

# Quantum Thermodynamics

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2019113005

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November, 2020

# Contents

<b>1</b>	<b>Abstract</b>	<b>3</b>
<b>2</b>	<b>Inspiration for this topic</b>	<b>3</b>
<b>3</b>	<b>Laws of Thermodynamics</b>	<b>3</b>
<b>4</b>	<b>Quantum Thermometry</b>	<b>5</b>
4.1	Optimal Thermometers . . . . .	6
<b>5</b>	<b>Carnot's Cycle</b>	<b>6</b>
5.1	Classical vs Quantum . . . . .	7
5.2	Quantum Thermodynamic Processes . . . . .	7
5.3	Quantum Carnot's Cycle . . . . .	10
5.4	Efficiency . . . . .	12
<b>6</b>	<b>Further topics</b>	<b>13</b>
	<b>References</b>	<b>15</b>

## 1 Abstract

We shall model the Carnot's engine using quantum mechanics and quantum thermodynamic processes and compare the efficiencies. We'll be going over the laws of thermodynamics and some quantum thermometry to understand how temperature is measured.

## 2 Inspiration for this topic

One of the limiting factors for performance in modern day devices is *heat*. We often see the term "can be *turbo boosted* up to" on laptop and computer descriptions. The reason for this is being the chips will generate more heat as load increases and hence thermal efficiency is critical for their performance. Obviously building a quantum level cooling system is going to be very complex. I'd like to model the simple Carnot cycle using quantum thermodynamics and compare its efficiency to the the classical model.

## 3 Laws of Thermodynamics

### 1. Zeroth law

*"If two systems are in thermal equilibrium with a third system, then they are in thermal equilibrium with each other."*

### 2. First law

$$dE = dQ - dW$$

Where  $E$  is the internal energy of the system,  $W$  is the work done and  $Q$  is heat supplied.

Conventionally in physics, work done by the system is considered to be positive and work done on the system is negative. Chemistry uses the

opposite sign convention. Also  $E$  is a state function. This means that the path of the process doesn't matter. Only the initial and final states matter.

### 3. Second law

- (a) *"No process is possible whose sole result is the extraction of energy from a heat bath, and the conversion of all that energy into work."* - Kelvin-Planck
- (b) *"No process is possible whose sole result is the transfer of heat from a body of lower temperature to a body of higher temperature."* - Clausius
- (c) *"No engine operating between two heat reservoirs can be more efficient than a Carnot engine operating between those same reservoirs."* - Carnot

A result of this is that the entropy of the universe never decreases with time.

$$\Delta S_{universe} \geq 0$$

### 4. Third law

Entropy change of a system will approach zero as the temperature of the system tends to zero.

$$\lim_{T \rightarrow 0} \Delta S = 0$$

### 5. Fourth law

If we consider the concept of thermodynamic flux and thermodynamic forces assuming that the thermodynamic system is in a state of local equilibrium, we can formulate the fourth law which is also known as the Onsager equation.

