}{2}(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R|\\ &- |\mathscr{D}_R\rangle\langle\mathscr{D}_L| - |\mathscr{D}_R\rangle\langle\mathscr{D}_R|).\end{aligned} \tag{4.9}$$

Term-3

$$\hat{I}_P\hat{\rho}_\perp\hat{\Pi} \otimes \hat{I}_D\hat{\rho}_D\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right).$$

Consider $\hat{I}_P \hat{\rho}_\perp \hat{\Pi}$ first

$$\hat{I}_P \hat{\rho}_\perp \hat{\Pi} = \left(\hat{P}_L + \hat{P}_R\right) \hat{\rho}_\perp \left(\hat{P}_L - \hat{P}_R\right),$$

$$\hat{I}_P \hat{\rho}_\perp \hat{\Pi} = \left(\hat{P}_L \hat{\rho}_\perp \hat{P}_L - \hat{P}_R \hat{\rho}_\perp \hat{P}_L - \hat{P}_L \hat{\rho}_\perp \hat{P}_R - \hat{P}_R \hat{\rho}_\perp \hat{P}_R\right).$$

But from Eq. (3.53) and (3.56)

$$\hat{P}_L \hat{\rho}_\perp \hat{P}_L = \frac{\hat{\rho}_R}{2},$$

$$\hat{P}_R \hat{\rho}_\perp \hat{P}_R = \frac{\hat{\rho}_L}{2}.$$

Where as

$$\hat{P}_L \hat{\rho}_\perp \hat{P}_R = 0,$$

$$\hat{P}_R \hat{\rho}_\perp \hat{P}_L = 0. \tag{4.10}$$

Hence

$$\hat{I}_P \hat{\rho}_\perp \hat{\Pi} = \frac{1}{2}\left(\hat{\rho}_L - \hat{\rho}_R\right).$$

Now we consider $\hat{I}_D \hat{\rho}_D \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)$:

$$\begin{aligned}\hat{I}_D \hat{\rho}_D \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right) =& \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)|\mathscr{D}_L\rangle\langle\mathscr{D}_R| \\ &- \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)|\mathscr{D}_R\rangle\langle\mathscr{D}_L|,\end{aligned}$$

$$\begin{aligned}\hat{I}_D \hat{\rho}_D \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right) =& \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L|\mathscr{D}_L\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\right) \\ &- \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right),\end{aligned}$$

$$\hat{I}_D \hat{\rho}_D \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right) = \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R| - |\mathscr{D}_L\rangle\langle\mathscr{D}_L| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right).$$

Term-3 becomes

$$\hat{I}_P\hat{\rho}_\perp\hat{\Pi}\otimes\hat{I}_D\hat{\rho}_D\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R|-|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right) \tag{4.11}$$
$$=\frac{1}{2}\left(\hat{\rho}_L-\hat{\rho}_R\right)\otimes\frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R|+|\mathscr{D}_R\rangle\langle\mathscr{D}_R|-|\mathscr{D}_L\rangle\langle\mathscr{D}_L|-|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right).$$

Term-4

$$\hat{\Pi}\hat{\rho}_\perp\hat{\Pi}\otimes\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R|-|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\hat{\rho}_D\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R|-|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right).$$

Consider $\hat{\Pi}\hat{\rho}_\perp\hat{\Pi}$ first

$$\hat{\Pi}\hat{\rho}_\perp\hat{\Pi}=\sum_{m=0}^{\infty}\left(|L_m\rangle\langle L_m|-|R_m\rangle\langle R_m|\right)\hat{\rho}_\perp\sum_{k=0}^{\infty}\left(|L_k\rangle\langle L_k|-|R_k\rangle\langle R_k|\right),$$

$$\hat{\Pi}\hat{\rho}_\perp\hat{\Pi}=\left(\hat{P}_L-\hat{P}_R\right)\hat{\rho}_\perp\left(\hat{P}_L-\hat{P}_R\right),$$

$$\hat{\Pi}\hat{\rho}_\perp\hat{\Pi}=\left(\hat{P}_L\hat{\rho}_\perp\hat{P}_L-\hat{P}_R\hat{\rho}_\perp\hat{P}_L-\hat{P}_L\hat{\rho}_\perp\hat{P}_R+\hat{P}_R\hat{\rho}_\perp\hat{P}_R\right).$$

Using Eq. (4.10)

$$\hat{\Pi}\hat{\rho}_\perp\hat{\Pi}=\frac{1}{2}\left(\hat{\rho}_L+\hat{\rho}_R\right).$$

Now we consider $\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R|-|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\hat{\rho}_D\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R|-|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)$:

$$\begin{aligned}&\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R|-|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\hat{\rho}_D\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R|-|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\\&=|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\hat{\rho}_D|\mathscr{D}_L\rangle\langle\mathscr{D}_R|-|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\hat{\rho}_D|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\\&-|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\hat{\rho}_D|\mathscr{D}_R\rangle\langle\mathscr{D}_L|+|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\hat{\rho}_D|\mathscr{D}_R\rangle\langle\mathscr{D}_L|.\end{aligned}$$

$$\begin{aligned}&|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\hat{\rho}_D|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\\&=|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\left(\frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L|+|\mathscr{D}_R\rangle\langle\mathscr{D}_L|+|\mathscr{D}_L\rangle\langle\mathscr{D}_R|+|\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right)|\mathscr{D}_L\rangle\langle\mathscr{D}_R|.\end{aligned}$$

