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Magnetic Otto Cycle for Quantum dot and Antidot Systems

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“Canto que ha sido valiente, siempre será canción nueva”

Victor Jara (1932-1973)

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Chapter 1

Introduction and Preliminary Concepts

Thermodynamics has been a cornerstone of physics, providing critical insights into the principles governing heat and work in physical systems. The foundational works of Carnot, Clausius, Kelvin, and Joule laid the groundwork for classical thermodynamics, which studies macroscopic systems in equilibrium [1]. Heat engines, in particular, have played a pivotal role in developing thermodynamic principles. By converting thermal energy into mechanical work, heat engines advanced scientific understanding. They spurred the Industrial Revolution, transforming society with innovations such as the steam engine and internal combustion engine [2].

In recent years, the field has expanded to include quantum heat engines[3], devices such as quantum engines and refrigerators that operate on working mediums composed of quantum systems. This field has proved to be a fruitful research area in the last decade [4–8]. These efforts have been focused principally on the study of the different thermodynamic cycles, such as the Otto and the Stirling cycles, in different regimes [9–13] and on the use of different quantum working substances such as spins [14–18], quantum dots [19, 20], and quantum harmonic oscillators [21–25]. Recent work has also examined the role that quantum properties, such as quantum coherence and quantum correlations, play in the performance of quantum thermal machines [26–31]. Endoreversible thermodynamics, where systems maintain local equilibrium while operating in finite time, bridges the gap between idealized theoretical models and practical, real-world applications. This approach allows engine performance optimization,

offering new perspectives on efficiency and performance limits [32]. A primary feature of interest of quantum thermal machines is their potential to surpass the performance of their classical counterparts [33, 34], which open the door to a new generation of highly efficient quantum engines and refrigerators for application in emerging quantum technologies.

The thesis is structured as follows: Chapter 1 introduces fundamental concepts of thermodynamics and the conventions used throughout the work. Chapter 2 presents the theoretical framework of thermal machines and endoreversible thermodynamics, including key results and the motivation for the research developed in Chapter 3 (already published in [35]) and Chapter 4. These chapters detail the results of two proposed quantum engines, along with an analysis of their thermodynamic behavior. Finally, Chapter 5 summarizes the main conclusions and outlines potential directions for future research.

1.1 Thermodynamic Concepts

Thermodynamics is the branch of physics that studies energy exchanges and the macroscopic properties of physical systems in equilibrium. In this context, the laws of thermodynamics are the basis for explaining the properties of a system, which generates classical thermodynamics. On the other hand, statistical mechanics is the theory that connects the macroscopic properties of systems with their microscopic behavior. It uses probabilistic concepts to explain how individual atoms and molecules contribute to the overall behavior of macroscopic systems, providing a deep understanding of thermodynamics from a molecular perspective. When the quantum effects are significant, classical thermodynamics and statistical mechanics extend to a new theory called quantum thermodynamics. It focuses on how the laws of thermodynamics apply to nanoscale-level systems and in situations where quantum coherence and entanglement play crucial roles.

The evolution of thermodynamics began with studies on heat and work. In 1824, Sadi Carnot introduced the concept of the Carnot cycle, highlighting the efficiency of heat engines and laying the groundwork for the second law of thermodynamics [1]. James Prescott Joule, through his experiments in the 1840s, demonstrated the equivalence between mechanical work and heat, consolidating the principle of energy conservation [1]. In 1850, Rudolf Clausius

formalized the second law of thermodynamics, introducing the concept of entropy to explain the irreversibility of natural processes [2].

Statistical mechanics emerged in the 19th century with the pioneering works of Ludwig Boltzmann and James Clerk Maxwell. Boltzmann developed his famous transport equation and the H-theorem, which relate entropy to the probability of microscopic states of a system [36]. Maxwell introduced the distribution of molecular speeds in gases, providing a probabilistic basis for understanding the macroscopic properties of gases from their molecular behaviors [36]. In the early 20th century, Josiah Willard Gibbs formalized the theory of ensembles, allowing calculating thermodynamic properties from the mechanics of molecules [36].

Quantum thermodynamics emerged with the advent of quantum mechanics in the early 20th century. In 1900, Max Planck introduced the concept of quanta to explain black-body radiation, a discovery that marked the beginning of quantum physics [36]. Integrating quantum mechanics with statistics led to the development of Bose-Einstein and Fermi-Dirac statistics, fundamental for understanding the behavior of indistinguishable particles at low temperatures [36]. More recently, in the 1990s, the concept of thermalization in isolated quantum systems, known as the eigenstate thermalization hypothesis, was developed to address how subsystems of quantum systems reach thermal equilibrium [36].

1.1.1 Work and Heat

In classical mechanics, the concept of mechanical work is well-known. When moving an object by applying a force, the amount of work generated is of the form

$$dW = \vec{F} \cdot d\vec{r}. \quad (1.1)$$

If we consider a system as a whole and it exerts work on the surroundings (or the opposite situation), the work generated is known as external work. We could also suppose that the system can be composed of subsystems, which exert work on each other; therefore, we will call it internal work. External work is the only one discussed in thermodynamics since we can define it in terms of its macroscopic variables such as pressure and volume [37]. Suppose we have a gas inside a container and exert pressure using a piston to compress the gas.