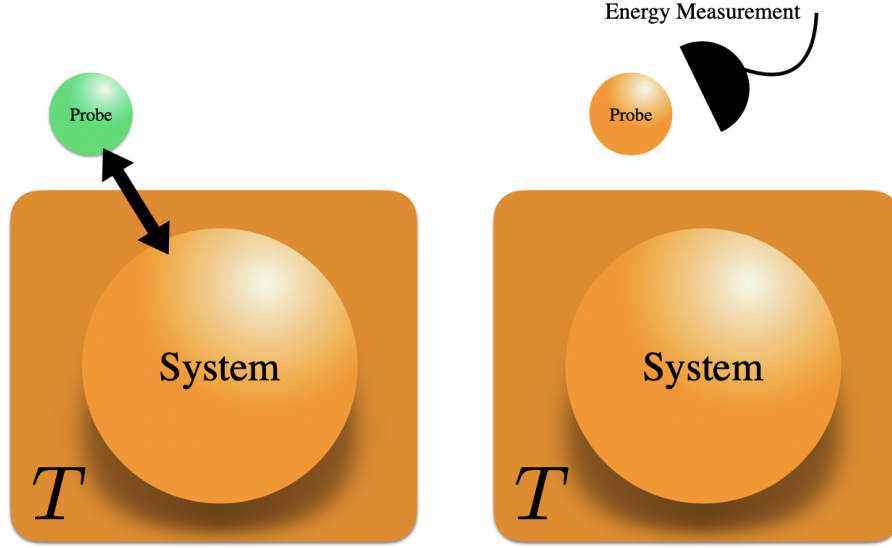
$$L_{i,j} = L_{j,i}$$

where  $L_{i,k}$  is the kinetic coefficient and is given by,

$$L_{i,k} = \frac{\partial J_k}{\partial F_i}, \quad (F_i = 0 \text{ at equilibrium})$$

where  $J$  is the thermodynamic flux and  $F$  is the thermodynamic force.

## 4 Quantum Thermometry



A quantum probe is a device used to measure the temperature of a quantum system. Temperature is fairly easy to measure in a classical system while the same doesn't apply quantum mechanically. We require a different system because temperature of quantum systems is neither observable classically nor quantum mechanically.

The quantum probe interacts with the quantum system until it is in equilibrium with it. We then measure the temperature of the probe. This is estimated using a model where higher the value of *Fisher Information*( $FI$ ), more the sensitivity. The maximum value of  $FI$  is known as Quantum Fisher Information (QFI). QFI is given by,

$$\mathcal{F}(\beta) = \beta^4 [\text{Var}(H)]^2$$

where  $\beta = \frac{1}{k_B T}$  and  $H$  is the Hamiltonian.

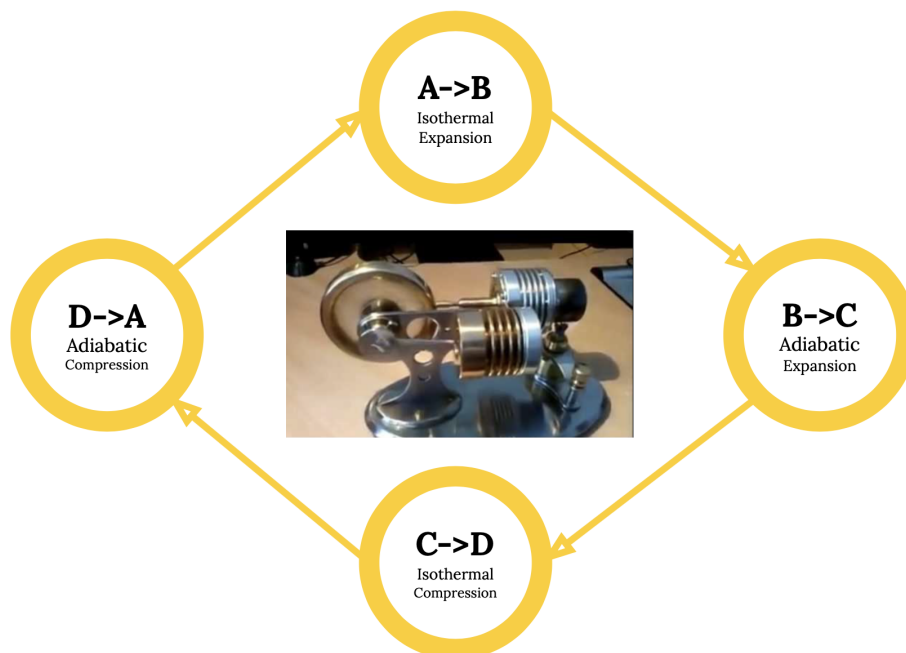
## 4.1 Optimal Thermometers

We said that maximising QFI will give us a more optimal thermometer. Clearly we can achieve this by maximising the variance of the Hamiltonian. We can achieve greater precision in two ways:

1. Increasing degeneracy
2. Introducing anharmonicity

When we exploit the degeneracy, the temperature range on which at which the probe functions optimally is reduced and hence we introduce anharmonicity to balance it.