$$\begin{aligned}|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\hat{\rho}_D|\mathscr{D}_L\rangle\langle\mathscr{D}_R|=&\frac{1}{2}|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\mathscr{D}_L\rangle\langle\mathscr{D}_L|\mathscr{D}_L\rangle\langle\mathscr{D}_R|+\frac{1}{2}|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\\&+\frac{1}{2}|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\mathscr{D}_L\rangle\langle\mathscr{D}_R|+\frac{1}{2}|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\mathscr{D}_R\rangle\langle\mathscr{D}_R|\mathscr{D}_L\rangle\langle\mathscr{D}_R|,\end{aligned}$$

using orthonormality conditions

$$
\begin{aligned}
|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\hat{\rho}_D|\mathscr{D}_L\rangle\langle\mathscr{D}_R| =& \frac{1}{2}|\mathscr{D}_L\rangle\cancelto{0}{\langle\mathscr{D}_R|\mathscr{D}_L\rangle}\langle\mathscr{D}_L|\mathscr{D}_L\rangle\langle\mathscr{D}_R| + \frac{1}{2}|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\mathscr{D}_L\rangle\langle\mathscr{D}_R| \\
&+ \frac{1}{2}|\mathscr{D}_L\rangle\cancelto{0}{\langle\mathscr{D}_R|\mathscr{D}_L\rangle}\cancelto{0}{\langle\mathscr{D}_R|\mathscr{D}_L\rangle}\langle\mathscr{D}_R| + \frac{1}{2}|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\mathscr{D}_R\rangle\cancelto{0}{\langle\mathscr{D}_R|\mathscr{D}_L\rangle}\langle\mathscr{D}_R|,
\end{aligned}
$$

$$
|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\hat{\rho}_D|\mathscr{D}_L\rangle\langle\mathscr{D}_R| = \frac{1}{2}|\mathscr{D}_L\rangle\cancelto{1}{\langle\mathscr{D}_R|\mathscr{D}_R\rangle}\cancelto{1}{\langle\mathscr{D}_L|\mathscr{D}_L\rangle}\langle\mathscr{D}_R|
$$

$$
\Rightarrow |\mathscr{D}_L\rangle\langle\mathscr{D}_R|\hat{\rho}_D|\mathscr{D}_L\rangle\langle\mathscr{D}_R| = \frac{1}{2}|\mathscr{D}_L\rangle\langle\mathscr{D}_R|,
$$

similarly

$$
|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\hat{\rho}_D|\mathscr{D}_L\rangle\langle\mathscr{D}_R| = \frac{1}{2}|\mathscr{D}_R\rangle\langle\mathscr{D}_R|,
$$

$$
|\mathscr{D}_L\rangle\langle\mathscr{D}_R|\hat{\rho}_D|\mathscr{D}_R\rangle\langle\mathscr{D}_L| = \frac{1}{2}|\mathscr{D}_L\rangle\langle\mathscr{D}_L|,
$$

$$
|\mathscr{D}_R\rangle\langle\mathscr{D}_L|\hat{\rho}_D|\mathscr{D}_R\rangle\langle\mathscr{D}_L| = \frac{1}{2}|\mathscr{D}_R\rangle\langle\mathscr{D}_L|.
$$

Hence

$$
\begin{aligned}
&\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\hat{\rho}_D\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right) \\
=& \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_R| - |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)
\end{aligned}
$$

Term-4 becomes

$$
\begin{aligned}
&\hat{\Pi}\hat{\rho}_\perp\hat{\Pi}\otimes\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\hat{\rho}_D\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right) \\
=& \frac{1}{2}\left(\hat{\rho}_L + \hat{\rho}_R\right)\otimes\frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_R| - |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right).
\end{aligned} \tag{4.12}
$$

Using Eq. (4.8), (4.9), (4.11), (4.12) in Eq. (4.6), we obtain

$$
\begin{aligned}
\hat{\rho}_{evolved,s} =& \frac{1}{2}\left[\frac{1}{2}\left(\hat{\rho}_L + \hat{\rho}_R\right) \otimes \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right] \\
&+\frac{1}{2}\left[\frac{1}{2}\left(\hat{\rho}_L - \hat{\rho}_R\right) \otimes \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L| - |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right] \\
&-\frac{1}{2}\left[\frac{1}{2}\left(\hat{\rho}_L - \hat{\rho}_R\right) \otimes \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R| - |\mathscr{D}_L\rangle\langle\mathscr{D}_L| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\right] \\
&-\frac{1}{2}\left[\frac{1}{2}\left(\hat{\rho}_L + \hat{\rho}_R\right) \otimes \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_R| - |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\right],
\end{aligned}
$$

for convenience, we will add Term-1 to Term-2 and Term-3 to Term-4

$$
\begin{aligned}
\hat{\rho}_{evolved,s} =& \frac{1}{2}\left[\frac{1}{2}\left(\hat{\rho}_L + \hat{\rho}_R\right) \otimes \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right] \\
&-\frac{1}{2}\left[\frac{1}{2}\left(\hat{\rho}_L + \hat{\rho}_R\right) \otimes \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_R| - |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\right] \\
&+\frac{1}{2}\left[\frac{1}{2}\left(\hat{\rho}_L - \hat{\rho}_R\right) \otimes \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L| - |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right] \\
&-\frac{1}{2}\left[\frac{1}{2}\left(\hat{\rho}_L - \hat{\rho}_R\right) \otimes \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R| - |\mathscr{D}_L\rangle\langle\mathscr{D}_L| - |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right)\right],
\end{aligned}
$$

$$
\begin{aligned}
\hat{\rho}_{evolved,s} =& \frac{1}{4}\left(\hat{\rho}_L + \hat{\rho}_R\right) \otimes \left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right) \\
&+\frac{1}{4}\left(\hat{\rho}_L - \hat{\rho}_R\right) \otimes \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| - |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right),
\end{aligned}
$$

$$
\begin{aligned}
\hat{\rho}_{evolved,s} =& \frac{1}{4}\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{\rho}_R \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| \\
&+\frac{1}{4}\hat{\rho}_L \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R| + \hat{\rho}_R \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R| \\
&+\frac{1}{4}\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| - \hat{\rho}_R \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| \\
&-\frac{1}{4}\hat{\rho}_L \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R| + \hat{\rho}_R \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|.
\end{aligned}
$$