The force applied can be written in terms of the pressure exerted and the area of the piston:

$$F = P_{\text{ext}} A \quad (1.2)$$

On the other hand, the volume of the gas can be written in terms of the displacement:

$$dV = A dx \quad (1.3)$$

Thus, the work generated is

$$dW = -P_{\text{ext}} dV \quad (1.4)$$

The choice of the negative sign is to clarify that the volume decreased, so it is a matter of convention. Following the above, we define work using the following convention:

- If the environment performs work on the system, the work for gas compression is positive: $\Delta V < 0 \Rightarrow W_{\text{comp}} > 0$
- If the system performs work on the environment, the work for the expansion of the gas is negative: $\Delta V > 0 \Rightarrow W_{\text{exp}} < 0$

If the external pressure is not constant, the work is not conservative, i.e., it depends on the chosen trajectory. We label this using the δ symbol which represents an inexact differential [1, 37, 38]:

$$\delta W = -P_{\text{ext}} dV \quad (1.5)$$

When work is performed on a system, it often increases the temperature, so another form of energy that is essential in thermodynamics is heat. We define heat as [1, 37, 38]

$$\delta Q = C dT \quad (1.6)$$

Here, C is known as the *heat capacity* of the system and T the temperature. Heat can flow from a system to its surroundings or the other way around, so again, we will use the next convention for the sign:

- If heat is entering the system, the heat transferred is positive because the temperature increases: $\Delta T > 0 \Rightarrow Q_{\text{in}} > 0$

- If heat is leaving the system, the heat transferred is negative because the temperature decreases: $\Delta T < 0 \Rightarrow Q_{\text{out}} < 0$

1.2 Laws of Thermodynamics

1.2.1 Zeroth Law

To start, let us consider a system which we want to describe using two independent coordinates X, Y . The *equilibrium* state will be defined as the one where X and Y have definite values and remain constant as long as the external conditions are not modified. Now, let us have two systems, each defined with its coordinates, separated by a wall that allows us to reach an equilibrium state between them. If the wall is *adiabatic*, the state Y, X of system A can coexist in equilibrium with the state Y', X' of system B for any possible value of each coordinate, as long as the wall resists the stresses caused by the difference between the two sets of coordinates. If the wall were *diathermic*, the values of both sets would change spontaneously until an equilibrium state of the whole set is reached. In the latter case, we have that both systems will be in *thermal equilibrium* with each other. Therefore, thermal equilibrium is the state reached by two (or more) systems, characterized by particular values of the coordinates of the system after they have been in communication with each other through a diathermal wall [1, 37, 39].

Now, suppose we have a third system, C , which is separated by a diathermic wall with A and B . In contrast, they are separated by a diathermic wall with A and B , while an adiabatic wall separates them, the whole assembly being separated from the surroundings by an adiabatic wall. Eventually, A and B will reach thermal equilibrium with C . If we separate the adiabatic wall between them by a diathermic one, we can see that nothing will happen since, by transitivity, these will also be in thermal equilibrium.

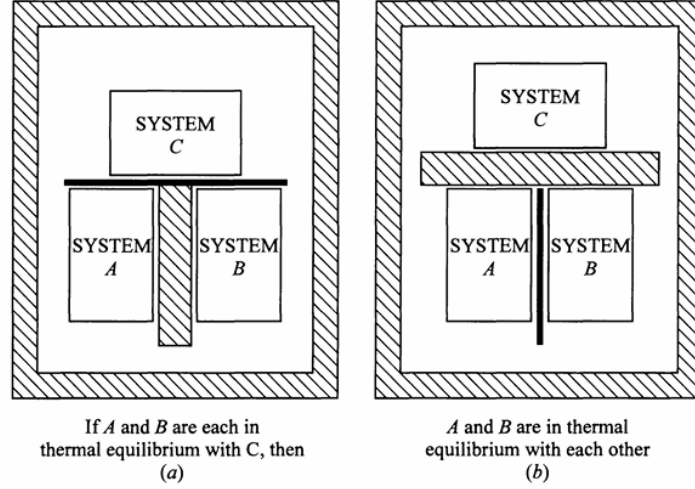


Figure 1.2.1: The Zeroth law of thermodynamics, where adiabatic walls are designated by diagonal shading, while diathermic walls by heavy lines [37].

With this, we enunciate what is known as the *zeroth law of thermodynamics*, according to R. H. Fowler: Two systems in thermal equilibrium with a third are in thermal equilibrium with each other [1, 37, 39].

1.2.2 First Law

Recall again from mechanics that when an object is moved from one point to another in a gravitational field, without friction, the work depends only on the initial and final positions but not on the trajectory traveled. On this basis, it was deduced that a function exists for the spatial coordinates of the body whose final value minus the initial value is equal to the work done. This function was called gravitational potential energy. Similarly, the electric potential energy appears when a charged object moves within an electric field. In thermodynamics, if a system moves from an initial to a final state, using only adiabatic transformations, the function of the coordinates that depends only on the end points and not on the trajectory will be equal to the adiabatic work [1, 37, 38]. This function is called *internal energy* and has the following form:

$$W_{i \rightarrow f} \text{ (adiabatic)} = U_f - U_i = \Delta U \quad (1.7)$$

When the change of state of the system is not done adiabatically, the work is not equal to the change in internal energy. This occurs because there is an exchange of heat between the system and the environment (which are at a

different temperature), so now the conservation of energy has the following form:

$$U_f - U_i = Q + W \quad (1.8)$$

This law of conservation of energy is known as the *first law of thermodynamics*. If we consider the change of internal energy for infinitesimal transformations, the first law becomes

$$dU = \delta W + \delta Q \quad (1.9)$$

Note that in a thermodynamic process leading a system from one equilibrium state to another, U depends only on the initial and final states (it is a state variable), while W and Q depend on the trajectory leading from an initial to a final state [1, 37, 38].

1.2.3 Second Law

From the first law, we find a principle of energy conservation involving open systems. However, that a process fulfills the first law does not necessarily mean it must occur. A clear example is when we leave a cup with a hot liquid in a room at a lower temperature. We know that the liquid will eventually cool down, and by conserving energy, the energy the liquid loses is gained by the surroundings. Now consider the reverse process, i.e., leaving the cup in the room and making it even hotter by transferring energy from the air. Even though this still obeys the first law, if the energy lost by the air is equal to that gained by the liquid, we know this can't occur naturally. There are many more examples, but the common denominator is that the process occurs in a particular direction, not vice versa. The first law does not refer to the direction of the process, only to the conservation of the energy of the process. This inability in the first law can be fixed with another general principle, known as the *second law of thermodynamics* [1, 37, 38].