## 5 Carnot's Cycle



Consider 4 states A, B, C and D.  $A \rightarrow B, C \rightarrow D$  Volume and pressure change,

while the temperature remains constant.  $B \rightarrow C, D \rightarrow A$  Volume and temperature change, while the entropy remains constant. Each of these processes are reversible.

## 5.1 Classical vs Quantum

Classically we the idea of using temperature is very well understood. Temperature is basically a measurement of energy in a sense. For example, internal energy of a molecule is given by  $\frac{f}{2}k_bT$  where  $f$  is the number of degrees of freedom of the molecule. In quantum mechanics, the equivalent of temperature is the expectation value of the Hamiltonian  $\langle H \rangle$ . We will also consider force while describing the quantum systems which is equivalent to pressure in classical systems (here equivalent doesn't mean exactly the same, rather comparable).

## 5.2 Quantum Thermodynamic Processes

In classical mechanics we consider this process using a mono-atomic gas in a cylinder and piston configuration. In quantum mechanics we'll be using the concept of *potential well*. The motion of the piston corresponds to the change in the length of the wall  $L$ . We'll be basing our calculation on a single quantum particle present in a quantum well and then consider infinite copies of such particles. The average of energies of all these particles will be given by the expectation value of the Hamiltonian.

Consider a particle of mass  $m$  in an one-dimensional potential well of length  $L$ . We know that the potential inside the well is zero and infinity outside. So the time independent Schrodinger equation satisfying the boundary

condition  $\psi(0) = \psi(L) = 0$  will be,

$$\begin{aligned}
E\psi(x) &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) \\
\psi(x) &= \sum_{n=1}^{\infty} a_n \phi_n(x) \text{ where } \sum_{n=1}^{\infty} |a_n|^2 = 1, \quad \phi_n(x) = \frac{\sqrt{2}}{\sqrt{L}} \sin\left(\frac{n\pi}{L}x\right) \\
E_n &= \frac{\pi^2 \hbar^2 n^2}{2mL^2} \\
(\text{Here, } n &= 1, 2, 3, \dots) \\
E(L) &= \langle H \rangle \\
F &= -\frac{dE(L)}{dL}
\end{aligned}$$

Where  $\psi(x)$  is the wave function,  $\phi_n(x)$  are the eigenstates,  $H$  is the Hamiltonian,  $E$  is the energy and  $F$  is the force.

Using the above information about the potential well, let us describe the some quantum thermodynamic processes.

### 1. **Adiabatic**

An adiabatic process is where the system is thermally isolated. Meaning that there is no heat transfer. From the first law of thermodynamics we see that work is converted to internal energy. Upon solving a couple of relations we arrive at the following,

$$PV^3 = C$$

where  $C$  is a constant. However this is true when we consider it classically.

Let us now look at it through quantum mechanics. We said that the motion of the piston is equivalent to the wall moving. Resulting in the change of length of the wall. However the system must remain in equilibrium. Hence the coefficients  $|a_n|^2$  will remain the same. Therefore we have,

$$\begin{aligned}
E(L) &= \sum_{n=1}^{\infty} |a_n|^2 E_n \\
F(L) &= \sum_{n=1}^{\infty} |a_n|^2 \frac{\pi^2 \hbar^2 n^2}{mL^3}
\end{aligned}$$



## 2. Free expansion

In this process there is no flow of heat and no work is done by the system. The temperature remains constant as there is no change in internal energy.

$$T = C$$

$$P_{final}V_{final} = P_{initial}V_{initial}$$

where  $C$  is a constant.

However this process is irreversible and we won't be using it in the Carnot's cycle. We won't be deriving the expression. Consider the length to be increased by a factor of  $\alpha$  which means that  $L' = \alpha L$ . The general equation that describe free expression quantum mechanically,

$$\sum_{m=1}^{\infty} \frac{\cos(mx)}{m^2 - u^2} = \frac{1}{2u} - \frac{\pi \cos([(2k+1)\pi - x]u)}{2u \sin(\pi u)}$$

where  $x = \frac{2\pi}{\alpha}$ ,  $u = \alpha n$  and  $k$  is the largest integer such that  $2\pi k \leq x$ .  $k = 0$  if the system expands (as  $\alpha > 1$ ).

