
AN INTRODUCTION TO QUANTUM THERMODYNAMICS

Parsa Rangriz
Department of Physics
Sharif University of Technology
Tehran, Iran
rangriz@physics.sharif.edu

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ABSTRACT

In this review letter, we mentioned some important remarks of quantum thermodynamics and their relations with quantum information theory. At first, we introduced some points of quantum open system and information theory and then applied them to quantum thermodynamics. Then, we generalized some materials such as laws and cycles of classical thermodynamics to the quantum-mechanical approaches.

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1 Introduction

If physical theories were people, thermodynamics would be the village witch. Over the course of three centuries, she smiled quietly as other theories and withered, surviving major revolutions in physics, like the advent of general relativity and quantum mechanics. The other theories find her somewhat odd, somehow different in nature from the rest, yet everyone comes to her for advice, and no-one dares to contradict her.

Her power and resilience lay mostly on her frank intention: thermodynamics has never claimed to be a means to understand the mysterious of the natural world, but rather a path towards efficient exploitation of said world. Her universality comes from the fact that she does not try to understand the microscopic details of particular systems. Instead, she only cares to identify which operations are easy and hard to implement in those systems, and which resources are freely available to an experimenter, in order to quantify the cost of state transformations. Although it may stand out within physics, this operational approach can be found in branches of computer science, economics and mathematics, and it plays a central role in quantum information theory.

In the early 20th century, information theory was constructed as the epitome of detachment from physics. Its basic premise was that we could think of information independently of its physical support.

But as it turned out, not all information was created equal. If we zoom in and try to encode information in the tiniest support possible, say the spin of an electron, we face some of the perplexing aspects of quantum physics. In short, we could not simply apply the old information theory to tasks involving quantum particles, and the scattered study of quirky quantum effects soon evolved into the fully-fledged discipline of quantum information theory. Today we see quantum theory as a generalization of classical probability theory, with density operators replacing probability distributions, measurement taking the place of events and quantum entropy measures the characterize operational tasks.

2 Quantum Open System

2.1 Noisy System: The Density Operator

As we learned in undergraduate quantum mechanics, the axioms provided a perfectly acceptable general formulation of the quantum theory. Yet under many circumstance, we find that the axioms appear to be violated. The trouble is that our axioms are intended to characterize the quantum behavior of the entire universe. In practice, the observations we make are always limited to a small part of much larger quantum system.

Our description of the state is then as an ensemble \mathcal{E} of quantum states where

$$\mathcal{E} = \{p_X(x), |\psi_x\rangle\}_{x \in \mathcal{X}} \quad (1)$$

In the above, X is a random variable with distribution $p_X(x)$. Each realization x of random variable X belongs to an alphabet \mathcal{X} . Thus, the realization x merely acts as an index, meaning that the quantum state is $|\psi_x\rangle$ with classical probability $p_X(x)$.

In this situation, if we want to measure the average of an observable like O on the system, we can write

$$\langle O \rangle = \sum_{x \in \mathcal{X}} p_X(x) \langle \psi_x | O | \psi_x \rangle \quad (2)$$

This equation could be rewrite as

$$\langle O \rangle = \text{tr}(O\rho) \quad (3)$$

where ρ is defined by

$$\rho \equiv \sum_{x \in \mathcal{X}} p_X(x) |\psi_x\rangle \langle \psi_x| \quad (4)$$

which it called density operator because it is the quantum generalization of a probability density function. From the definition, we can immediately infer that ρ has the following properties:

1. ρ is self-adjoint: $\rho = \rho^\dagger$
2. ρ is positive: $\rho \geq 0$
3. $\text{tr}(\rho) = 1$

We can also refer to the density operator as the state of a given quantum system because it is possible it to use it to calculate probabilities for any measurement performed on that system. So the state of a quantum system is given by a density operator ρ , which is a positive semi-definite operator with trace equal to one. Let $D(\mathcal{H})$ denote the set of all density operators acting on a Hilbert space \mathcal{H} .

One of the most important states is the maximally mixed state π . It is the density operator corresponding to a uniform ensemble of orthogonal state $\{\frac{1}{d}, |x\rangle\}$, where d is the dimensions of the Hilbert space. The maximally mixed state π is then equal to

$$\pi \equiv \frac{1}{d} \sum_{x \in \mathcal{X}} |x\rangle \langle x| = \frac{I}{d} \quad (5)$$

The purity $P(\rho)$ of a density operator ρ is equal to

$$P(\rho) \equiv \text{tr}(\rho^\dagger \rho) = \text{tr}(\rho^2) \quad (6)$$

The purity is one particular measure of the noisiness of a quantum state. The purity of a pure state is equal to one and the purity of a mixed state is strictly less than one. A state is pure if it can be written as $\rho = |\psi\rangle \langle \psi|$ for some unit vector ψ

2.2 Noiseless Unitary Evolution of a Noisy State

We first consider noiseless evolution according to some unitary U . Suppose we have the ensemble \mathcal{E} with density operator ρ . Suppose without loss of generality that the state is $|\psi_x\rangle$. Then the evolution postulate of the noiseless quantum theory gives that the state after the unitary evolution is as follows: $U|\psi_x\rangle$. This result implies that the evolution leads to a new ensemble

$$\mathcal{E} = \{p_X(x), U|\psi_x\rangle\}_{x \in \mathcal{X}} \quad (7)$$

The density operator of the evolved ensemble is

$$\rho' = \sum_{x \in \mathcal{X}} p_X(x) U |\psi_x\rangle \langle \psi_x| U^\dagger = U \left(\sum_{x \in \mathcal{X}} p_X(x) |\psi_x\rangle \langle \psi_x| \right) U^\dagger = U \rho U^\dagger \quad (8)$$

2.3 Noiseless Measurement of a Noisy State

In similar fashion, we can analyze the result of a measurement on a system with ensemble description \mathcal{E} . Suppose that we perform a projective measurement with projection $\{\Pi_j\}_j$ where $\sum_j \Pi_j = I$.

Let us suppose that the state is in the ensemble \mathcal{E} is $|\psi_x\rangle$. Then the noiseless quantum theory predicts that the probability of obtaining outcome j conditioned on the index x is

$$p_{J|X}(j|x) = \langle \psi_x | \Pi_j | \psi_x \rangle \quad (9)$$

and the resulting state is

$$\frac{\Pi_j |\psi_x\rangle}{\sqrt{p_{J|X}(j|x)}} \quad (10)$$

Supposing that we receive outcome j , then we have a new ensemble:

$$\mathcal{E}_j = \left\{ p_{X|J}(x|j), \frac{\Pi_j |\psi_x\rangle}{\sqrt{p_{J|X}(j|x)}} \right\}_{x \in \mathcal{X}} \quad (11)$$

Therefore the density operator for this ensemble is

$$\sum_{x \in \mathcal{X}} p_{X|J}(x|j) \frac{\Pi_j |\psi_x\rangle \langle \psi_x| \Pi_j}{p_{J|X}(j|x)} = \frac{\Pi_j \rho \Pi_j}{p_J(j)} \quad (12)$$

2.4 Noisy Non-Unitary Evolution of a Noisy State

We now consider non-unitary evolution of system \mathbf{S} that interacts with environment \mathbf{E} . We note that \mathbf{S} and \mathbf{E} correspond to Hilbert spaces $\mathcal{H}_\mathbf{S}$ and $\mathcal{H}_\mathbf{E}$, respectively. We assume that the initial state of the total system is given by a product state

$$\rho_{tot} \equiv \rho \otimes |\psi\rangle \langle \psi| \quad (13)$$

where the state of \mathbf{E} is assumed to be described by a state vector $|\psi\rangle$. We note that the generality is not lost by this assumption, because every mixed state can be described by a vector with a sufficiently large Hilbert space. After unitary evolution U of $\mathbf{S} + \mathbf{E}$, the total state is given by

$$\rho'_{tot} = U \rho_{tot} U^\dagger \quad (14)$$

which leads to \mathbf{S} 's state

$$\rho' = \text{tr}_{\mathbf{E}}(\rho'_{tot}) \quad (15)$$

Let $\{|k\rangle\}$ be an $\mathcal{H}_{\mathbf{E}}$'s basis. Then we have

$$\rho' = \sum_k \langle k| U |\psi\rangle \rho |\psi\rangle U^\dagger |k\rangle \quad (16)$$

By introducing notation

$$M_k \equiv \langle k| U |\psi\rangle \quad (17)$$

and we finally obtain

$$\rho' = \sum_k M_k \rho M_k^\dagger \quad (18)$$

This equation is called Kraus representation and M_k 's are called Kraus operators. We note that the Kraus operators satisfy

$$\sum_k M_k^\dagger M_k = \sum_k \langle \psi| U^\dagger |k\rangle \langle k| U |\psi\rangle = \langle \psi| I_{tot} |\psi\rangle = I_S \quad (19)$$

This equation confirms that the trace of ρ is conserved

$$\text{tr}(\rho') = \text{tr}(\rho) \quad (20)$$

2.5 Noisy Measurement of a Noisy State: POVM

We next discuss the general formulation of quantum measurements involving measurement errors. The measurement process can be formulated by indirect measurement models, in which the measured system \mathbf{S} interact with a probe \mathbf{P} . Let ρ be the measured state of \mathbf{S} and σ be the initial state of \mathbf{P} . The initial state of the composite system is then $\rho \otimes \sigma$. Let U be the unitary operator which characterizes the interaction between \mathbf{S} and \mathbf{P} as

$$\rho \otimes \sigma \rightarrow U(\rho \otimes \sigma)U^\dagger \quad (21)$$

After this unitary evolution, we can extract the information about measured state $|\psi\rangle$ by performing the projection measurement of observer R of $\mathbf{S} + \mathbf{P}$. We write the spectrum decomposition of R as

$$R \equiv \sum_i r(i) \Pi_R(i) \quad (22)$$

where $r(i) \neq r(j)$ for $i \neq j$, and $\Pi_R(i)$'s are projection operators with $\sum_i \Pi_R(i) = I$.