Above equation can be simplified as

$$
\hat{\rho}_{evolved,s} = \frac{1}{2}\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{\rho}_R \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right). \tag{4.13}
$$

Here, we can see that particle and demon become correlated as a result of interaction. If particle is located on the left side of partition then the state of demon is necessarily $|\mathscr{D}_L\rangle$ and if particle is located on the right side of partition then the state of demon is

$|\mathscr{D}_R\rangle$. This corresponds to exactly what we were expecting from strong or projective measurements.

4.5 Entropy

Let us calculate the entropy of both the particle and the demon before and after measurement. This, we can do with the help of partial trace.

4.5.1 Entropy of Demon before Interaction

From Eq. (4.1), density operator of demon before interaction can be written as

$$\hat{\rho}_D = \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L| + |\mathscr{D}_L\rangle\langle\mathscr{D}_R|\right).$$

From Eq. (4.13) we know this is a pure state having only one eigenvalue, so entropy will be zero.

$$S\left(\hat{\rho}_D\right) = 0. \tag{4.14}$$

4.5.2 Entropy of Demon after Interaction

First we need to determine the density operator of demon after interaction. Taking partial trace of Eq. (4.13) with respect to particle, we will get the reduce density operator of demon.

$\hat{\rho}_{D,evolved}$ is the state of demon after evolution which can be obtained as

$$\hat{\rho}_{D,evolved} = Tr_p\left[\hat{\rho}_{evolved,s}\right],$$

$$\hat{\rho}_{D,evolved} = Tr_p\left(\frac{1}{2}\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{\rho}_R \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right).$$

Carrying out the trace

$$\begin{aligned}\hat{\rho}_{D,evolved} = &\sum_{m=0}^{\infty}\langle L_m|\left(\frac{1}{2}\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{\rho}_R \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right)|L_m\rangle \\ &+ \sum_{m=0}^{\infty}\langle R_m|\left(\frac{1}{2}\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{\rho}_R \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right)|R_m\rangle,\end{aligned}$$

$$\begin{aligned}\hat{\rho}_{D,evolved} =& \frac{1}{2}\sum_{m=0}^{\infty}\langle L_m|\hat{\rho}_L|L_m\rangle \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| \\ &+\frac{1}{2}\sum_{m=0}^{\infty}\langle L_m|\hat{\rho}_R|L_m\rangle \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R| \\ &+\frac{1}{2}\sum_{m=0}^{\infty}\langle R_m|\hat{\rho}_L|R_m\rangle \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| \\ &+\frac{1}{2}\sum_{m=0}^{\infty}\langle R_m|\hat{\rho}_R|R_m\rangle \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|.\end{aligned} \tag{4.15}$$

Taking one term at time:

Term-1

$$\sum_{m=0}^{\infty}\langle L_m|\hat{\rho}_L|L_m\rangle =\sum_{m=0}^{\infty}\langle L_m|\frac{1}{Z_L}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega(2n+\frac{3}{2})}|L_n\rangle\langle L_n|L_m\rangle,$$

$$\sum_{m=0}^{\infty}\langle L_m|\hat{\rho}_L|L_m\rangle =\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{1}{Z_L}e^{-\beta\hbar\omega(2n+\frac{3}{2})}\langle L_m|L_n\rangle\langle L_n|L_m\rangle,$$

for $m=n$

$$\sum_{m=0}^{\infty}\langle L_m|\hat{\rho}_L|L_m\rangle =\sum_{n=0}^{\infty}\frac{1}{Z_L}e^{-\beta\hbar\omega(2n+\frac{3}{2})}. \tag{4.16}$$

Term-2

$$\sum_{m=0}^{\infty}\langle L_m|\hat{\rho}_R|L_m\rangle =\sum_{m=0}^{\infty}\langle L_m|\frac{1}{Z_R}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega(2n+\frac{3}{2})}|R_n\rangle\langle R_n|L_m\rangle,$$

$$\sum_{m=0}^{\infty}\langle L_m|\hat{\rho}_R|L_m\rangle =\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{1}{Z_R}e^{-\beta\hbar\omega(2n+\frac{3}{2})}\langle L_m|R_n\rangle\langle R_n|L_m\rangle,$$

for $m=n$

$$\sum_{m=0}^{\infty}\langle L_m|\hat{\rho}_R|L_m\rangle = 0. \tag{4.17}$$

Term-3

$$\sum_{m=0}^{\infty}\langle R_m|\hat{\rho}_L|R_m\rangle \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| =\sum_{m=0}^{\infty}\langle R_m|\frac{1}{Z_L}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega(2n+\frac{3}{2})}|L_n\rangle\langle L_n|R_m\rangle,$$

$$\sum_{m=0}^{\infty}\langle R_m|\hat{\rho}_L|R_m\rangle \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| =\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{1}{Z_L}e^{-\beta\hbar\omega(2n+\frac{3}{2})}\langle R_m|L_n\rangle\langle L_n|R_m\rangle,$$

for $m=n$

$$\sum_{m=0}^{\infty}\langle R_m|\hat{\rho}_L|R_m\rangle\otimes|\mathscr{D}_L\rangle\langle\mathscr{D}_L|=0. \tag{4.18}$$