## 3. Isothermal

Here the temperature remains constant. Thus there is no change in internal energy. However, the system does work. Therefore we have the following relation,

$$PV = C$$

where  $C$  is a constant.

Quantum mechanically, the particle can move to a higher energy state. Thus we'll be considering our initial state to be a linear combination of eigenstates.

$$E(L) = \sum_{n=1}^{\infty} |a_n|^2 E_n$$
$$\sum_{n=1}^{\infty} |a_n|^2 = 1$$

Here  $|a_n|^2$  do not assume constant values as they must change in order to keep the expectation value of the Hamiltonian constant.

### 5.3 Quantum Carnot's Cycle

This is also known as the *two-state quantum heat engine* as it assumes two energy states during the cycle. Let us begin the process by considering a potential well whose length of wall is  $L_1$ . The expectation value of the Hamiltonian and force respectively are,

$$E_H = \frac{\pi^2 \hbar^2}{2mL_1^2}$$

$$F = \frac{\pi^2 \hbar^2}{mL_1^3}$$

**Step I:** Isothermal expansion

We know that the system will transition to the first excited state during this process. Thus we represent the state of the system as a linear combination of two eigenvalues.

$$\psi(x) = a_1(L) \frac{\sqrt{2}}{\sqrt{L}} \sin\left(\frac{2\pi}{L}x\right) + a_2(L) \frac{\sqrt{2}}{\sqrt{L}} \sin\left(\frac{\pi}{L}x\right)$$

$$(|a_1|^2 + |a_2|^2 = 1)$$

Calculating the expectation value of the Hamiltonian and equating it to  $E_H$  we get,

$$\langle H \rangle = \frac{\pi^2 \hbar^2}{2mL_2^2} (4 - 3|a_1|^2) = \frac{\pi^2 \hbar^2}{2mL_1^2}$$

$$L_2^2 = (4 - 3|a_1|^2) L_1^2$$

$$(L_2)_{max} = 2L_1$$

Now let us calculate the force and verify if it follows the classical relation of pressure and volume.

$$F_1(L) = |a_1|^2 \frac{\pi^2 \hbar^2}{mL_1^3} + (1 - |a_1|^2) \frac{4\pi^2 \hbar^2}{mL_1^3}$$

$$= \frac{\pi^2 \hbar^2}{mL_1^2 L_2}$$

$$LF_1(L) = C$$

where  $C$  is a constant.

**Step II:** Adiabatic expansion

In this process the expectation value of the Hamiltonian remains the same while it expands to  $L_3$ . The values of expectation value of the Hamiltonian and the force respectively is,

$$E_H = \frac{2\pi^2\hbar^2}{mL^2}$$
$$F_2(L) = \frac{4\pi^2\hbar^2}{mL^3}$$

From the expression of force we clearly see that,

$$L^3 F(L) = C$$

where  $C$  is a constant.

**Step III:** Isothermal compression

During this process the expectation value of the Hamiltonian remains the same while the length decreases to  $L_4$ . Using the same logic from step I, we can say that  $L_4 = \frac{1}{2}L_3$ . The values of expectation value of the Hamiltonian and the force respectively is,

$$E_H = \frac{2\pi^2\hbar^2}{mL_3^2}$$
$$F_3(L) = \frac{4\pi^2\hbar^2}{mL_3^2 L}$$

From the expression of force we clearly see that,

$$L F(L) = C$$

where  $C$  is a constant.

**Step IV:** Adiabatic compression

In this process the expectation value of the Hamiltonian remains the same while it returns to the original length  $L_1$ . The values of expectation value

of the Hamiltonian and the force respectively is,

$$E_H = \frac{\pi^2 \hbar^2}{2mL^2}$$

$$F_4(L) = \frac{\pi^2 \hbar^2}{mL^3}$$

From the expression of force we clearly see that,

$$L^3 F(L) = C$$

where  $C$  is a constant.