From the Born rule, the probability of obtaining outcome $r(i)$ is given by

$$p_k = \text{tr}(\Pi_R(k)(U(\rho \otimes \sigma)U^\dagger)) \quad (23)$$

By introducing

$$\Lambda_k \equiv \text{tr}_{\mathbf{P}}(U(I \otimes \sigma)U^\dagger) \quad (24)$$

we can express p_k as

$$p_k = \text{tr}(\Lambda_k \rho) \quad (25)$$

The set $\{\Lambda_k\}$ is called a positive operator-valued measure (POVM). We next consider post-measurement states. Suppose that we get outcome k . Then the corresponding post-measurement state ρ_k is given by

$$\rho_k = \text{tr}_{\mathbf{P}}(\Pi_R(k)(U(\rho \otimes \sigma)U^\dagger)\Pi_R(k))/p_k \quad (26)$$

Let $\sigma = \sum_j q_j |\psi_j\rangle \langle \psi_j|$ be the spectral decomposition with $\{|\psi_j\rangle\}$ being an orthonormal basis. Then we have

$$\rho_k = \sum_{j,l} q_j \langle \psi_l | \Pi_R(k) U |\psi_j\rangle \rho \langle \psi_j | U^\dagger \Pi_R(k) |\psi_l\rangle / p_k \quad (27)$$

and define the Kraus operators as

$$M_{k;jl} \equiv \sqrt{q_j} \langle \psi_l | \Pi_R(k) U |\psi_j\rangle \quad (28)$$

which is also called measurement operators in this situation. We finally have

$$\rho_k = \frac{1}{p_k} \sum_{j,l} M_{k;jl} \rho M_{k;jl}^\dagger \quad (29)$$

and

$$\Lambda_k = \sum_{j,l} M_{k;jl}^\dagger M_{k;jl} \quad (30)$$

3 Information Theory

3.1 Classical Information Theory

We first introduce the concept of entropy, which is a measure of the uncertainty of a random variable. Let X be a discrete random variable with alphabet \mathcal{X} and probability mass function $p(x) = \Pr\{X = x\}, x \in \mathcal{X}$.

3.1.1 Shannon Entropy

The entropy $H(X)$ of a discrete random variable X is defined by

$$H(X) = - \sum_{x \in \mathcal{X}} p(x) \log p(x) \quad (31)$$

It is easy to prove that $H(X) \geq 0$.

3.1.2 Joint Entropy and Conditional Entropy

We defined the entropy of a single random variable. We now extend the definition to a pair of random variables. There is nothing really new in this definition because (X, Y) can be considered to be a single vector-valued random variable.

The joint entropy $H(X, Y)$ of a pair of discrete random variables (X, Y) with a joint distribution $p(x, y)$ is defined as

$$H(X, Y) = - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log p(x, y) \quad (32)$$

We also define the conditional entropy of a random variable given another as the expected value of the entropies of the conditional distributions, averaged over the conditioning random variable.

If $(X, Y) \sim p(x, y)$, the conditional entropy $H(Y|X)$ is defined as

$$\begin{aligned} H(Y|X) &= \sum_{x \in \mathcal{X}} p(x) H(Y|X = x) \\ &= - \sum_{x \in \mathcal{X}} p(x) \sum_{y \in \mathcal{Y}} p(y|x) \log p(y|x) \\ &= - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log p(y|x) \end{aligned} \quad (33)$$

The naturalness of the definition of joint entropy and conditional entropy is exhibited by the fact that the entropy of a pair of random variables is the entropy of one plus the conditional entropy of the other. This is proved in the following theorem:

$$H(X, Y) = H(X) + H(Y|X) \quad (34)$$

3.1.3 Relative Entropy and Mutual Information

The entropy of a random variable is a measure of the uncertainty of the random variable; it is a measure of the amount of information required on the average to describe the random variable. In this section we introduce two related concepts: relative entropy and mutual information.

The relative entropy is a measure of the distance between two distributions. In statistics, it arises as an expected logarithm of the likelihood ratio. The relative entropy $D(p||q)$ is a measure of the inefficiency of assuming that the distribution is q when the true distribution is p .

The relative entropy between two probability mass function $p(x)$ and $q(x)$ is defined as

$$D(p||q) = \sum_{x \in \mathcal{X}} p(x) \log \frac{p(x)}{q(x)} \quad (35)$$

We now introduce mutual information, which is a measure of the amount of information that one random variable contains about another random variable. It is the reduction in the uncertainty of one random variable due to the knowledge of the other.

Consider two random variables X and Y with a joint probability mass function $p(x, y)$ and marginal probability mass function $p(x)$ and $p(y)$. The mutual information $I(X; Y)$ is the relative entropy between the joint distribution and the product distribution $p(x)p(y)$:

$$I(X; Y) = \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log \frac{p(x, y)}{p(x)p(y)} = D(p(x, y) || p(x)p(y)) \quad (36)$$

3.1.4 Entropy and Mutual Information

We can rewrite the definition of mutual information $I(X; Y)$ as

$$I(X; Y) = \sum_{xy} \log \frac{p(x|y)}{p(x)} = H(X) - H(X|Y) \quad (37)$$

By symmetry, it also follows that

$$I(X; Y) = H(Y) - H(Y|X) \quad (38)$$

Since $H(X, Y) = H(X) + H(Y|X)$, as shown in previous sections, we have

$$I(X; Y) = H(X) + H(Y) - H(X, Y) \quad (39)$$

3.1.5 Inequalities

Let $p(x), q(x), x \in \mathcal{X}$, be two probability mass function. Then it is easy to show that

$$D(p||q) \geq 0 \quad (40)$$

with equality if and only if $p(x) = q(x)$ for all x . Hence, for any two random variables, X, Y ,

$$I(X, Y) \geq 0 \quad (41)$$

with equality if and only if X and Y are independent.

3.2 Quantum Information Theory

3.2.1 Quantum Entropy

We might expect a measure of the entropy of a quantum system to be vastly different from the classical measure of entropy from the previous section because a quantum system possesses not only classical uncertainty but also quantum uncertainty that arises from the uncertainty principle. But recall that the density operator captures both types of uncertainty and allows us to determine probabilities from the outcomes of any measurement on a given system.

Suppose that Alice prepares some quantum system A in a state $\rho_A \in D(\mathcal{H})$. Then the entropy $H(A)_\rho$ of the state is defined as follows:

$$H(\rho_A) \equiv -\text{tr}\{\rho_A \log \rho_A\} \quad (42)$$

The entropy of a quantum system is also known as the von Neumann entropy or the quantum entropy.

We now discuss several mathematical properties of the quantum entropy: non-negativity, its minimum value, its maximum value and so far. Some of these properties follow from the analogous properties in the classical world because the quantum entropy of a density operator is the Shannon entropy of its eigenvalues. We state them formally below:

The quantum entropy $H(\rho)$ is non-negative for any density operator ρ :

$$H(\rho) \geq 0 \quad (43)$$

The minimum value of the quantum entropy is zero, and it occurs when the density operator is a pure state and the maximum value of the quantum entropy is $\log d$ where d is the dimension of the system, and it occurs for the maximally mixed state.

Let $\rho_x \in D(\mathcal{H})$ and let $p_X(x)$ be a probability distribution. The entropy is concave in the density operator:

$$H(\rho) \geq \sum_x p_X(x) H(\rho_x) \quad (44)$$

The physical interpretation of concavity is as before for classical entropy.