Term-4

$$\sum_{m=0}^{\infty}\langle R_m|\hat{\rho}_R|R_m\rangle=\sum_{m=0}^{\infty}\langle R_m|\frac{1}{Z_R}\sum_{n=0}^{\infty}e^{-\beta\hbar\omega(2n+\frac{3}{2})}|L_n\rangle\langle L_n|R_m\rangle,$$

$$\sum_{m=0}^{\infty}\langle R_m|\hat{\rho}_R|R_m\rangle=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{1}{Z_R}e^{-\beta\hbar\omega(2n+\frac{3}{2})}\langle R_m|R_n\rangle\langle R_n|R_m\rangle,$$

for $m=n$

$$\sum_{m=0}^{\infty}\langle R_m|\hat{\rho}_R\sum_{k=0}^{\infty}|R_k\rangle=\sum_{n=0}^{\infty}\frac{1}{Z_R}e^{-\beta\hbar\omega(2n+\frac{3}{2})}. \tag{4.19}$$

Using Eq. (4.16), (4.17), (4.18), (4.19) in Eq. (4.15)

$$\begin{aligned}\hat{\rho}_{D,evolved}=&\frac{1}{2}\sum_{n=0}^{\infty}\frac{1}{Z_L}e^{-\beta\hbar\omega(2n+\frac{3}{2})}\otimes|\mathscr{D}_L\rangle\langle\mathscr{D}_L|\\&+\frac{1}{2}\sum_{n=0}^{\infty}\frac{1}{Z_R}e^{-\beta\hbar\omega(2n+\frac{3}{2})}\otimes|\mathscr{D}_R\rangle\langle\mathscr{D}_R|.\end{aligned}$$

Form Eq. (3.59) and (3.62)

$$Z_L=\sum_{n=0}^{\infty}e^{-\beta\hbar\omega(2n+\frac{3}{2})},$$

$$Z_R=\sum_{n=0}^{\infty}e^{-\beta\hbar\omega(2n+\frac{3}{2})}.$$

Hence

$$\hat{\rho}_{D,evolved}=\frac{1}{2}\frac{1}{Z_L}Z_L\otimes|\mathscr{D}_L\rangle\langle\mathscr{D}_L|+\frac{1}{2}\frac{1}{Z_R}Z_R\otimes|\mathscr{D}_R\rangle\langle\mathscr{D}_R|.$$

Therefore demon's evolved state is

$$\hat{\rho}_{D,evolved}=\frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L|+|\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right).$$

Now let us check $\hat{\rho}_{D,evolved}$ is a mixed state or not;

$$\hat{\rho}^2_{D,evolved}=\frac{1}{4}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L|+|\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right),$$

$$Tr\left(\hat{\rho}^2_{D,evolved}\right) = \langle\mathscr{D}_L|\left(\frac{1}{4}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right)|\mathscr{D}_L\rangle$$
$$+\langle\mathscr{D}_R|\left(\frac{1}{4}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right)|\mathscr{D}_R\rangle,$$

$$Tr\left[\hat{\rho}^2_{D,evolved}\right] = \frac{1}{4} + \frac{1}{4},$$

$$Tr\left[\hat{\rho}^2_{D,evolved}\right] = \frac{1}{2} < 1.$$

Hence the state of demon is a maximally mixed state. Its entanglement entropy can be calculated as

$$S\left(\hat{\rho}_{D,evolved}\right) = -k_B Tr\left[\left(\hat{\rho}_{D,evolved} ln \hat{\rho}_{D,evolved}\right)\right].$$

For convenience, we can represent $\hat{\rho}_{D,evolved}$ in matrix form using basis $\{|\mathscr{D}_L\rangle, |\mathscr{D}_R\rangle\}$, matrix elements are

$$\langle\mathscr{D}_L|\hat{\rho}_{D,evolved}\;|\mathscr{D}_L\rangle = \langle\mathscr{D}_L|\frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)|\mathscr{D}_L\rangle = \frac{1}{2},$$
$$\langle\mathscr{D}_L|\hat{\rho}_{D,evolved}\;|\mathscr{D}_R\rangle = \langle\mathscr{D}_L|\frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)|\mathscr{D}_R\rangle = 0,$$

$$\langle\mathscr{D}_R|\hat{\rho}_{D,evolved}\;|\mathscr{D}_R\rangle = \langle\mathscr{D}_L|\frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)|\mathscr{D}_R\rangle = \frac{1}{2},$$

$$\langle\mathscr{D}_R|\hat{\rho}_{D,evolved}\;|\mathscr{D}_L\rangle = \langle\mathscr{D}_L|\frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)|\mathscr{D}_R\rangle = 0.$$

$\hat{\rho}_{D,evolved}$ in matrix form will become

$$\hat{\rho}_{D,evolved} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}.$$

Therefore

$$S\left(\hat{\rho}_{D,evolved}\right) = -k_B Tr\left[\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} ln \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}\right],$$

$$S\left(\hat{\rho}_{D,evolved}\right) = -k_B Tr\left[\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \begin{pmatrix} ln\left(1/2\right) & 0 \\ 0 & ln\left(1/2\right) \end{pmatrix}\right],$$

$$S\left(\hat{\rho}_{D,evolved}\right) = -k_B Tr\begin{pmatrix} 1/2 ln\left(1/2\right) & 0 \\ 0 & 1/2 ln\left(1/2\right) \end{pmatrix},$$

$$S\left(\hat{\rho}_{D,evolved}\right) = -k_B\left[\frac{1}{2}ln\left(\frac{1}{2}\right) + \frac{1}{2}ln\left(\frac{1}{2}\right)\right],$$

$$S\left(\hat{\rho}_{D,evolved}\right) = k_B ln2 \tag{4.20}$$

This is the maximum entropy of demon as it is a two state quantum pointer variable. On the other hand, we can also calculate the entropy of particle before and after interaction.