## 5.4 Efficiency

Efficiency of a system is given by,

$$\eta = \frac{W}{Q_H}$$

$$= \frac{W}{W + Q_C}$$

$$= 1 - \frac{T_C}{T_H}$$

where  $W$  is the work done,  $Q_H$  is the high-temperature reservoir and  $Q_C$  is the low-temperature reservoir.

Let us calculate the work done in the quantum mechanical system.

$$W = \int_{L_1}^{2L_1} F_1(L) dL + \int_{2L_1}^{L_3} F_2(L) dL + \int_{L_3}^{\frac{L_3}{2}} F_3(L) dL + \int_{\frac{L_3}{2}}^{L_1} F_4(L) dL$$

$$= \frac{\pi^2 \hbar^2}{m} \left( \frac{1}{L_1^2} - \frac{4}{L_3^2} \right) \ln(2)$$

Let us calculate the  $Q_H$  in the quantum mechanical system.

$$Q_H = \int_{L_1}^{2L_1} F_1(L) dL$$

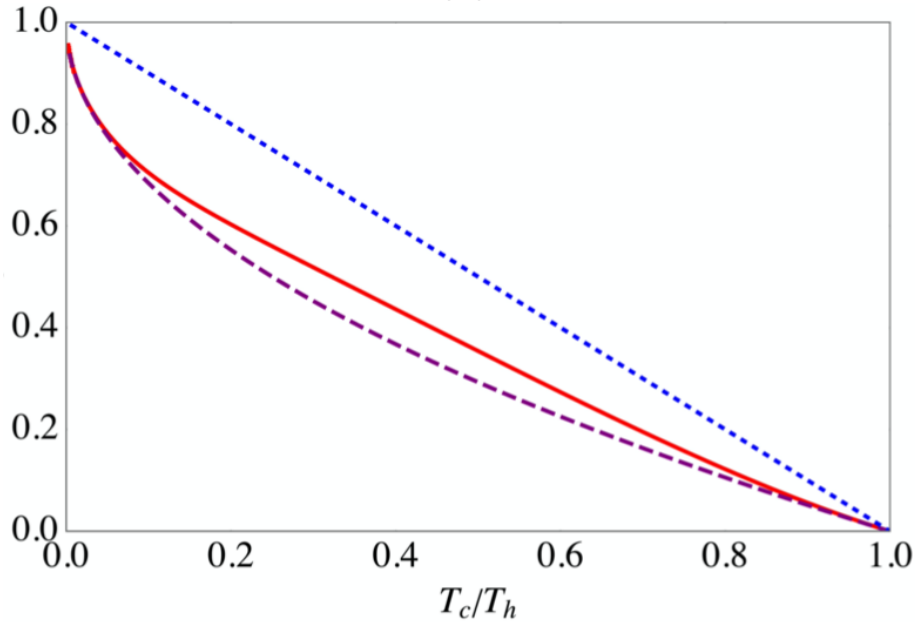
$$= \frac{\pi^2 \hbar^2}{mL_1^2} \ln(2)$$

Therefore efficiency of the system is given by,

$$\begin{aligned}\eta &= \frac{W}{Q_H} \\ &= 1 - 4 \frac{L_1^2}{L_3^2} \\ &= 1 - \frac{E_C}{E_H}\end{aligned}$$

As we've said that we'd be considering the expectation value of the Hamiltonian in the place of temperature which is nothing but the energy, we see that the  $\eta_{\text{classical carnot engine}} = \eta_{\text{quantum carnot engine}}$ .

## 6 Further topics



### 1. Other quantum cycles

We can also look into the Otto cycle, Brownian engine, etc. Although they are all less efficient than the Carnot's engine. This an efficiency

vs  $\frac{T_c}{T_h}$  graph. Here the dotted blue line represents the efficiency of the Carnot's cycle, red line represents the endoreversible Otto cycle and the dotted purple line represents Curzon-Ahlborn cycle

## 2. Work extraction from arrays of quantum batteries

Examples of these include Qubit quantum batteries, Qutrit quantum batteries, etc. It is shown that *"the work extracted is  $n$  times the work that could have been extracted from a single battery if and only if the final state is the tensor product of single- battery states"*. We can further explore the powerful charging of such batteries.

## References

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