The second law allows for the setting of theoretical limits in operating systems such as thermal and refrigerating machines and the prediction of the degree of completion of chemical reactions. From the first law we have that it holds for both reversible and irreversible processes:

$$dU = \delta W_{\text{rev}} + \delta Q_{\text{rev}} = \delta W_{\text{irr}} + \delta Q_{\text{irr}} \quad (1.10)$$

From here we can see that if there is a conservation in the variation of internal energy, then the work done in a reversible process is not equal to that of the irreversible one, the same happens for the heat transferred. For example, for an ideal gas, in isothermal expansion we have that the absolute value of the work done is greater in the reversible process compared to the irreversible one, while for compression the *work required* is less in the reversible one.

In general, then, it is generally

$$\delta W_{\text{rev}} < \delta W_{\text{irr}} \quad (1.11)$$

while the absolute value of the waste heat is always higher in a reversible process than in an irreversible process

$$\delta Q_{\text{irr}} < \delta Q_{\text{rev}} \quad (1.12)$$

Thus, the equality of equation (1.10) is maintained. This means that for a reversible process, less work is needed, while for an irreversible, one part of that “extra” work is converted into heat, which is radiated out of the system (with a negative sign).

From the reversible cycle processes, it can be obtained that the inexact differential of the transferred heat is possible to convert it to another exact differential, adding an integrating factor such that

$$dS = \frac{\delta Q_{\text{rev}}}{T} \quad (1.13)$$

this new quantity S is known as the entropy of the system, and by being able to express it using an exact differential, we are indicating that this extensive quantity only depends on the initial and final states in a reversible process. The entropy change between an initial and final state is:

$$S_f - S_i = \int_i^f \frac{\delta Q_{\text{rev}}}{T} \quad (1.14)$$

we can notice that if the change starts and ends in the same state, then

$$\oint \frac{\delta Q_{\text{rev}}}{T} = 0 \quad (1.15)$$

The above equation is known as the *Clausius theorem*. In general, for a cyclic transformation with a defined temperature, it is satisfied that

$$\oint \frac{\delta Q}{T} \leq 0 \quad (1.16)$$

where the integral extends throughout this transformation. The entropy change in a process that is not necessarily reversible generates that

$$\int_i^f \frac{\delta Q}{T} \leq S_f - S_i \quad (1.17)$$

Therefore, a reversible path between the initial and final state will be the one that minimizes the entropy change, while for a closed system subjected to an irreversible process, the infinitesimal change of entropy satisfies that

$$dS > \frac{\delta Q}{T_{\text{surroundings}}} \quad (1.18)$$

obtaining the statement of the second law of thermodynamics: The entropy of a thermally isolated system never decreases.

All isolated systems tend spontaneously to thermodynamic equilibrium, given by the state that maximizes their entropy. Thus, we have that spontaneous processes are irreversible, with increased entropy, since there is no way to naturally gain energy by transferring heat from a colder system to a hotter one, thus defining the direction in which processes occur [38].

Chapter 2

Thermal Machines

A thermal machine is a device that operates through a series of processes in a cyclic manner to convert heat into mechanical work. This set of processes is known as a thermodynamic cycle and operates within a temperature range. The substance to and from which heat is transferred is called the working fluid or substance. From the previous chapter, we know that these cyclic processes must occur in such a direction that they comply with the laws of thermodynamics, which is why thermal machines are defined as devices that perform a certain amount of net positive work through the transfer of heat from a higher body to a lower body temperature. Usually, the term thermal engine is also used to include other types of device that produce work, either by heat transfer or combustion, even though they do not operate in a thermodynamic cycle. The internal combustion engine and gas turbines are examples of such devices; calling them thermal machines is acceptable.

In this sense, a steam power plant is a case of a thermal machine that uses water (steam) as a working substance, as we can see in 2.0.1. A certain amount of heat, Q_h , is transferred from a higher temperature reservoir, which may be the product of combustion in a furnace, a reactor, or another fluid heated in a reactor. In addition, a quantity of heat Q_l is expelled to a lower temperature reservoir, usually the cooled water in a condenser. However, what is important here is that a net work is produced during the cycle. Generally, the notation for Q_h refers to the heat added from the hot reservoir to the system, while Q_l is the heat lost transferred from the system to the cold reservoir. The above implies that since the internal energy change in a cycle is zero, then the net work done by the machine is equal to the difference between the heat in and

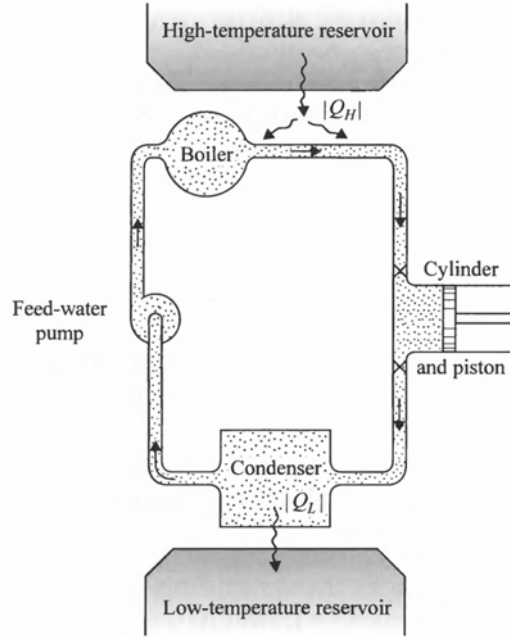


Figure 2.0.1: Schematic diagram of a simple steam engine [37].

the heat out:

$$W_{\text{net}} = Q_h - Q_l \quad (2.1)$$

The fraction of the input energy (Q_h) that is converted into work (W_{net}) is known as the thermal efficiency or thermal performance:

$$\eta = \frac{W_{\text{net}}}{Q_h} = \frac{Q_h - Q_l}{Q_h} = 1 - \frac{|Q_l|}{Q_h} \quad (2.2)$$

Adding an absolute value to the heat released is considered negative because it is the heat lost by the system. By working only with positive quantities, the efficiency is well-defined. However, in the literature, there are different expressions for this depending on the convention to be used.