4.5.3 Entropy of Particle Before Interaction

From Eq. (3.50), we can write the density operator of particle before measurement as

$$\hat{\rho}_{\perp} = \frac{1}{Z_{\perp}}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(2n+\frac{3}{2}\right)}\left(|L_n\rangle\langle L_n| + |R_n\rangle\langle R_n|\right),$$

we can also calculate the above equation by taking the partial trace of Eq. (4.4) with respect to demon i.e.

$$Tr_D\left[\hat{\rho}_{\perp,s}\right] = Tr_D\left[\hat{\rho}_{\perp}\otimes\hat{\rho}_D\right] = \hat{\rho}_{\perp}.$$

From Eq. (3.44) (we have already calculated)

$$S\left(\hat{\rho}_{\perp}\right) = k_B\left\{\beta\hbar\omega ln\left[coth\left(\beta\hbar\omega\right)\right] - ln\left[sinh\left(\beta\hbar\omega\right)\right]\right\}.$$

4.5.4 Entropy of Particle After Interaction

We can write density operator of particle after interaction by taking the partial trace of the evolved composite density operator $\hat{\rho}_{evolved}$ (Eq. (4.13)) with respect to demon.

$\hat{\rho}_{p,evolved}$ is the state of particle after evolution which can be obtained from partial trace:

$$\hat{\rho}_{p,evolved} = Tr_D\left[\hat{\rho}_{evolved}\right],$$

$$\hat{\rho}_{evolved,p} = Tr_D\left[\frac{1}{2}\left(\hat{\rho}_L\otimes|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{\rho}_R\otimes|\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right],$$

$$\begin{aligned}\hat{\rho}_{evolved,p} =& \langle\mathscr{D}_L|\left[\frac{1}{2}\left(\hat{\rho}_L\otimes|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{\rho}_R\otimes|\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right]|\mathscr{D}_L\rangle\\ &+\langle\mathscr{D}_R|\left[\frac{1}{2}\left(\hat{\rho}_L\otimes|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{\rho}_R\otimes|\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right]|\mathscr{D}_R\rangle,\end{aligned}$$

$$\hat{\rho}_{evolved,p} = \frac{1}{2}\hat{\rho}_L \otimes \langle\mathscr{D}_L|\mathscr{D}_L\rangle\langle\mathscr{D}_L|\mathscr{D}_L\rangle + \frac{1}{2}\hat{\rho}_R \otimes \langle\mathscr{D}_L|\mathscr{D}_R\rangle\langle\mathscr{D}_R|\mathscr{D}_L\rangle$$
$$+\frac{1}{2}\hat{\rho}_L \otimes \langle\mathscr{D}_R|\mathscr{D}_L\rangle\langle\mathscr{D}_L|\mathscr{D}_R\rangle + \frac{1}{2}\hat{\rho}_R \otimes \langle\mathscr{D}_R|\mathscr{D}_R\rangle\langle\mathscr{D}_R|\mathscr{D}_R\rangle,$$

using orthonormality conditions

$$\hat{\rho}_{evolved,p} = \frac{1}{2}\hat{\rho}_L \otimes 1 + \frac{1}{2}\hat{\rho}_R \otimes 1,$$

$$\hat{\rho}_{evolved,p} = \frac{1}{2}\left(\hat{\rho}_L + \hat{\rho}_R\right),$$

using Eq. (3.58)

$$\hat{\rho}_{evolved,p} = \hat{\rho}_{\perp}.$$

Now , entropy of particle after interaction will be

$$S(\hat{\rho}_{evolved,p}) = S\left(\hat{\rho}_{\perp}\right) = k_B\left\{\beta\hbar\omega ln\left[coth\left(\beta\hbar\omega\right)\right] - ln\left[sinh\left(\beta\hbar\omega\right)\right]\right\}.$$

So, we can see that entanglement entropy of particle does not change as a result of interaction.

4.6 Evolution as a Result of Expansion

As a result of interaction, the states of particle and demon become correlated. If demon is in state $|\mathscr{D}_L\rangle$ then particle is located on the left side of partition and if the demon is in state $|\mathscr{D}_R\rangle$ then the particle is located on the right side of partition. Once the particle is projected onto one side of barrier then particle pushes the barrier either to left or right side depending upon the location of particle. When particle pushes the barrier then system evolves with time. For this evolution, we need a Hamiltonian.

4.6.1 Total Hamiltonian for Evolution

From Eq. (4.13) we can see that states of particle and demon are correlated. When particle is located on the right side of partition, the state of demon must be $|\mathscr{D}_R\rangle$and particle pushes the barrier towards left side. In this situation Hamiltonian can be written as

$$\hat{H}_{\leftarrow} \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|. \tag{4.21}$$

$\hat{H}_{\leftarrow}$ represents the Hamiltonian for the barrier translated towards left side if the state of demon is $|\mathscr{D}_R\rangle$. Once the particle is projected onto the right side of barrier then $\hat{H}_{\leftarrow}$

acts on particle.