Let $\rho_x \in D(\mathcal{H})$ and $U : \mathcal{H} \rightarrow \mathcal{H}'$ be an isometry. The entropy of a density operator is invariant with respect to isometries, in the following sense:

$$H(\rho) = H(U\rho U^\dagger) \quad (45)$$

3.2.2 Joint Quantum Entropy

The joint quantum entropy $H(AB)_\rho$ of the density operator $\rho_{AB} \in D(\mathcal{H}_A \otimes \mathcal{H}_B)$ for a bipartite system AB follows naturally from the definition of quantum entropy:

$$H(\rho_{AB}) = -\text{tr}\{\rho_{AB} \log \rho_{AB}\} \quad (46)$$

The marginal entropies $H(\rho_A)$ and $H(\rho_B)$ of a pure bipartite state $|\phi\rangle_{AB}$ are equal:

$$H(\rho_B) = H(\rho_A) \quad (47)$$

while the joint entropy $H(|\phi\rangle_{AB} \langle\phi|)$ vanishes:

$$H(|\phi\rangle_{AB} \langle\phi|) = 0 \quad (48)$$

Let $\rho_A \in D(\mathcal{H}_A)$ and $\sigma_B \in D(\mathcal{H}_B)$. The quantum entropy is additive for tensor-product states:

$$H(\rho_A \otimes \sigma_B) = H(\rho_A) + H(\sigma_B) \quad (49)$$

One can verify this property simply by diagonalization both density operators and resorting to the additivity of the joint Shannon entropies of the eigenvalues.

3.2.3 Conditional Quantum Entropy

The definition of conditional quantum entropy that has been most useful in quantum information theory. Let $\rho_{AB} \in D(\mathcal{H}_A \otimes \mathcal{H}_B)$. The conditional quantum entropy $H(\rho_A|\rho_B)$ of ρ_{AB} is equal to the difference of the joint quantum entropy $H(\rho_{AB})$ and the marginal entropy $H(\rho_B)$:

$$H(\rho_A|\rho_B) \equiv H(\rho_{AB}) - H(\rho_B) \quad (50)$$

The above definition is the most natural one, both because it is straightforward to compute for any bipartite state and because it obeys many relations that the classical conditional entropy obeys.

3.2.4 Quantum Mutual Information

The standard informational measure of correlations in the classical world is the mutual information, and such a quantity plays a prominent role in measuring classical and quantum correlations in the quantum world as well.

The quantum mutual information of a bipartite state $\rho_{AB} \in D(\mathcal{H}_A \otimes \mathcal{H}_B)$ is defined as follows:

$$I(\rho_A; \rho_B) \equiv H(\rho_A) + H(\rho_B) - H(\rho_{AB}) \quad (51)$$

The following relations hold for quantum mutual information, in analogy with the classical case:

$$I(\rho_A; \rho_B) = H(\rho_A) - H(\rho_A|\rho_B) = H(\rho_B) - H(\rho_B|\rho_A) \quad (52)$$

The quantum mutual information $I(\rho_A; \rho_B)$ of any bipartite quantum state ρ_{AB} is non-negative:

$$I(\rho_A; \rho_B) \geq 0 \quad (53)$$

The quantum relative entropy $D(\rho||\sigma)$ between a density operator $\rho \in D(\mathcal{H})$ and a positive semi-definite operator σ is defined as follows:

$$D(\rho||\sigma) \equiv \text{tr}\{\rho[\log \rho - \log \sigma]\} \quad (54)$$

It is easy to prove that

$$D(\rho||\sigma) \geq 0 \quad (55)$$

and $D(\rho||\sigma) = 0$ if and only if $\rho = \sigma$

3.2.5 Holevo Bound

Another important quantity related to the mutual information is "the Holevo χ quantity". Let $X \equiv \{x\}$ be a set of classical probability variables, and $\{\rho_x\}_{x \in X}$ be a set of density operators that are not necessarily mutually orthogonal. Let $\rho = \sum_x p_x \rho_x$ with $\mathbf{p} \equiv \{p_x\}$ being a probability distribution. Then the Holevo χ quantity is given by

$$\chi \equiv H(\rho) - \sum_k p_k H(\rho_k) \quad (56)$$

The Holevo bound is formulated as follows. An agent called Alice prepares a state ρ_k and send it to an other agent called Bob. Bob performs a quantum measurement on the system with POVM $\{\Lambda_y\}_{y \in Y}$, where Y is the set of measurement outcomes. The joint distribution of X and Y is given by

$$p(x, y) = \text{tr}[\Lambda_y \rho_x] p_x \quad (57)$$

which gives the marginal distribution of y as

$$q(y) \equiv \sum_x p(x, y) = \text{tr}[\Lambda_y \rho] \quad (58)$$

Let $\mathbf{q} \equiv \{q(y)\}$. Then the classical mutual information between X and Y is given by

$$I(X : Y) = \sum_{x, y} p(x, y) \ln \frac{p(x, y)}{p(x)q(y)} \quad (59)$$

The Holevo bound states that the classical mutual information is bounded by the Holevo χ quantity as

$$I(X : Y) \leq \chi \quad (60)$$

3.2.6 QC-Mutual Information

We next discuss "QC-mutual information" which will play crucial role in the generalizations of the second law of thermodynamics. Here "QC" denotes "quantum-classical"; as we will see later, QC-mutual information characterizes a kind of correlation between a quantum system and a classical system.

We consider density operator ρ of quantum system \mathbf{S} , and perform a quantum measurement on it. Let $\{E_y\}_{y \in Y}$ be the POVM of the measurement, where Y is the set of measurement outcomes. The probability of obtaining y is given by $p(y) = \text{tr}[\Lambda_y \rho]$. Let $\mathbf{p} \equiv \{p(y)\}$ and $H(\mathbf{P}) \equiv -\sum_y p(y) \ln p(y)$. The QC-mutual information associated the POVM is then defined as

$$I_{QC} = H_Q(\rho) + H_C(\mathbf{S}) + \sum_y \text{tr} \left(\sqrt{\Lambda_y} \rho \sqrt{\Lambda_y} \ln \left(\sqrt{\Lambda_y} \rho \sqrt{\Lambda_y} \right) \right) \quad (61)$$

where H_Q is a quantum entropy and H_C is a classical entropy. We note that, the QC-mutual information can be written as

$$I_{QC} \equiv H_Q(\rho) - \sum_y p(y) H(\rho^{(y)}) \quad (62)$$

where

$$\rho^{(y)} \equiv \frac{1}{p(y)} \sqrt{\Lambda_y} \rho \sqrt{\Lambda_y} \quad (63)$$

4 Quantum Master Equations

4.1 Quantum Dynamical Semigroups

In general the dynamics of the reduced system defined by the exact equations

$$\rho_S(t) = \text{tr}_B(U(t, t_0) \rho(t_0) U^\dagger(t, t_0)) \quad (64)$$

and

$$\frac{d}{dt} \rho_S(t) = -i \text{tr}_B[H(t), \rho(t)] \quad (65)$$

will be quite involved. However, under the condition of short environmental correlation times one may neglect memory effects and formulate the reduced system dynamics in terms of a quantum dynamics semigroup.

Let us suppose that we are able to prepare at the initial time $t = 0$ the state of the total system $\mathbf{S} + \mathbf{B}$ as an uncorrelated product state $\rho(0) = \rho_S(0) \otimes \rho_B$, where $\rho_S(0)$ is the initial state of the reduced system \mathbf{S} and ρ_B represents some reference state of the environment, a thermal equilibrium, for example. The transformation describing the change of the reduced system from the initial time $t = 0$ to some $t > 0$ may then be written in the form

$$\rho_S(0) \rightarrow \rho_S(t) V(t) \rho_S(0) \equiv \text{tr}_B(U(t, 0) [\rho_S(0), \rho_B] U^\dagger(t, 0)) \quad (66)$$

If we regard the reference state ρ_B and the final time to be fixed, this relation defines a map from the space $D(\mathcal{H}_S)$ of density operator of the reduced system into itself,

$$V(t) : D(\mathcal{H}_S) \rightarrow D(\mathcal{H}_S) \quad (67)$$

This map, describing the state change of the open system over time t , is called a dynamical map. If the characteristic time scales over which the reservoir correlation functions decay are much smaller than the characteristic time scale of the systematic system evolution, it is justified to neglect memory effects in the reduced system dynamics. As in the classical theory one thus expects Markovian-type behavior. For the homogeneous case the latter may be formalized with the help of the semigroup property:

$$V(t_1)V(t_2) = V(t_1 + t_2), \quad t_1, t_2 > 0 \quad (68)$$

4.2 The Markovian Quantum Master Equation

Given a quantum dynamical semigroup there exists, under certain mathematical conditions, a linear map \mathcal{L} , the generator of the semigroup, which allows us to represent the semigroup in exponential form,

$$V(t) = \exp(\mathcal{L}t) \quad (69)$$

This representation immediately yields a first-order differential equation for the reduced density operator of the open system,

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}\rho_S(t) \quad (70)$$

which is called the Markovian quantum master equation.