2.1 Quasi-static Cycles

2.1.1 Ideal Gas Carnot Engine

During one part of the cycle performed by a working substance in an engine, part of the heat is absorbed by the hot reservoir, and then, in the other part of the cycle, an amount is dissipated by the cold reservoir. The engine then

operates between these two reservoirs. As there is heat dissipated to the cold reservoir, the second law tells us that there is no 100% efficiency of this machine, so it is important to know what the maximum efficiency that can be obtained for an engine working between the two reservoirs and with that, how such an engine would be. Nicolas Léonard Sadi Carnot asked himself these questions, and in 1824 he answered them in his work called "Réflexions sur la Puissance Motrice du Feu," designing an ideal engine that works using the well-known Carnot Cycle.

A Carnot cycle is a set of processes that can be performed in any thermodynamic system, be it hydrostatic, chemical, electrical, magnetic, etc. The working system or substance is first thought to be in thermal equilibrium, with the reservoir at a high temperature T_h . An engine operating with a cycle is known as the Carnot engine. As the four stages of the cycle are reversible, then the Carnot engine is reversible. A representation of the Carnot cycle using a $P - V$ is as follows:

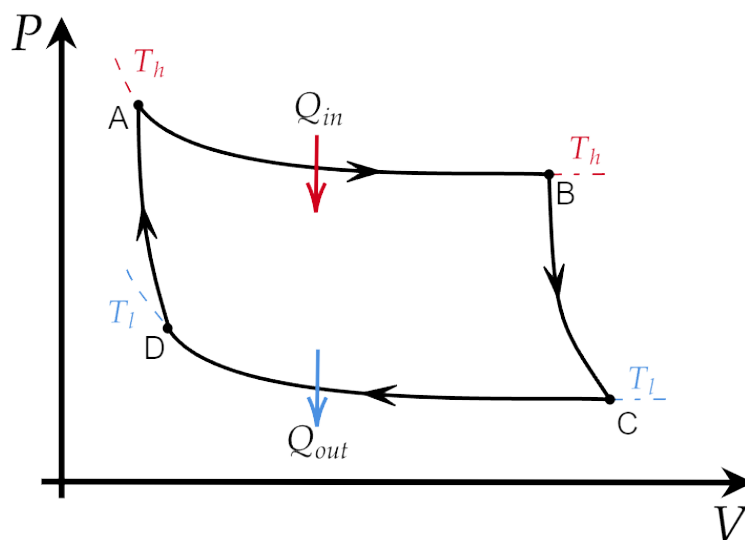


Figure 2.1.1: Pressure and volume diagram for the Carnot cycle.

Considering a working substance as an ideal gas, we can analyze the stages of this graph:

- Step $A \rightarrow B$: Isothermal expansion at temperature T_h . Since $T_A = T_B =$

T_h , then from the equation of state, we have that:

$$PV = Nk_B T \longrightarrow PV = cte \longrightarrow P_A V_A = P_B V_B \quad (2.3)$$

In addition, the internal energy depends on the temperature, but since the process is isothermal, then

$$U = \frac{3}{2} Nk_B T_h \longrightarrow U_{AB} = 0 \quad (2.4)$$

Then, from the first law of thermodynamics

$$Q_{AB} = -W_{AB} = \int_{V_A}^{V_B} \frac{Nk_B T_h}{V} dV = Nk_B T_h \ln \left(\frac{V_B}{V_A} \right) \quad (2.5)$$

Furthermore, Q_{AB} is the incoming, i.e., $Q_{AB} = Q_h$, and since $V_B > V_A$, then $Q_{AB} > 0$.

- Step B $\rightarrow$ C: Adiabatic expansion from V_B to V_C . In this case, we have a temperature change from T_h to T_l . From the equation of state, we have that

$$TV^{\gamma-1} = cte \longrightarrow T_h V_B^{\gamma-1} = T_l V_C^{\gamma-1} \longrightarrow \frac{V_C}{V_B} = \left(\frac{T_h}{T_l} \right)^{\frac{3}{2}} \quad (2.6)$$

Moreover, being an adiabatic process we know that $Q_{BC} = 0$ and from the first law of thermodynamics:

$$W_{BC} = U_{BC} = c_V (T_l - T_h) \quad (2.7)$$

- Step C $\rightarrow$ D: Isothermal compression at temperature T_l . Since $T_C = T_D = T_l$, then from the equation of state, we have that:

$$PV = Nk_B T \longrightarrow PV = cte \longrightarrow P_C V_C = P_D V_D \quad (2.8)$$

In addition, internal energy depends on the temperature, thus

$$U = \frac{3}{2} Nk_B T_l \longrightarrow U_{CD} = 0 \quad (2.9)$$

Therefore, from the first law

$$Q_{CD} = -W_{CD} = \int_{V_C}^{V_D} \frac{Nk_B T_l}{V} dV = Nk_B T_l \ln \left(\frac{V_D}{V_C} \right) \quad (2.10)$$