From Eq. (3.71)

$$\hat{H}_{\leftarrow}(t) = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 + \alpha\delta\left(\hat{q} - q_o(t)\right),$$

$$q_o : 0 \to -\infty.$$

When particle is located on the left side of partition, state of demon must be $|\mathscr{D}_L\rangle$ and particle pushes the barrier towards right side. In this situation Hamiltonian can be written as

$$\hat{H}_{\rightarrow} \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|. \tag{4.22}$$

$\hat{H}_{\rightarrow}$ represents the Hamiltonian for the barrier translated towards right side if state of demon is $|\mathscr{D}_L\rangle$. Once particle is projected onto the left side of barrier then $\hat{H}_{\rightarrow}$ acts on particle.

$$\hat{H}_{\rightarrow}(t) = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 + \alpha\delta\left(\hat{q} - q_o(t)\right),$$

$$q_o : 0 \to \infty.$$

From Eq. (4.22) and (4.21), we can construct the total Hamiltonian $\hat{H}_T$.

$$\hat{H}_T = \hat{H}_{\rightarrow} \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{H}_{\leftarrow} \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|. \tag{4.23}$$

4.6.2 Unitary Operator for Evolution

Let us construct unitary operator $\hat{U}_T$ corresponding to Hamiltonian $\hat{H}_T$

$$\hat{U}_T = e^{-i\hat{H}_T\delta t},$$

$$\hat{U}_T = e^{-i\left(\hat{H}_{\rightarrow}\otimes|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{H}_{\leftarrow}\otimes|\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\delta t},$$

$$\hat{U}_T = e^{-i\hat{H}_{\rightarrow}\otimes|\mathscr{D}_L\rangle\langle\mathscr{D}_L|\delta t}e^{-i\hat{H}_{\leftarrow}\otimes|\mathscr{D}_R\rangle\langle\mathscr{D}_R|\delta t}. \tag{4.24}$$

Let us consider each exponential separately:

$$\begin{aligned} e^{-i\hat{H}_{\rightarrow}\otimes|\mathscr{D}_L\rangle\langle\mathscr{D}_L|\delta t} =& \hat{I}_P \otimes \hat{I}_D + -i\hat{H}_{\rightarrow} \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\delta t \\ &+ \left(-i\hat{H}_{\rightarrow} \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\delta t\right)^2 + \ldots \end{aligned}$$

Using

$$\hat{I}_D = |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|.$$

we obtain

$$\begin{aligned} e^{-i\hat{H}_{\rightarrow}\otimes|\mathscr{D}_L\rangle\langle\mathscr{D}_L|\delta t} =& \hat{I}_P \otimes (|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|) + \left(-i\hat{H}_{\rightarrow}\right) \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\delta t \\ &+ \frac{1}{2!}\left(-i\hat{H}_{\rightarrow}\right)^2 \otimes (|\mathscr{D}_L\rangle\langle\mathscr{D}_L|)^2 (\delta t)^2 + ..., \end{aligned}$$

$$\begin{aligned} e^{-i\hat{H}_{\rightarrow}\otimes|\mathscr{D}_L\rangle\langle\mathscr{D}_L|\delta t} =& \hat{I}_P \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{I}_P \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R| + \left(-i\hat{H}_{\rightarrow}\delta t\right) \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| \\ &+ \frac{1}{2!}\left(-i\hat{H}_{\rightarrow}\delta t\right)^2 \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + ..., \end{aligned}$$

$$e^{-i\hat{H}_{\rightarrow}\otimes|\mathscr{D}_L\rangle\langle\mathscr{D}_L|\delta t} = \hat{I}_P \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R| + \left(\hat{I}_P + \left(-i\hat{H}_{\rightarrow}\delta t\right) + \frac{1}{2!}\left(-i\hat{H}_{\rightarrow}\delta t\right)^2 + ...\right) \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|,$$

since

$$e^{-i\hat{H}_{\rightarrow}\delta t} = \hat{I}_P + \left(-i\hat{H}_{\rightarrow}\delta t\right) + \frac{1}{2!}\left(-i\hat{H}_{\rightarrow}\delta t\right)^2 + ... \equiv \hat{U}_{\rightarrow}$$

therefore

$$e^{-i\hat{H}_{\rightarrow}\otimes|\mathscr{D}_L\rangle\langle\mathscr{D}_L|\delta t} = \hat{I}_P \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R| + \hat{U}_{\rightarrow} \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|. \tag{4.25}$$

$\hat{U}_{\rightarrow}$ only acts on the particle.
Similarly 2^{nd} exponential can be written as

$$e^{-i\hat{H}_{\rightarrow}\otimes|\mathscr{D}_R\rangle\langle\mathscr{D}_R|\delta t} = \hat{I}_P \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{U}_{\leftarrow} \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|. \tag{4.26}$$

Using Eq. (4.25) and (4.26) in Eq. (4.24)

$$\hat{U}_T = \left(\hat{I}_P \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R| + \hat{U}_{\rightarrow} \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\right) \times \left(\hat{I}_P \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{U}_{\leftarrow} \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right),$$

$$\begin{aligned} \hat{U}_T =& \hat{I}_P\hat{I}_P \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{U}_{\rightarrow}\hat{I}_P \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\mathscr{D}_L\rangle\langle\mathscr{D}_L| \\ &+ \hat{I}_P\hat{U}_{\leftarrow} \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\mathscr{D}_R\rangle\langle\mathscr{D}_R| + \hat{U}_{\rightarrow}\hat{U}_{\leftarrow} \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\mathscr{D}_R\rangle\langle\mathscr{D}_R|, \end{aligned}$$

using orthonormality conditions

$$\hat{U}_T = \hat{U}_{\rightarrow} \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{U}_{\leftarrow} \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|,$$

$$\hat{U}_T^{\dagger} = \hat{U}_{\rightarrow}^{\dagger} \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{U}_{\leftarrow}^{\dagger} \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|. \tag{4.27}$$

Now we can use the unitary operator $\hat{U}_T$ to determine the evolved state during expansion.