Let us construct the most general form for the generator \mathcal{L} of a quantum dynamical semigroup. To this end, we consider first the simple case of a finite-dimensional Hilbert space \mathcal{H}_S , $\dim \mathcal{H}_S = N$. The corresponding Liouville space is a complex space of dimension N^2 and we choose a complete basis of orthonormal operators $F_i, i = 1, 2, \dots, N^2$, in this space such that we have

$$(F_i, F_j) \equiv \text{tr}_S(F_i^\dagger F_j) = \delta_{ij} \quad (71)$$

For convenience one of the basis operators is chosen to be proportional to the identity, namely $F_{N^2} = (1/N)^{1/2}I_S$, such that the other basis operators are traceless, that is $\text{tr}_S F_i = 0$ for $i = 1, 2, \dots, N^2 - 1$. Applying the completeness relation to each of the operators $K_{\alpha\beta}(t)$ defined in the following relations:

A dynamical map can be characterized completely in terms of operators pertaining to open system's Hilbert space \mathcal{H}_S . To this end, we use the spectral decomposition of the density operator ρ_B of the environment,

$$\rho_B = \sum_{\alpha} \lambda_{\alpha} |\phi_{\alpha}\rangle \langle \phi_{\alpha}| \quad (72)$$

Here, the $|\phi_{\alpha}\rangle$ form an orthonormal basis in \mathcal{H}_B and the λ_{α} are non-negative real numbers satisfying $\sum_{\alpha} \lambda_{\alpha} = 1$. Definition 66 then immediately yields the following representation,

$$V(t)\rho_S = \sum_{\alpha, \beta} K_{\alpha\beta} \rho_S K_{\alpha\beta}^\dagger \quad (73)$$

where the $K_{\alpha\beta}$, being operators in \mathcal{H}_S , are defined by

$$K_{\alpha\beta} = \sqrt{\lambda_{\beta}} \langle \phi_{\alpha} | U(t, 0) | \phi_{\beta} \rangle \quad (74)$$

where

$$\sum_{\alpha, \beta} K_{\alpha\beta}^\dagger K_{\alpha\beta} = I_S \quad (75)$$

Then we have

$$K_{\alpha\beta} = \sum_{i=1}^{N^2} F_i (F_i, K_{\alpha\beta}(t)) \quad (76)$$

With the help of the representation 73 we can write the action of the dynamical map $V(t)$ as

$$V(t)\rho_S = \sum_{i, j=1}^{N^2} c_{ij} F_i \rho_S F_j^\dagger \quad (77)$$

where

$$c_{ij} = \sum_{\alpha\beta} (F_i, K_{\alpha\beta}(t)) (F_j, K_{\alpha\beta}(t))^* \quad (78)$$

The coefficient matrix $c = (c_{ij})$ is easily seen to be Hermitian and positive.

The definition 70 of the generator \mathcal{L} now gives, by virtue of equation 77,

$$\begin{aligned} L\rho_S &= \lim_{\epsilon \rightarrow \infty} \frac{1}{\epsilon} (V(\epsilon)\rho_S - \rho_S) \\ &= \lim_{\epsilon \rightarrow \infty} \left(\frac{1}{N} \frac{c_{N^2 N^2}(\epsilon) - N}{\epsilon} \rho_S + \frac{1}{\sqrt{N}} \sum_{i=1}^{N^2-1} \left(\frac{c_{i N^2}(\epsilon)}{\epsilon} F_i \rho_S + \frac{c_{N^2 i}(\epsilon)}{\epsilon} \rho_S F_i^\dagger \right) \right) \end{aligned} \quad (79)$$

Next, we define coefficient a_{ij} by

$$\begin{aligned} a_{N^2 N^2} &= \lim_{\epsilon \rightarrow 0} \frac{c_{N^2 N^2} - N}{\epsilon} \\ a_{i N^2} &= \lim_{\epsilon \rightarrow 0} \frac{c_{i N^2}(\epsilon)}{\epsilon}, \quad i = 1, 2, \dots, N^2 - 1 \\ a_{ij} &= \lim_{\epsilon \rightarrow 0} \frac{c_{ij}(\epsilon)}{\epsilon}, \quad i, j = 1, \dots, N^2 - 1 \end{aligned} \quad (80)$$

and introduce the quantities

$$F = \frac{1}{\sqrt{N}} \sum_{i=1}^{N^2-1} a_{i N^2} F_i \quad (81)$$

and

$$G = \frac{1}{2N} a_{N^2 N^2} I_S + \frac{1}{2} (F^\dagger + F) \quad (82)$$

as well as the Hermitian operator

$$H = \frac{1}{2i} (F^\dagger - F) \quad (83)$$

We note that the matrix formed by the coefficient a_{ij} is Hermitian and positive. With the help of these definitions we can write the generator as

$$\mathcal{L}\rho_S = -i[H, \rho_S] + \{G, \rho_S\} + \sum_{i,j=1}^{N^2-1} a_{i,j} F_i \rho_S F_j^\dagger \quad (84)$$

Since the semigroup is trace preserving we have for all density operators ρ_S

$$0 = \text{tr}_S(\mathcal{L}\rho_S) = \text{tr}_S \left(\left(2G + \sum_{i,j=1}^{N^2-1} a_{i,j} F_j^\dagger F_i \right) \rho_S \right) \quad (85)$$

from which we deduce that

$$G = -\frac{1}{2} \sum_{i,j=1}^{N^2-1} a_{i,j} F_j^\dagger F_i \quad (86)$$

Hence, we get from 84 the first standard form of the generator,

$$\mathcal{L}\rho_S = -i[H, \rho_S] + \sum_{i,j=1}^{N^2-1} a_{ij} \left(F_i \rho_S F_j^\dagger - \frac{1}{2} \{F_j^\dagger F_i, \rho_S\} \right) \quad (87)$$

Since of the coefficient matrix $a = (a_{ij})$ is positive it may be diagonalized with help an appropriate unitary transformation u , $uau^\dagger = \text{diag}(\gamma_1, \gamma_2, \dots, \gamma_{N^2-1})$ where the eigenvalues γ_i are non-negative. Introducing a new set of operators A_k through

$$F_i = \sum_{k=1}^{N^2-1} u_{ki} A_k \quad (88)$$

the following diagonal form of the generator is obtained

$$\mathcal{L}\rho_S = -i[H, \rho_S] + \sum_{k=1}^{N^2-1} \gamma_k \left(A_k \rho_S A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S - \frac{1}{2} \rho_S A_k^\dagger A_k \right) \quad (89)$$

which it called LGKS equation.

5 Laws of Thermodynamics

5.1 The 1st Law in Unitary Evolution

An arbitrary quantum system with a finite number of energy levels is used here as the working substance. The Hamiltonian of the working substance can be written as

$$\mathcal{H} = \sum_n E_n |n\rangle \langle n| \quad (90)$$

where $|n\rangle$ is the n -th eigenstate of the system and E_n is its corresponding eigenenergy. Without loss of generality, we choose the eigenenergy of the ground state $|0\rangle$ as a reference point. Then the Hamiltonian can be written as

$$\mathcal{H} = \sum_n (E_n - E_0) |n\rangle \langle n| \quad (91)$$

The internal energy E of the working substance can be expressed as

$$E = \langle \mathcal{H} \rangle = \sum_n P_n E_n \quad (92)$$

for a given occupation distribution with probabilities P_n in the n -th eigenstate.

Now we need to identify the quantum analogues of the heat exchange dQ and the work performed dW . From the past equation we have

$$dE = \sum_n (E_n dP_n + P_n dE_n) \quad (93)$$

In classical thermodynamics, the first law of thermodynamics is expressed as

$$dE = dQ + dW \quad (94)$$

where $dQ = TdS$, and $dW = \sum_i Y_i dy_i$. T is the temperature and S is the entropy; y_i is the generalized coordinates and Y_i is the generalized force conjugated to y_i . Due to the relationship $H = -\sum_i P_i \ln P_i$ between the entropy H and the probabilities P_i , we can make the following identification

$$dQ = \sum_n E_n dP_n \quad (95)$$

$$dW = \sum_n P_n dE_n \quad (96)$$

These equations imply that the work performed corresponds to the change in the eigenenergies E_n , and this is in accordance with the fact that work can only be performed through a change in the generalized coordinates of the system, which in turn gives rise to a change in the eigenenergies.

5.2 The 1st Law in Non-Unitary Evolution

Quantum thermodynamics is based on a series of idealizations in similar fashion to the ideal gas model which serves classical thermodynamics. The theory of quantum open system is the inspiration for many of these idealizations.