Futhermore, Q_{CD} is the heat released, i.e., $Q_{CD} = Q_l$, and since $V_C > V_D$, then $Q_{CD} < 0$. The absolute value of this remains

$$|Q_{CD}| = Nk_B T_l \ln \left(\frac{V_C}{V_D} \right) \quad (2.11)$$

- Step D $\rightarrow$ A: Adiabatic compression from V_D to V_A . Know the temperature goes from T_l to T_h . From the equation of state:

$$TV^{\gamma-1} = cte \longrightarrow T_l V_D^{\gamma-1} = T_h V_A^{\gamma-1} \longrightarrow \frac{V_D}{V_A} = \left(\frac{T_h}{T_l} \right)^{\frac{3}{2}} \quad (2.12)$$

In addition, being an adiabatic process we know that $Q_{DA} = 0$ and from the first law:

$$W_{DA} = U_{DA} = c_V(T_h - T_l) \quad (2.13)$$

Note that if we add up all the variations of internal energy, we have

$$\begin{aligned} U_{\text{Total}} &= U_{AB} + U_{BC} + U_{CD} + U_{DA} \\ &= 0 + c_V(T_l - T_h) + 0 + c_V(T_h - T_l) = 0 \end{aligned}$$

Then since $U_{\text{Total}} = 0$, we have that it is indeed a thermodynamic cycle. Furthermore, since

$$\frac{V_C}{V_B} = \left(\frac{T_h}{T_l} \right)^{\frac{3}{2}}, \quad \frac{V_D}{V_A} = \left(\frac{T_h}{T_l} \right)^{\frac{3}{2}}$$

Then

$$\frac{V_C}{V_B} = \frac{V_D}{V_A} \longrightarrow \frac{V_D}{V_C} = \frac{V_A}{V_B} \quad (2.14)$$

Relating the heats exchanged in steps 1 and 3:

$$\frac{Q_h}{T_h} + \frac{Q_l}{T_l} = 0 \quad (2.15)$$

And this equation is valid for any *reversible process*. Calculating the quotient

between the heat input and the heat released:

$$\frac{|Q_l|}{Q_h} = \frac{NK_B T_l \ln(V_C/V_D)}{NK_B T_h \ln(V_B/V_A)} = \frac{T_l}{T_h} \quad (2.16)$$

With the above, we obtain the efficiency:

$$\eta = 1 - \frac{|Q_l|}{Q_h} = 1 - \frac{T_l}{T_h} \quad (2.17)$$

2.1.1.1 Carnot theorem

The following theorem is generated thanks to the Carnot engine: No engine operating between two given reservoirs is more efficient than a Carnot machine between those same reservoirs.

To prove this, let us consider two engines: The Carnot engine, which we will call R , which is reversible, and another engine, I , which is irreversible. Both engines operate between the same reservoirs and are adjusted to generate the same amount of work $|W|$. For R :

$$\eta_R = \frac{|W|}{|Q_h|} \quad (2.18)$$

While for I :

$$\eta_I = \frac{|W|}{|Q'_h|} \quad (2.19)$$

Let us assume that the efficiency of the engine I is greater than that of R , then

$$\eta_I > \eta_R \longrightarrow \frac{|W|}{|Q'_h|} > \frac{|W|}{|Q_h|} \longrightarrow |Q_h| > |Q'_h| \quad (2.20)$$

Now let us have motor I drive motor R backward like a Carnot refrigerator. The engine and refrigerator work together as a self-contained machine since the engine manages all the work required to operate the refrigerator.

The net heat extracted from the cold reservoir is

$$(|Q_h| - |W|) - (|Q'_h| - |W|) = |Q_h| - |Q'_h| \quad (2.21)$$

which is positive. The heat dissipated to the cold reservoir is the same as before. Therefore, this self-contained machine transfers $|Q_h| - |Q'_h|$ units of heat from a cold reservoir to a hot reservoir without any work done by the surroundings.

The problem with this is that it violates the second law by Clausius's theorem, so our assumption that $\eta_I > \eta_R$ is false, and thus Carnot's theorem is proved. The above can then be expressed as

$$\eta_I \leq \eta_R \quad (2.22)$$

A result of the above is that if two Carnot engines work on the same reservoirs, they have the same efficiency. This can be demonstrated analogously to what was previously done. It is then concluded that if they have the same efficiency, the working substance to which we apply the Carnot cycle does not influence the efficiency of the cycle.

2.1.2 Ideal Gas Otto Engine

Just as there is the Carnot Cycle, several other cycles can be worked with. The main difference between the Carnot and Otto cycles is that the former operates based on isothermal and adiabatic processes, while the latter on isochoric and isentropic processes. The Otto cycle is an idealized approximation of the gasoline engine. The working fluid (a mixture of air and vapor gasoline) is first adiabatically compressed ($A \rightarrow B$), then heated to constant volume ($B \rightarrow C$). In the real case, the fluid reacts at this stage, burning, and then the number of moles changes; however, in the Otto engine, this is not considered. In the third step the fluid expands adiabatically ($C \rightarrow D$), to finally be cooled isochorically ($D \rightarrow A$) to its initial state A. Moreover, in the gasoline engine, the adiabatic compression is not quasi-static, so it will not be isentropic. However, the Otto cycle provides an idealized perspective for analyzing gasoline engines. With the above, then we have the following S-V representation of the cycle:

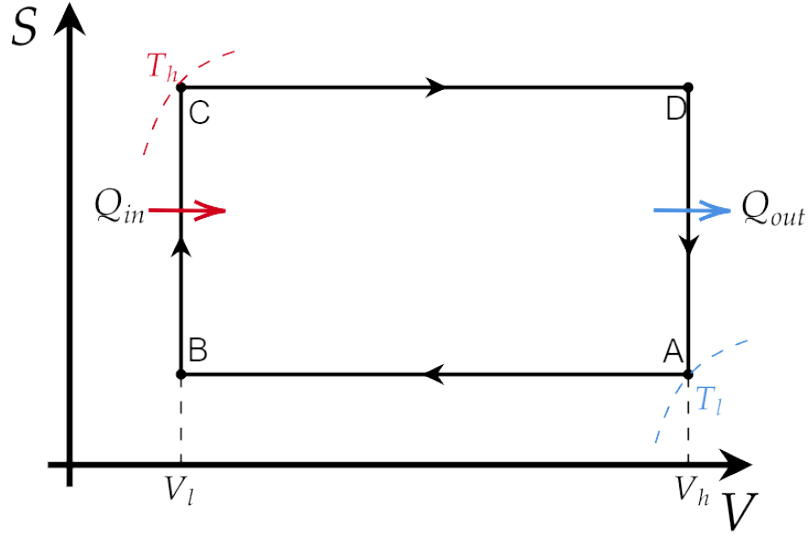


Figure 2.1.2: Entropy and volume diagram for the Otto cycle.

From here we can analyze the following for an ideal gas as with Carnot:

- Step A $\rightarrow$ B: Isentropic compression from V_h a V_l . The temperature goes from T_A to T_B . From the equation of state, we have that

$$TV^{\gamma-1} = cte \longrightarrow T_A V_A^{\gamma-1} = T_B V_B^{\gamma-1} \quad (2.23)$$

Moreover, since the process is adiabatic, then $Q_{AB} = 0$, thus, from the first law:

$$W_{AB} = U_{AB} = c_V(T_B - T_A) \quad (2.24)$$

- Step B $\rightarrow$ C: Isochoric heating at V_l . Since it is an isochoric process, $V_B = V_C = V_l$ and $W_{BC} = 0$. Thus, from the first law, we have that

$$Q_{BC} = U_{BC} = c_V(T_C - T_B) \quad (2.25)$$

Note that since $T_C > T_B$, then $Q_{BC} > 0$ and corresponds to $Q_{in} = Q_h$.

- Step C $\rightarrow$ D: Isentropic expansion from V_C to V_D . The temperature goes from T_C to T_D . From the equation of state, we have that

$$TV^{\gamma-1} = cte \longrightarrow T_C V_C^{\gamma-1} = T_D V_D^{\gamma-1} \quad (2.26)$$

Furthermore, since the process is adiabatic, then $Q_{AB} = 0$, with this:

$$W_{CD} = U_{CD} = c_V(T_D - T_C) \quad (2.27)$$

- Stage D $\rightarrow$ A: Isochoric cooling at V_h . We have $V_A = V_D = V_h$ and $W_{DA} = 0$ for the isochoric process. With this, using the first law:

$$Q_{DA} = U_{DA} = c_V(T_A - T_D) \quad (2.28)$$

Note that since $T_D > T_A$, then $Q_{DA} < 0$ and corresponds to $Q_{\text{out}} = Q_l$. The absolute value of this would then be

$$|Q_l| = c_V(T_D - T_A) \quad (2.29)$$

If we calculate the total variation of internal energy, we have the following:

$$\begin{aligned} U_{\text{Total}} &= U_{AB} + U_{BC} + U_{CD} + U_{DA} \\ &= c_V(T_B - T_A) + c_V(T_C - T_B) + c_V(T_D - T_C) + c_V(T_A - T_D) = 0 \end{aligned}$$

Lets remember that in the isochoric processes $V_A = V_D$ and $V_B = V_C$, then from equations (2.23) and (2.26), the temperatures are related as follows:

$$\frac{T_A}{T_D} = \frac{T_B}{T_C} \quad (2.30)$$

And with that, we can find that the efficiency of the cycle is

$$\eta = 1 - \frac{|Q_l|}{Q_h} = 1 - \frac{c_V(T_D - T_A)}{c_V(T_C - T_B)} = 1 - \frac{T_A}{T_B} = 1 - \left(\frac{V_B}{V_A}\right)^{\gamma-1} \quad (2.31)$$

Defining $\frac{V_A}{V_B} = r$, known as the compression ratio, then:

$$\eta = 1 - \frac{1}{r^{\gamma-1}} \quad (2.32)$$

Here, unlike Carnot, Otto cycle efficiency does depend on the properties on the working medium.

2.2 Endoreversible Cycles

In the previous section, we reviewed quasi-static thermodynamic cycles, characterized by thermal equilibrium at the end of the stages where the working substance is connected to the thermal reservoirs. The clearest example of an ideal system with reversible processes is the Carnot engine, where we find an upper limit to the efficiency of any system. However, this efficiency cannot be achieved in practice because most of the processes we observe are not reversible and are not always in thermodynamic equilibrium, so it is necessary to consider this in a more realistic model.

Let us consider a system consisting of smaller subsystems interacting with each other and the surroundings. Assume that the subsystems carry out reversible internal processes so that any irreversible process occurs through interactions between them or with the environment. We will call this an endoreversible system, defined by the subsystems' properties and interactions. Thus, the processes of these subsystems are called endoreversible processes [40–45].

As a first example of an endoreversible cycle, we will review the Novikov engine [46, 47]. Figure shows the schematic of the Novikov engine and a T-S diagram. The Novikov engine consists of a Carnot engine with a hot and cold reservoir at temperatures T_h and T_l , respectively. The system is in direct contact with the external low-temperature heat bath while it is coupled to an external high-temperature heat bath through a finite heat conductance K . We will consider that the heat baths are infinite, such that the energy flux with the working substance does not change its temperature.