4.6.3 Evolution during Expansion

$\hat{\rho}_{evolved,s}$ is the state of composite system after evolution (from Eq. (4.13))

$$\hat{\rho}_{evolved,s} = \frac{1}{2}\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{\rho}_R \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right).$$

Let us call the state during expansion $\hat{\rho}'_{evolved,s}$

$$\hat{\rho}'_{evolved,s} = \hat{U}_T \hat{\rho}_{evolved,s} \hat{U}_T^{\dagger},$$

$$\hat{\rho}'_{evolved,s} = \hat{U}_T \left(\frac{1}{2}\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{\rho}_R \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\right)\hat{U}_T^{\dagger},$$

$$\hat{\rho}'_{evolved,s} = \frac{1}{2}\hat{U}_T\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\right)\hat{U}_T^{\dagger} + \frac{1}{2}\hat{U}_T\left(\hat{\rho}_R \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\hat{U}_T^{\dagger}. \tag{4.28}$$

Let us consider each term of the above equation separately:

Term-1

$$\hat{U}_T\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\right)\hat{U}_T^{\dagger},$$

using Eq. (3.54) and (4.27)

$$\hat{U}_T\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\right) = \left(\hat{U}_{\rightarrow} \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{U}_{\leftarrow} \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|,$$

$$\hat{U}_T\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\right) = \left(\hat{U}_{\rightarrow}\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{U}_{\leftarrow}\hat{\rho}_L \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\mathscr{D}_L\rangle\langle\mathscr{D}_L|\right),$$

using orthonormality conditions

$$\hat{U}_T\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\right) = \hat{U}_{\rightarrow}\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|.$$

Now applying $\hat{U}_T^{\dagger}$ from the left

$$\hat{U}_T\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\right)\hat{U}_T^\dagger = \hat{U}_\rightarrow \hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\hat{U}_T^\dagger,$$

$$\hat{U}_T\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\right)\hat{U}_T^\dagger = \hat{U}_\rightarrow \hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\left(\hat{U}_\rightarrow^\dagger \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L| + \hat{U}_\leftarrow^\dagger \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right),$$

$$\begin{aligned}\hat{U}_T\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\right)\hat{U}_T^\dagger =& \hat{U}_\rightarrow \hat{\rho}_L \hat{U}_\rightarrow^\dagger \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\mathscr{D}_L\rangle\langle\mathscr{D}_L| \\ &+ \hat{U}_\rightarrow \hat{\rho}_L \hat{U}_\leftarrow^\dagger \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\mathscr{D}_R\rangle\langle\mathscr{D}_R|,\end{aligned}$$

using orthonormality conditions

$$\hat{U}_T\left(\hat{\rho}_L \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\right)\hat{U}_T^\dagger = \hat{U}_\rightarrow \hat{\rho}_L \hat{U}_\rightarrow^\dagger \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|. \tag{4.29}$$

Similarly,
Term-2

$$\hat{U}_T\left(\hat{\rho}_R \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)\hat{U}_T^\dagger = \hat{U}_\leftarrow \hat{\rho}_R \hat{U}_\leftarrow^\dagger \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|. \tag{4.30}$$

Finally using Eq. (4.29) and (4.30) in Eq. (4.28)

$$\hat{\rho}'_{evolved,s} = \frac{1}{2}\left(\hat{U}_\rightarrow \hat{\rho}_L \hat{U}_\rightarrow^\dagger \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\right) + \frac{1}{2}\left(\hat{U}_\leftarrow \hat{\rho}_R \hat{U}_\leftarrow^\dagger \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right).$$

Once the barrier is pushed all the way to infinity, we are back to the initial state:

$$\hat{U}_\rightarrow \hat{\rho}_L \hat{U}_\rightarrow^\dagger = \hat{\rho}_{in},$$

$$\hat{U}_\leftarrow \hat{\rho}_R \hat{U}_\leftarrow^\dagger = \hat{\rho}_{in},$$

$$\Rightarrow \hat{\rho}'_{evolved,s} = \frac{1}{2}\left(\hat{\rho}_{in} \otimes |\mathscr{D}_L\rangle\langle\mathscr{D}_L|\right) + \frac{1}{2}\left(\hat{\rho}_{in} \otimes |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right),$$

$$\hat{\rho}'_{evolved,s} = \hat{\rho}_{in} \otimes \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right). \tag{4.31}$$

This is the state of system at the end of cycle. We can see that quantum particle returns to its initial state but demon is in a mixed state at the end of cycle. However, it was in a pure state initially. So in order to restart the cycle, it is necessary to reset the demon to its initial or ready state $|\mathscr{D}_o\rangle$.

4.7 Resetting Demon's State

This means that we need to reset the final state of demon to initial state $\hat{\rho}_D$.

$$|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R| \longrightarrow \hat{\rho}_D.$$

From Eq. (4.1)

$$\frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right) \longrightarrow \frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L|\right).$$

We know that demon is a two state system $\{|\mathscr{D}_L\rangle, |D_R\rangle\}$ having maximum entropy $k_B ln2$.

From Eq. (4.14) and (4.20)

- $\frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)$ has entropy $k_B ln2$ which is the maximum value, so it has no free energy available.
- $\frac{1}{2}\left(|\mathscr{D}_L\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_L| + |\mathscr{D}_R\rangle\langle\mathscr{D}_R|\right)$ has entropy 0, so it has $k_B ln2$ free energy available.