It is customary to assume that the entire world is a large system and, therefore, time evolution is governed by a unitary transformation generated by a global Hamiltonian. For the combined system bath scenario the global Hamiltonian can be decomposed into:

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_B + \mathcal{H}_{SB} \quad (97)$$

where \mathcal{H}_S is the system's Hamiltonian, \mathcal{H}_B the bath Hamiltonian and \mathcal{H}_{SB} the system-bath interaction. Formally the state of the system can be obtained from a partial trace over the combined system: $\rho'_S = \text{tr}_B \rho'_{SB} = \text{tr}_B U \rho_{SB} U^\dagger$ where U is generated by the total Hamiltonian: $U = e^{-i\mathcal{H}t}$.

There are two major strategies to derive such equations. The first is based on the weak system-bath coupling expansion which leads to an integro-differential equation for the system state ρ_S :

$$\frac{d}{dt} \rho_S(t) = -i[\mathcal{H}_S, \rho_S] + \int_0^t \mathcal{K}(t, t') \rho_S(t') dt' \quad (98)$$

where \mathcal{K} is the memory kernel, and an additional assumption that at $t = 0$ the system and bath are uncorrelated:

$$\rho = \rho_S \otimes \rho_B \quad (99)$$

Assuming the bath dynamics is fast, the equation reduced to a differential form:

$$\frac{d}{dt}\rho_S = -i[\mathcal{H}_S, \rho_S] + \mathcal{L}_D \rho_S \quad (100)$$

where \mathcal{L}_D is the generator of dissipative dynamics.

The alternative approach to reduced dynamics searches for the most general form of the generator of Markovian dynamics or in more technical terms: A quantum dynamical completely positive semigroup. Kraus has shown that starting from an uncorrelated initial system and bath state, a reduced map $\mathcal{L}_S(t)$ to the final time has always the structure.

$$\rho_S(t) = \mathcal{L}_S(t)\rho_S(0) = \sum_j K_j \rho_S(0) K_j^\dagger \quad (101)$$

where K are system operators. When adding a Markovian assumption $\Lambda_S(t) = e^{\mathcal{L}t}$ the differential generator \mathcal{L} of the map becomes

$$\frac{d}{dt}\rho_S = \mathcal{L}\rho_S = -i[\mathcal{H}_S, \rho_S] + \sum_j \left(A_j \rho_S A_j^\dagger - \frac{1}{2} \{A_j^\dagger A_j, \rho_S\} \right) \quad (102)$$

where A are system operators and \mathcal{H}_S is a re-normalized system Hamiltonian. In previous sections we called this LGKS equation. The Heisenberg representation supplies a direct link to quantum thermodynamical observables. The dynamics of an observable represented by the operator O it has the form

$$\frac{dO}{dt} = \mathcal{L}^* O = i[\mathcal{H}_S, O] + \sum_j \left(A_j O V_j^\dagger - \frac{1}{2} \{A_j^\dagger A_j, O\} \right) + \frac{\partial O}{\partial t} \quad (103)$$

The first law is devoted to the elusive concept of energy conservation. If the universe is closed and passive then its energy is conserved. This implies that the total evolution is unitary, where the dynamics is generated by a total Hamiltonian \mathcal{H} . As a result the total energy expectation $\langle \mathcal{H} \rangle$ is constant.

Quantum thermodynamics focuses on the balance of energy of system coupled to bath. The local energy is the sum of the heat currents in and out of the system: Heat flow from the environments and power from an external source. The time derivation of the system's energy balance becomes:

$$\frac{dE_S}{dt} = \sum_j \mathcal{J}_j + \mathcal{P} \quad (104)$$

where \mathcal{J}_j is the heat current from the j th bath, and \mathcal{P} is the external power. The quantum version of the first law is obtained by inserting the system Hamiltonian \mathcal{H}_S into the operator dynamic equation.

$$\frac{dE_S}{dt} = \left\langle \frac{\partial \mathcal{H}_S}{\partial t} \right\rangle + \langle \mathcal{L}_D(\mathcal{H}_S) \rangle = \left\langle \frac{\partial \mathcal{H}_S}{\partial t} \right\rangle + \sum_j \mathcal{J}_j \quad (105)$$

since $[\mathcal{H}_S, \mathcal{H}_S] = 0$ only the dissipative part of \mathcal{L} appears. The heat currents \mathcal{J}_j can be identified as:

$$\mathcal{J}_j = \langle A_j \mathcal{H}_S A_j^\dagger - \frac{1}{2} \{A_j^\dagger A_j, \mathcal{H}_S\} \rangle \quad (106)$$

and the power becomes:

$$\mathcal{P} = \left\langle \frac{\partial \mathcal{H}_S}{\partial t} \right\rangle \quad (107)$$

5.3 The 2nd Law in Unitary Evolution

5.3.1 Equivalence of Entropies

We next review how to derive the second law based on microscopic dynamics. Starting with the statement of the second law, we derive it by a standard method in non-equilibrium statistical mechanics. We formulate the theory such that the total system of the thermodynamic system and the heat baths obey the unitary evolution, and assume that the initial states of the heat bath are in the canonical distribution.

Now suppose that thermodynamic system S is contacted with a huge bath with temperature T . In terms of statistical mechanics, thermodynamics quantities in thermal equilibrium can be calculated by using probability models. One of the most useful probability models is the canonical distribution:

$$\rho_{can} \equiv \frac{e^{-\beta\mathcal{H}}}{Z} \quad (108)$$

where \mathcal{H} is the Hamiltonian of the system, and

$$Z \equiv \text{tr}[e^{\beta\mathcal{H}}] \quad (109)$$

With the canonical distribution, free energy F can be calculated as

$$F = -T \ln Z \quad (110)$$

and internal energy E as

$$E = \text{tr}[\mathcal{H}\rho_{can}] \quad (111)$$

From above equations, we obtain

$$S_{thermo} = \beta(E - F) = -\text{tr}[\rho_{can} \ln \rho_{can}] \equiv H(\rho_{can}) \quad (112)$$

which implies that the thermodynamic entropy and the von Neumann entropy are equivalent in the canonical distribution.

5.3.2 Single Heat Bath

We now want to consider a single bath which is contacted with the system. For this purpose, we define the partition function and the Helmholtz free energies with temperature T corresponding to the initial and final Hamiltonians:

$$Z_i \equiv \text{tr}[e^{-\beta\mathcal{H}_i}], \quad Z_f \equiv \text{tr}[e^{-\beta\mathcal{H}_f}] \quad (113)$$

and

$$F_i \equiv -T \ln Z_i, \quad F_f \equiv -T \ln Z_f \quad (114)$$

The initial state of the system is assumed to be the canonical distribution at T :

$$\rho_i = \rho_{can,i} \equiv \frac{e^{-\beta\mathcal{H}_i}}{Z_i} \quad (115)$$

Then the final state of the system is given by

$$\rho_f = U\rho_i U^\dagger \quad (116)$$

which is not necessarily equal to the canonical distribution.

Since the von Neumann entropy $H(\cdot)$ is time-invariant under unitary evolutions, we obtain

$$H(\rho_i) = H(\rho_f) \quad (117)$$

On the other hand, from Klein's inequality, we have

$$H(\rho_f) \leq -\text{tr}[\rho_f \ln \rho_{can,f}] \quad (118)$$

From the previous part, we can show that

$$H(\rho_i) = \beta(\text{tr}[\mathcal{H}_i \rho_i] - F_i) \quad (119)$$

Therefore we know that

$$\text{tr}[\mathcal{H}_f \rho_f] - \text{tr}[\mathcal{H}_i \rho_i] \geq F_f - F_i \quad (120)$$

We note that the left-hand side of the above equation is the difference of the energies of the initial and final states. Since the system is not in contact with another heat bath, we can identify the energy difference with the work performed on the system. Therefore, we obtain

$$W \equiv \text{tr}[\mathcal{H}_f \rho_f] - \text{tr}[\mathcal{H}_i \rho_i] \quad (121)$$

Hence,

$$W \geq \Delta F \quad (122)$$

which is the second law of thermodynamics for isothermal processes.

We stress that we did not assume that the final state of the system is the canonical distribution. In fact, we cannot say that even the temperature is well-defined in the final state. The final free energy F_f is only formally defined by using the final Hamiltonian \mathcal{H}_f and the initial temperature T , which is a standard formulation in modern non-equilibrium statistical physics. Since the final state is arbitrary, inequality can be applied to an arbitrary non-equilibrium process in which only the initial state is in the canonical distribution. We also stress that we did not assume that the system is large; inequality can be applied even to small systems.

Also, we note that the difference between the work and the free-energy change is given by the relative entropy:

$$W - \Delta F = TD(\rho_f || \rho_{f,can}) \quad (123)$$

which implies that $W - \Delta F$ is given by the gap between the final state and the canonical distribution.