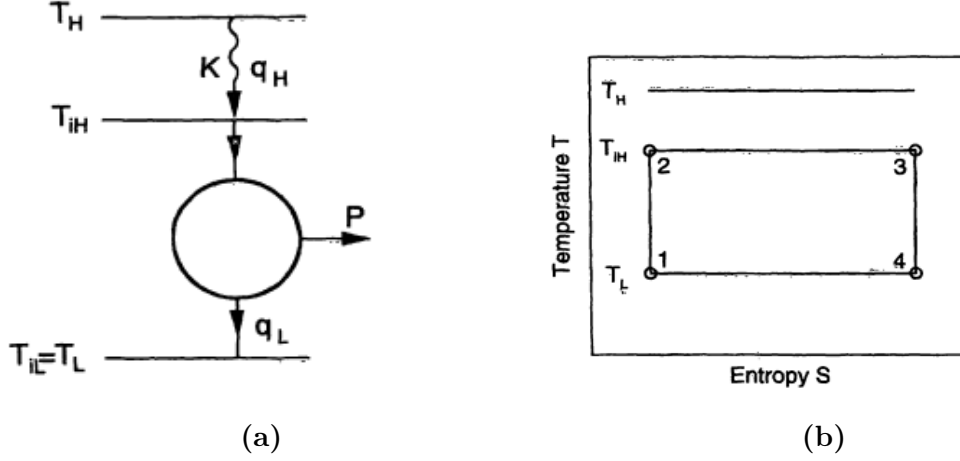


Figure 2.2.1: (a) Novikov engine. The wall connecting the hot reservoir has a thermal conductivity constant K . (b) Temperature and entropy diagram for the Novikov cycle. The hot reservoir is at temperature $T_h > T_{ih}$ [40].

Since the heat conductance K limits the heat flow through the system, the engine's efficiency is also limited. In addition, we will assume that the heat flux transported from the heat bath to the engine follows a simple Fourier or Newtonian heat conduction law (we choose $\tau = 1$ for simplification), i.e., the heat flux is proportional to the temperature difference

$$Q_h = K(T_h - T_{ih}) \quad (2.33)$$

where T_h is the temperature of the hot reservoir and T_{ih} is the temperature that the working substance reaches when connected to that reservoir. Notice that because the system doesn't fully thermalize with the reservoir, then $T_{ih} < T_h$. On the other hand, when the working substance is connected to the cold reservoir, the temperature T_{il} is the same as the bath temperature $T_{il} = T_l$. From Clausius theorem, we have that in the cyclic process:

$$\frac{Q_h}{T_{ih}} = \frac{Q_l}{T_{il}} = 0 \quad (2.34)$$

Then, the net work performed by the engine is

$$W = Q_h - Q_l = Q_h \left(1 - \frac{T_l}{T_{ih}}\right) = K(T_h - T_{ih}) \left(1 - \frac{T_l}{T_{ih}}\right) \quad (2.35)$$

Since Q_h happens during a finite time, then the power delivered by the engine is

$$P = \frac{W}{\tau} = K(T_h - T_{ih}) \left(1 - \frac{T_l}{T_{ih}} \right) \quad (2.36)$$

Where $\tau = 1$ is the total cycle time. For given reservoirs and heat conductance, work, heat, and power output only depend on T_{ih} , then we can find the maximum power differentiating concerning T_{ih} :

$$\frac{dP}{dT_{ih}} = K \left(\frac{T_l T_h}{T_{ih}^2} - 1 \right) = 0 \longrightarrow T_{ih} = \sqrt{T_l T_h} \quad (2.37)$$

Then, the maximum power is

$$P_{\max} = K(\sqrt{T_l} - \sqrt{T_h})^2 \quad (2.38)$$

And with this, the efficiency at maximum power is [40]

$$\eta = 1 - \frac{T_l}{T_{ih}} = 1 - \sqrt{\frac{T_l}{T_h}} \quad (2.39)$$

Although we are assuming conditions that limit the engine's efficiency due to endoreversibility, the efficiency obtained does not depend on the conductivity and temperature of the working substance, only on the reservoirs. With this simple example, we have found an interesting limit for engines at maximum power. We will now study a more general version of the Novikov engine, limiting the flux transferred in both reservoirs for the Carnot cycle.

2.2.1 Finite time Carnot Engine and Curzon-Ahlborn Efficiency

For the endoreversible case, we can assume linear dependence of the heat transferred again using Fourier's law. In the isothermal expansion ($B \rightarrow A$), we will assume that the working substance is slightly cooler than the reservoir at T_h . Then, the heat flowing into the working substance is

$$Q_{AB} = Q_{\text{in}} = \lambda_h \tau_h (T_h - T_{hw}) \quad (2.40)$$

While in the isothermal compression ($C \rightarrow D$), we will have that the working substance is slightly hotter than the cold reservoir at T_l ; thus, the heat leaving

the system is

$$Q_{CD} = Q_l = \lambda_l \tau_l (T_{lw} - T_l) \quad (2.41)$$

where T_{hw} , T_{lw} are the temperatures of the working substance, λ_h , λ_l are the hot and cold heat transfer coefficients and τ_h , τ_l the times of the strokes.

We can also assume that adiabatic processes are reversible concerning the local temperatures of the medium. This implies that we can again use the Clausius theorem to relate the heat transferred and the temperatures of the working system:

$$\frac{Q_h}{T_{hw}} = \frac{Q_l}{T_{lw}} \longrightarrow \frac{\tau_h}{\tau_l} = \frac{\lambda_l T_{hw} (T_{lw} - T_l)}{\lambda_h T_{lw} (T_h - T_{hw})} \quad (2.42)$$

The power output of the engine is

$$P = \frac{W}{\tau_{cyc}} = \frac{Q_h - Q_l}{\gamma(\tau_h + \tau_l)} \quad (2.43)$$

where the denominator refers to the total cycle time and

$$\gamma \equiv \tau_{cyc}/(\tau_h + \tau_l) \rightarrow \tau_{cyc} = \gamma(\tau_h + \tau_l) \quad (2.44)$$

is a multiplicative factor that accounts for the adiabatic strokes for simplification. Following the work from Curzon and Ahlborn [48], we defined $x = T_h - T_{hw}$ and $y = T_{lw} - T_l$, and using equation (2.42), the power output is

$$P = \frac{\lambda_h \lambda_l x y (T_h - T_l - x - y)}{\gamma(\lambda_l T_h y + \lambda_h T_l x + x y (\lambda_h - \lambda_l))} \quad (2.45)$$