So, if we want to go from final state of demon to initial state i.e. from mixed state to pure state, we have to provide $k_B ln2$ energy during each cycle. By this transformation of mixed state to pure state, entropy of demon becomes zero. This decrease in entropy of demon balances the thermodynamical entropy of particle [29].

Hence for the complete (particle + demon) closed system

$$\triangle \boldsymbol{S} = \boldsymbol{0}.$$

This result **negates the apparent violation of** 2^{nd} **Law of thermodynamics** during the complete cycle of quantum Szilard engine. Hence, we can say that second law of thermodynamics is valid for the quantum Szilard engine as expected.

Chapter 5

Discussion and Conclusions

The detailed analysis of quantum harmonic Szilard engine shows that all thermodynamics functions shown in Figure 5.1 can be calculated analytically at the end of each stage of the cycle.

Thermodynamical quantities	Before Barrier Insertion	After Barrier insertion	After Measurement
Free energy $A_x = \frac{-1}{\beta}\ln(Z_x)$	$A_{in} = \frac{1}{\beta}\ln[2\sinh(\frac{\beta\hbar\omega}{2})]$	$A_{\perp} = \frac{1}{\beta}\ln[\sinh(\beta\hbar\omega)] + \frac{\hbar\omega}{2}$	$A_R = \frac{1}{\beta}\ln[\sinh(\beta\hbar\omega)] + \frac{\hbar\omega}{2} + \frac{1}{\beta}\ln 2$
Average energy $E_x = -\frac{1}{Z_x}\frac{d}{d\beta}(Z_x)$	$E_{in} = \frac{1}{2}\hbar\omega[\coth(\frac{\beta\hbar\omega}{2})]$	$E_{\perp} = \hbar\omega[\coth(\beta\hbar\omega)] + \frac{\hbar\omega}{2}$	$E_R = \hbar\omega[\coth(\frac{\beta\hbar\omega}{2})] + \frac{\hbar\omega}{2}$
Entropy $S_x = -\frac{d}{dT}(A_{in})$	$S_{in} = k_B\{\frac{\beta\hbar\omega}{2}\coth(\frac{\beta\hbar\omega}{2}) - ln[2\sinh(\frac{\beta\hbar\omega}{2})]\}$	$S_{\perp} = k_B\{\beta\hbar\omega\coth(\beta\hbar\omega) - ln[\sinh(\beta\hbar\omega)]\}$	$S_R = k_B\{\beta\hbar\omega\coth(\beta\hbar\omega) - ln[\sinh(\beta\hbar\omega)]\} - k_B\ln 2$

Figure 5.1: Thermodynamic functions calculated at the end of each stage for a cycle.

This analysis shows that average energy of system increases which implies that barrier insertion cannot be done quantum mechanically at zero energy cost. The effects of barrier insertion can be observed significantly at low temperature i.e. increase in entropy etc., however, entropy remains same before and after barrier insertion in the high temperature limit. We then perform a projective measurement, assuming Maxwell's demon operating the engine is not treated dynamically that results in the localization of particle either on the left or right side of harmonic well. The entropy of system decreases by an amount $k_B ln2$; an amount of useful work $k_B T ln2$ can be extracted from the thermal bath that leads to the violation of second law of thermodynamics.

In full quantum analysis, demon is treated dynamically to show explicitly that he cannot operate the engine for more than one cycle. During a cycle, the entropy(information entropy) of demon increases by an amount $k_B ln2$ in obtaining the information whether the particle is located on the left or right side of harmonic well. At the end of each cycle, it can be seen from the quantum analysis that particle returns to its initial state, however demon remains in a mixed state. For a cyclic process, initial and final state of system must be same. So in order to continue the cycle, demon needs to reset its final state to initial state which leads to lowering the entropy. To erase this 1-bit of information, at least $k_B T ln2$ amount of energy is required according to Landaure's principle [6], which is as same as obtained from single cycle of engine.

Thus, we conclude that the second law of thermodynamics is apparently violated when demon is not treated dynamically. However, second law of thermodynamics is not violated when a more complete analysis is carried out with the demon operating the engine treated dynamically because decrease in the thermodynamics entropy is compensated by increase in the information entropy of demon. Work extracted from thermal bath is used to reset the state of demon in order to run the engine in a cyclic manner which negates the extraction of net useful work. Hence, second law of thermodynamics remains intact throughout.

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[25] This corresponds to the usual notion of measurement by a classical apparatus so central to the Copenhagen interpretation of quantum mechanics. See Chapter 5 of Ref. 20 for a detailed description of the measurement postulate and the Born rule in this framework. Appendix D of the same reference extends these notions to the case of mixed states (where the Born rule is sometimes known as Luders rule).

[26] Although there is energy output from the engine, the quasi-static assumption implies zero net power. This is a familiar idealization in thermodynamics, as the Carnot engine also evolves quasi-statically during its cycle. Relaxing this quasi-static condition reduces the efficiency of the engine.

[27] For a discussion of the definition and properties of the tensor product with respect to quantum systems with multiple degrees of freedom see Chapter 5 of Ref. 20.

[28] Technically $\hat{I}_D$should be replaced by the quantum Hamiltonian of the pointer variable. However, we neglect the quantum dynamics of the pointer variable in this work. This can safely be done as long as the two energy eigenvalues corresponding to $|\mathscr{D}_L\rangle$ and $|\mathscr{D}_R\rangle$ are separated by less than $\hbar/\tau$ (where τ is the characteristic time scale of the problem).

[29] Of course, one could consider a quantum demon at a temperature $T_D < T$, in which case the energy required to "reset" the demon is less than the amount extracted from one engine cycle. However, in this case, the engine is no longer monothermal, so there is no violation of the second law of thermodynamics

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