5.3.3 Multi Heat Baths

We next consider a thermodynamic process \mathbf{S} that can contact heat baths $\mathbf{B}_1, \mathbf{B}_2, \dots, \mathbf{B}_n$ at respective temperature T_1, T_2, \dots, T_n . We assume that the total of \mathbf{S} and \mathbf{B}_m 's obeys a unitary evolution and the initial state of the total system is given by

$$\rho_i \equiv \rho^S \otimes \rho_{can}^{B_1} \otimes \dots \otimes \rho_{can}^{B_n} \quad (124)$$

where ρ^S is an arbitrary initial state of \mathbf{S} , and

$$\rho_{can}^{B_m} \equiv \frac{e^{-\beta H^{B_m}}}{Z^{B_m}} \quad (125)$$

is the canonical distribution with $Z^{B_m} = \text{tr}[e^{-\beta H^{B_m}}]$. We write the free energies of the heat baths as $F^{B_m} \equiv T_m \ln Z^{B_m}$.

The unitary evolution of the total system is given by

$$\rho_f = U \rho_i U^\dagger \quad (126)$$

We write $\rho_f^S \equiv \text{tr}_{B_1, \dots, B_n}[\rho_f]$

Duo to the unitary evolution invariance of the von Neumann entropy, we obtain

$$H(\rho_i) = H(\rho_f) \quad (127)$$

On the other hand, we have

$$H(\rho_i) = H(\rho_i^S) + \sum_m \beta_m (\text{tr}[\rho_i H^{B_m}] - F^{B_m}) \quad (128)$$

From Klein's inequality, we also have

$$H(\rho_f) = S(\rho_f^S) + \sum_m \beta_m (\text{tr}[\rho_f H^{B_m}] \geq \text{tr}[\rho_f \ln(\rho_f)]) \quad (129)$$

where we used $-\text{tr}[\rho_f^S \ln \rho_f^S] = H(\rho_f^S)$. Therefore we obtain

$$H(\rho_f^S) - H(\rho_i^S) \geq \sum_m \beta_m Q_m \quad (130)$$

where

$$Q_m \equiv \text{tr}[\rho_i H^{B_m}] - \text{tr}[\rho_f H^{B_m}] \quad (131)$$

is the heat that is absorbed by system \mathbf{S} from heat bath \mathbf{B}_m . This inequality can be regarded as a generalization of Clausius's inequality to non-equilibrium initial and final distribution.

Non-equilibrium steady state. We first consider a simple case in which system \mathbf{S} is in contact with two heat baths T_H and T_L with $T_H > T_L$, and \mathbf{S} is in a non-equilibrium steady state with a constant heat flow $Q_H = -Q_L \equiv Q$. Since \mathbf{S} is in a steady state, we may assume $H(\rho_i^S) = H(\rho_f^S)$. Therefore inequality reduces to

$$(\beta_H - \beta_L)Q \leq 0 \quad (132)$$

and therefore $Q \leq 0$, implying that the heat flows from the hot bath to the cold one.

Isothermal process. We next consider the case in which there is a single heat bath at temperature T . In this case, inequality reduces to

$$H(\rho_f^S) - H(\rho_i^S) \geq \beta Q \quad (133)$$

We then assume that the initial state of \mathbf{S} is the canonical distribution as

$$\rho_i^S = \rho_{can,i}^S \equiv \frac{e^{-\beta \mathcal{H}_i^S}}{Z_i^S} \quad (134)$$

where $Z_i^S \equiv \text{tr}[e^{-\beta \mathcal{H}_i^S}]$. We also introduce notations as

$$F_i^S = -T \ln Z_i^S \quad (135)$$

From Klein's inequality, we obtain

$$H(\rho_f^S) - H(\rho_i^S) \leq \beta(\Delta E^S - \Delta F^S) \quad (136)$$

where

$$\Delta E^S \equiv \text{tr}[\mathcal{H}_f^S \rho_f^S] - \text{tr}[\mathcal{H}_i^S \rho_i^S] \quad (137)$$

Hence, the first law of thermodynamics holds as

$$\Delta E^S - \Delta F^S \geq Q \implies \Delta E^S = Q + W^S \quad (138)$$

5.4 The 2nd Law in Non-Unitary Evolution

In this section, we review a generalized second law with a quantum measurement and feedback control.

5.4.1 Entropy Inequality

We first discuss the entropy balance of a quantum system that obeys a quantum measurement and feedback in addition to unitary evolution. Let ρ_i be an arbitrary initial density operator of a finite-dimensional quantum system, which evolve follows:

Step 1: Unitary evolution. From time 0 to t_1 , the system undergoes unitary evolution U_i . At time t_1 , the density operator is given by $\rho_1 = U_i \rho_i U_i^\dagger$

Step 2: Measurement. From time t_1 to t_2 , we perform a quantum measurement on the system. We assume that the measurement is described by measurement operator $\{M_k\}$ with k 's being measurement outcome, which leads to POVM

$$\Lambda \equiv M_k^\dagger M_k \quad (139)$$

We obtain each outcome k with probability

$$p_k = \text{tr}(\Lambda_k \rho_1) \quad (140)$$

Here we assumed that every single measurement operator corresponds a single measurement outcome as $\Lambda = M_k^\dagger M_k$. Let $\mathbf{p} \equiv \{p_k\}$. The post-measurement state corresponding to outcome k is given by

$$\rho_2^{(k)} = \frac{1}{p_k} M_k \rho_1 M_k^\dagger \quad (141)$$

and the ensemble average is given by

$$\rho_2 = \sum_k p_k \rho_2^{(k)} = \sum_k M_k \rho_1 M_k^\dagger \quad (142)$$

Step 3: Feedback control. From t_2 to t_3 , we perform feedback control; the corresponding unitary operator U_k depends on measurement outcome k . The post-feedback state corresponding to outcome k is given by

$$\rho_3^{(k)} = U_k \rho_2^{(k)} U_k^\dagger = \sum_k U_k M_k \rho_1 M_k^\dagger U_k^\dagger \quad (143)$$

Step 4: Unitary evolution. After the feedback from t_3 to τ , the system evolves according to unitary operator U_f which is independent of outcome k . The final state is $\rho_f = U_f \rho_3 U_f^\dagger$.

The entire time evolution is then given by

$$\rho_f = \mathcal{E}(\rho_i) \equiv \sum_k U_f U_k M_k U_i \rho_i U_i^\dagger M_k^\dagger U_k^\dagger U_f^\dagger \quad (144)$$

The difference in the von Neumann entropy H between the initial and final states can be bounded as follows:

$$\begin{aligned} H(\rho_i) - H(\rho_f) &= H(\rho_1) - H(\rho_3) \leq H(\rho_1) - \sum_k p_k H(\rho_3^{(k)}) \\ &= H(\rho_1) - \sum_k p_k H(\rho_2^{(k)}) = H(\rho_1) + \sum_k \text{tr} \left(\sqrt{\Lambda_k} \rho_1 \sqrt{\Lambda_k} \ln \frac{\sqrt{\Lambda_k} \rho_1 \sqrt{\Lambda_k}}{p_k} \right) \end{aligned} \quad (145)$$

Hence,

$$H(\rho_i) - H(\rho_f) \leq I_{QC} \quad (146)$$

where the equality is achieved if and only if all of $\rho_3^{(k)}$'s are the same. Intuitively speaking, this condition means that the feedback control is perfect, i.e., we used all the obtained information by feedback control.

5.4.2 Generalized Second Laws

We now consider the energetics of feedback control on thermodynamics systems, in terms of the work, the heat, and the free energy. We consider a thermodynamic process of system \mathbf{S} which can be in contact with heat baths $\mathbf{B}_1, \mathbf{B}_2, \dots, \mathbf{B}_n$, at respective temperature T_1, T_2, \dots, T_n .

We assume that the total system of \mathbf{S} and heat baths \mathbf{B}_m obeys a unitary evolution expect for the process of a measurement. We assume that the initial state of the total system is given by

$$\rho_i \equiv \rho_i^S \otimes \rho_{can}^{B_1} \otimes \cdots \otimes \rho_{can}^{B_n} \quad (147)$$

where ρ_i^S is an arbitrary initial of \mathbf{S} . The total density operator evolves as described in Step 1 to 5 in the previous subsection. To transform inequity $H(\rho_i) - H(\rho_f) \leq I_{QC}$ to energetic inequalities, we can apply the same argument as in the previous subsection. First of all, equality 127 is replaced by inequality 146 in the presence of feedback control. We then obtain

$$H(\rho_f^S) - H(\rho_i^S) \geq \sum_m \beta_m Q_m - I_{QC} \quad (148)$$

which is a generalization of inequality 130 to the situation in which the system is subject to feedback control.

If there is a single heat bath and the initial distribution of \mathbf{S} is a canonical distribution, 148 reduces to

$$W \geq \Delta F - TI_{QC} \quad (149)$$

where W is given by ???. This inequality is a generalization of inequality 133 to feedback-controlled processes. By introducing notation $W_{ext} \equiv -W$, the inequality can be written as

$$W_{ext} \leq -\Delta F + TI_{QC} \quad (150)$$

This inequality implies that we can extract work greater than $-\Delta F$ from a single heat bath with feedback control, but that we cannot extract work larger than $-\Delta F + TI_{QC}$. If $I_{QC} = 0$, the inequality reduces to 122. On the other hand, in the case of a classical and error-free measurement, the inequality becomes [6]

$$W_{ext} \leq -\Delta F + TH(\mathbf{P}) \quad (151)$$

6 Quantum Cycles

6.1 Quantum Isothermal Process

Let us now consider the quantum versions of some thermodynamics processes. First we study quantum isothermal processes. In quantum isothermal processes, the working substance, such as a particle confined in a potential energy well, is kept in contact with a heat bath at a constant temperature. The particle can perform positive work to the outside, and meanwhile absorb heat from the bath. Both the energy gaps and the occupation probabilities need to change simultaneously, so that the system remains in an equilibrium state with the heat bath at every instant. Specifically, let us consider a two-level system with the excited state $|e\rangle$, the ground state $|g\rangle$, and a single energy spacing Δ . In the quasi-static quantum isothermal process, the ratio $r = P_e/P_g$ of the two occupation probabilities must satisfy the Boltzmann distribution $r = P_e/P_g = \exp(-\beta\Delta)$ and also the normalization condition $P_e + P_g = 1$. Δ changes slowly with time t , and accordingly r can be written as

$$r = r(t) = \frac{P_e}{P_g} = e^{\beta\Delta} \quad (152)$$

where $\beta = \frac{1}{T}$ and T is the temperature.

6.2 Effective Temperature

We can also define an effective temperature T_{eff} for any two-level system according to the ratio $r(t)$ and the level spacing Δ . For a two-level system with energy levels E_e and E_g , even in a non-equilibrium state, we can imagine that it is a virtual equilibrium state with the effective temperature

$$T_{eff} = \frac{1}{\beta_{eff}} = \Delta \left(\ln \frac{P_g}{P_e} \right)^{-1} \quad (153)$$

as long as the level spacing Δ and the energy distribution P_g and P_e are know.

6.3 Quantum Adiabatic Process

A classical adiabatic thermodynamic process can be formulated in terms of a microscopic quantum adiabatic thermodynamic process. Because quantum adiabatic processes proceed slow enough such that the generic quantum adiabatic condition is satisfied, then the population distribution remain unchanged, $dP_n = 0$. According to equation 95, $dQ = 0$,

there is no heat exchange in a quantum adiabatic process, but work can still nonzero according to equation 96. A classical adiabatic process, however, does not necessarily require the occupation probabilities to be kept invariant. For example, when the process proceeds very fast, and the quantum adiabatic condition is not satisfied, internal excitations will likely occur, but there is no heat exchange between the working substance and the external heat bath. This thermodynamic process is classical adiabatic but not quantum adiabatic. Thus it can be verified that a classical adiabatic process includes, as a subset, a quantum adiabatic process; but the inverse is not valid.

The evolution of the density operator is given by

$$\frac{d\rho}{dt} = -i[\mathcal{H}(\omega), \rho] \quad (154)$$

The change of the energy $\langle E \rangle = \text{Tr} H(\omega)\rho$ due to the explicit time dependence of ω on the adiabats becomes

$$\frac{d}{dt}\langle E \rangle_a = \text{tr} \left\{ \left(\frac{d}{dt} \mathcal{H} \right) \rho \right\} \quad (155)$$

The work in a time period t is then

$$W(t) = \int_0^t \frac{d}{dt'} \langle E \rangle_a dt' = \langle E(t) \rangle_a - \langle E(0) \rangle_a \quad (156)$$

Notice that $W > 0$ when the system energy increases and $W < 0$ when the cycle realizes useful work on the environment.

6.4 Quantum Isochoric Process

A quantum isochoric process has similar properties to that of a classical isochoric processes. In a quantum isochoric process, the working substance is placed in contact with a heat bath. No work is done in this process while heat is exchanged between the working substance and the heat bath. This is the same as that in a classical isothermal process. In a quantum isochoric process the occupation probabilities P_n and thus the entropy S change, until the working substance finally reaches thermal equilibrium with the heat bath only at the end of this process.

The system is in contact with a heat bath at temperature T_α while the external control is equal to ω_α , with $\alpha = c, h$. When the working medium couples weakly to a heat bath, the Markovian relaxation towards thermal equilibrium is described by GKLS equation

$$\frac{d\rho}{dt} = -i[H(\omega_\alpha), \rho] + \mathcal{L}_\alpha(\rho) \quad (157)$$

where

$$\mathcal{L}(\rho) = \sum_j \kappa_j \left(V_j \rho V_j^\dagger - \frac{1}{2} \{V_j^\dagger V_j, \rho\} \right) \quad (158)$$

In this expression V_j are transition operators between neighboring energy levels of \mathcal{H} and κ_j the corresponding transition rates.

The energy change in the isochore is

$$\frac{d}{dt}\langle E \rangle_i = \text{tr} \{ \mathcal{H}(\omega_\alpha) \mathcal{L}_\alpha(\rho) \} \quad (159)$$

The heat exchange with the baths is a time period t is then

$$Q_\alpha(t) = \int_0^t \frac{d}{dt'} \langle E \rangle_i dt' = \langle E(t) \rangle_i - \langle E(0) \rangle_i \quad (160)$$

which is positive when energy flows towards the system.

6.5 Pressure in Quantum-Mechanical System

In order to study the quantum isobaric process, we must first study pressure in an arbitrary quantum-mechanical system. Let us recall that in some previous section, heat and work have been extended to quantum-mechanical system and expressed as function of the eigenenergies E_n and probability P_n . The first law of thermodynamics has also been generalized to quantum-mechanical system as follows:

$$dQ = \sum_n E_n dP_n \quad (161)$$

$$dW = \sum_n P_n dE_n \quad (162)$$

and

$$dE = dQ + dW = \sum_n (E_n dP_n + P_n dE_n) \quad (163)$$

The density operator of the system can be written as $\rho = \sum_n P_n |n\rangle \langle n|$. dQ and dW depict the heat exchange and work done, respectively, during a thermodynamic process. From classical thermodynamics we know that the first law can be expressed as $dE = dQ + dW = TdS + \sum_n Y_n dy_n$. Inversely, the generalized force conjugate to the generalized coordinate y_n can be expressed as

$$Y_n = -\frac{dW}{dy_n} \quad (164)$$

For example, when the generalized coordinate is chosen to be the volume V , we have its corresponding generalized force-pressure $P = -dW/dV$. Motivated by the definition the generalized force for a classical system, we define analogously the force for a quantum-mechanical system

$$\mathcal{F} = -\frac{dW}{dL} = -P_n \frac{dE_n}{dL} \quad (165)$$

where L is the generalized coordinate corresponding to the force \mathcal{F} . In obtaining equation 165, we have used the expression of work for a quantum system $dW = \sum_n P_n dE_n$. For a single particle in a 1D box, the generalized coordinate is the width of the potential, and the eigenenergies for such a system depends on the generalized coordinate

$$E_n(L) = (\pi\hbar n)^2 / (2mL^2) \quad (166)$$

Here \hbar is Planck's constant; n is the quantum number; m is the mass of the particle. We obtain the derivative of $E_n(L)$ over L straightforwardly

$$\frac{dE_n}{dL} = -2\frac{E_n(L)}{L} \quad (167)$$

When the system is in thermal equilibrium with a heat bath at an inverse temperature $\beta = 1/T$, the force exerting on either wall of the potential can be calculated by substituting $\frac{dE_n}{dL}$ and the Gibbs distribution $P_n = 1/Z e^{-\beta E_n}$ into equation 165. Alternatively, the expression of force in a quantum-mechanical system can be obtained in a statistical mechanical way

$$\mathcal{F} = -\left(\frac{\partial F}{\partial L}\right)_T = T \left(\frac{\partial \ln Z}{\partial L}\right)_T = T \frac{1}{Z} \frac{\partial}{\partial L} \sum_n e^{-\beta E_n} = -\sum_n P_n \frac{dE_n}{dL} \quad (168)$$

where $F = -T \ln Z$ is the free energy of the quantum system.

6.6 Quantum Isobaric Process

Having clarified force for a quantum-mechanical system, in the following we study how to extend the classical isobaric process is a quasi-static thermodynamic process, in which the pressure of the system remains a constant. The time scale of relaxation of the system with the heat bath is much shorter than the time scale of controlling the volume of the system. In a classical isobaric process, in order to achieve a constant pressure, we must carefully control the temperature of the heat bath, when we change the volume of the classical system. For example, for the classical idea gas with the equation of state $PV = NT$, the temperature of the system in the isobaric process is required to be proportional to the volume of the gas heat bath with the generalized coordinate may not be so obvious as the classical ideal gas, because we usually do not know the equation of state of a quantum-mechanical system. Let us consider the quantum isobaric process on a one dimensional box. For such a quantum-mechanical system, the pressure on the wall can be obtained from equation 165,

$$\begin{aligned} F &= -\sum_n P_n(L) \frac{dE_n(L)}{dL} = -\sum_n \frac{\exp(-\beta(L)E_n(L))}{Z(L)} \frac{dE_n(L)}{dL} \\ &= -\frac{4}{L} \sqrt{\frac{\pi\hbar^2\beta(L)}{2mL^2}} \left(-\frac{\partial}{\partial\beta(L)} \sum_n \exp\left(-\beta(L)\frac{\pi^2\hbar^2 n^2}{2mL^2}\right) \right) = \frac{1}{L\beta(L)} \end{aligned} \quad (169)$$

Equation 169 can be regarded as the equation of state $FL = T$ for the 1DB obtained from equation 165 and it means that if we want to keep the pressure F as a constant, we must control the temperature of the system to be proportional to the width of the potential well $\beta(L) = 1/(FL)$ when the system inside the box pushes one of the walls to perform work. This property of the 1DB is the same as the classical ideal gas

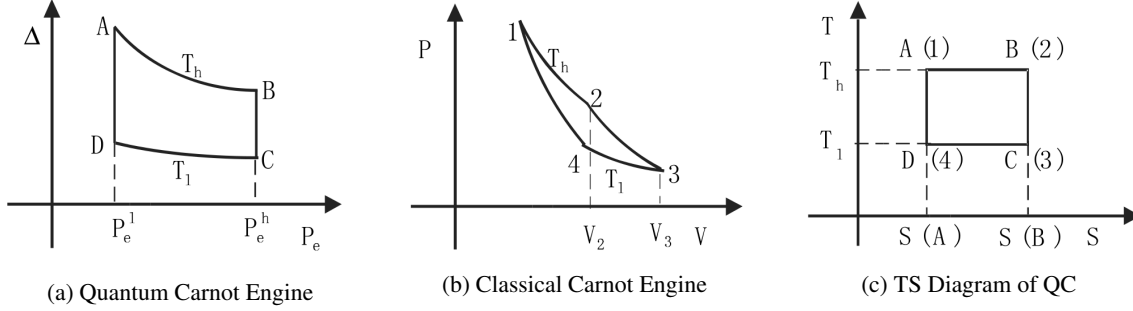


Figure 1: Carnot Engine

6.7 Quantum Carnot Cycle

in the previous sections, we defined quantum isothermal process. Based on this definition, in this section, we study the QC cycle and its properties. The QC cycle (Figure 1), just like its classical counterpart, consists of two quantum isothermal process ($A \rightarrow B$ and $C \rightarrow D$) and two quantum adiabatic process ($B \rightarrow C$ and $D \rightarrow A$). During the isothermal expansion process from A to B , the particle confined in the potential well is kept in contact with a heat bath at temperature T_h , while the energy levels of the system change much slower than the relaxation of the system, so that the particle is always kept in thermal equilibrium with the heat bath. Below, we consider both cases: two-level and multi-level systems.

6.7.1 Thermodynamic Reversibility

It is well known that quantum mechanical reversibility are associated with quantum mechanical unitary evolution. Different from quantum mechanical reversibility, thermodynamic reversibility accompanies the heat bath and the effective temperature of the working substance. We emphasize that, in order to ensure that the cycle is thermodynamic reversible, two conditions on the quantum adiabatic process required: (1) after the quantum adiabatic process ($B \rightarrow C$), we can use an effective temperature T_l to characterize the working substance and (2) the effective temperature T_l of the working substance, after the quantum adiabatic process, equals the temperature T_l of the heat bath of the following quantum isothermal process ($C \rightarrow D$). When either condition is not satisfied, a thermalization process of the working substance is inevitable before the quantum isothermal process ($C \rightarrow D$). In the thermalization process, the total entropy increase of the working substance plus the heat bath is nonzero. Hence, this thermalization process is irreversible.

6.7.2 Work and Efficiency

Now we analyze the operation efficiency η_C of the QC introduced above. For simplicity, instead of applying equation $dQ = \sum_n E_n dP_n$, we use $dQ = TdS$ to calculate the heat exchange dQ in any quantum isothermal process (QIT). Because the temperature of the heat bath is kept invariant in the quantum isothermal process, the heat absorbed Q_{in}^{QIT} and released Q_{out}^{QIT} in the quantum isothermal expansion and compression processes can be calculated as follows

$$\begin{aligned} Q_{in}^{QIT} &= T_h(S(B) - S(A)) > 0 \\ Q_{out}^{QIT} &= T_l(S(C) - S(D)) > 0 \end{aligned} \quad (170)$$

where T_h and T_l are the temperatures of the two different heat baths, and

$$S(i) = - \sum_n \frac{\exp(-\beta_i E_n(i))}{Z(i)} (-\beta_i E_n(i) - \ln Z(i)) \quad (171)$$

are the entropies of the working substance at different instants $i = A, B, C, D$ (see figure 1). Here, $\beta_{A,B} = 1/T_h$, $\beta_{C,D} = 1/T_l$. In obtaining the above result, we have used the Boltzmann distribution of thermal equilibrium state, i.e., $\rho = (1/Z) \sum_n -\beta E_n |n\rangle \langle n|$, where $Z = \text{tr } e^{\beta H}$ is the partition function.

Now, we would like to calculate the work W_C done during a QC cycle and its operation efficiency η_C . From equations 170 and the first law of thermodynamics we obtain the net work done during a QC cycle

$$W_C = Q_{in}^{QIT} - Q_{out}^{QIT} = (T_h - T_l)(S(B) - S(A)) \quad (172)$$

where we have used the relations $S(B) = S(C)$ and $S(A) = S(D)$. This equivalence is due to the fact that the occupation probabilities and thus the entropy remain invariant in any quantum adiabatic process. The efficiency η_C of the QC is

$$\eta_C = \frac{W_C}{Q_{in}^{QIT}} = 1 - \frac{T_l}{T_h} \quad (173)$$

which is just the efficiency of a classical Carnot engine.

Let us assume that bath at temperature T_h at the instant B before the adiabatic process ($B \rightarrow C$). In this case the quantum state is described by a density operator

$$\rho(B) = \frac{1}{Z} \sum_n \exp(-\beta_h E_n(B)) |n(B)\rangle \langle n(B)| \quad (174)$$

After the adiabatic process is completed, at instant C in Fig 1, the eigenenergies of the working substance become $E_n(C)$, and the working substance reaches an effective temperature T_l . The occupation probabilities P_n of the working substance are kept unchanged during the adiabatic process ($B \rightarrow C$), and they satisfy the Boltzmann distribution. Thus, for any eigenstates $|n\rangle$ and $|m\rangle$, the occupation probabilities P_n and P_m satisfy

$$\frac{P_n(B)}{P_m(B)} = \frac{\exp(-\beta_h E_n(B))}{\exp(-\beta_h E_m(B))} = \frac{P_n(C)}{P_m(C)} = \frac{\exp(-\beta_l E_n(C))}{\exp(-\beta_l E_m(C))} \quad (175)$$

That is

$$E_n(C) - E_m(C) = \frac{T_l}{T_h} (E_n(B) - E_m(B)) \quad (176)$$

for any m, n .

From 176 we see that the ratio of the temperature in the efficiency (equation 173) of the QC can also be replaced by the ratio of the energy gaps

$$\eta_C = 1 - \frac{E_n(C) - E_m(C)}{E_n(B) - E_m(B)} \quad (177)$$

References

- [1] John Goold, Marcus Huber, Arnau Riera, L dia del Rio, Paul Skrzypczyk. *The Role of Quantum Information in Thermodynamics*. Journal of Physics A: Mathematical and Theoretical. Volume 49, Number 14. 2016.
- [2] Mark M. Wilde. *Quantum Information Theory (Second Edition)*. Cambridge University Press. 2014.
- [3] Thomas M. Cover, Joy A. Thomas. *Elements of Information Theory (Second Edition)*. John Wiley & Sons Inc. Publication. 2016
- [4] Heinz-Peter Breuer, Francesco Petruccione. *The Theory of Open Quantum Systems*. Oxford University Press. 2002.
- [5] Ronnie Kosloff. *Quantum Thermodynamics*. Entropy 15, No. 6, 2100-2128, 2013.
- [6] Takahiro Sagawa. *Thermodynamics of Information Processing in Small Systems*. Progress of Theoretical Physics, Volume 127, Issue 1, 2012.
- [7] H. T. Quan, Yu-xi Liu, C. P. Sun, Franco Nori. *Quantum Thermodynamic Cycles and Quantum Heat Engines*. Phys. Rev. E 76, 031105. 2017.
- [8] H. T. Quan *Quantum Thermodynamic Cycles and Quantum Heat Engines. II*. Phys. Rev. E 79, 041129. 2009