Notice that the power is now expressed in terms of the thermal reservoirs and the previously introduced x and y variables. Maximizing the power concerning x , y :

$$\frac{\partial P}{\partial x} = 0 \longrightarrow \lambda_l T_h y (T_h - T_l - x - y) = x(\lambda_l T_h y + \lambda_h T_l x + x y (\lambda_h - \lambda_l)) \quad (2.46)$$

$$\frac{\partial P}{\partial y} = 0 \longrightarrow \lambda_h T_l x (T_h - T_l - x - y) = y(\lambda_l T_h y + \lambda_h T_l x + x y (\lambda_h - \lambda_l)) \quad (2.47)$$

From this, we obtain the values of x and y :

$$x = \frac{T_h(1 - \sqrt{\frac{T_l}{T_h}})}{1 + \sqrt{\frac{\lambda_h}{\lambda_l}}} \quad (2.48)$$

$$y = \frac{T_l(\sqrt{\frac{T_h}{T_l}} - 1)}{1 + \sqrt{\frac{\lambda_h}{\lambda_l}}} \quad (2.49)$$

Now, the efficiency is given by

$$\eta = 1 - \frac{Q_l}{Q_h} = 1 - \frac{T_{lw}}{T_{hw}} = 1 - \frac{T_l + y}{T_h - x} \quad (2.50)$$

Replacing equations (2.48) and (2.49) we obtain the efficiency at maximum power:

$$\eta = 1 - \sqrt{\frac{T_l}{T_h}} \quad (2.51)$$

This is known as the Curzon–Ahlborn efficiency [48], or, due to the identical result obtained in equation (2.39), it is sometimes referred to as the Chambadal–Novikov–Curzon–Ahlborn efficiency. Similarly to the Carnot efficiency, it depends solely on the temperatures of the hot and cold reservoirs, and not on the properties of the working substance or the characteristics of the walls.

2.2.2 Finite Time Otto Engine and Efficiency at Maximum Power

A similar analysis can be done for the Otto cycle, but since the cycle depends on the working substance, we will only make a general analysis. In this part, we will follow the work of Deffner [22] for the general idea of the endoreversible Otto cycle and show some significant results that motivate this thesis.

As discussed previously, the Otto cycle consists of two isentropic strokes and two isochoric strokes. In the isentropic strokes, there is no heat exchange between the working substance and the environment ($Q = 0$), so in isentropic compression, the work produced is

$$W_{AB} = W_{\text{comp}} = U(T_B, \lambda_B) - U(T_A, \lambda_A) \quad (2.52)$$

Where we have that the internal energy depends on the temperature T and a working parameter λ , such as the volume of a gas, the frequency of a harmonic oscillator, or the external magnetic field.

The work parameter remains constant during the isochoric strokes, so no work is produced ($W = 0$). During the isochoric heating, the working substance is connected to the hot reservoir, and heat flows into the system:

$$Q_{BC} = Q_{\text{in}} = U(T_C, \lambda_B) - U(T_B, \lambda_B) \quad (2.53)$$

Since the working substance does not thermalize with the reservoir, we have

$$T(0) = T_B \quad T(\tau_h) = T_C \quad T_B < T_C \leq T_h$$

where τ_h is the duration of the stroke. We can notice that the Otto cycle does not have isothermal strokes, so the heat flux rate is not constant, in contrast to the Carnot cycle. Fourier's law, in this case, is written as

$$\frac{dT}{dt} = -\alpha_h(T(t) - T_h) \quad (2.54)$$

where α_h is a constant depending on the working substance's heat conductivity and heat capacity. Solving this equation, we obtain

$$T_C - T_h = (T_B - T_h) \exp(-\alpha_h \tau_h) \quad (2.55)$$

Analogously, for the isentropic expansion stroke, there is no heat exchanged, but work produced:

$$W_{CD} = W_{\text{exp}} = U(T_D, \lambda_A) - U(T_C, \lambda_B) \quad (2.56)$$

For the isochoric cooling, we have no work, but heat is transferred from the working substance to the cold reservoir:

$$Q_{DA} = Q_{\text{out}} = U(T_A, \lambda_A) - U(T_D, \lambda_A) \quad (2.57)$$

where the temperature during the stroke is

$$T(0) = T_D \quad T(\tau_l) = T_A \quad T_l \leq T_A < T_D$$

Fourier's law, in this case, is

$$\dot{T} = -\alpha_l(T(t) - T_l) \quad (2.58)$$

and solving this, we find:

$$T_A - T_l = (T_D - T_l) \exp(-\alpha_l \tau_l) \quad (2.59)$$

From equations (2.55) and (2.59), we have relations between the four temperatures at points A , B , C and D . During isentropic strokes, the entropy remains constant between the points A and B and between points C and D , so in these strokes, we can find two relations between the temperatures at the four points. This can be found in two different ways:

- By matching the points in the isentropic strokes

$$S(T_A, \lambda_A) = S(T_B, \lambda_B) \quad (2.60)$$

$$S(T_C, \lambda_C) = S(T_D, \lambda_D) \quad (2.61)$$

- By solving the first-order differential equation in the isentropic trajectory, which has the form

$$dS(T, \lambda) = \left(\frac{\partial S}{\partial T} \right)_\lambda dT + \left(\frac{\partial S}{\partial \lambda} \right)_T d\lambda = 0 \quad (2.62)$$

Solving for the temperatures using equations (2.55), (2.59) and (2.61) or (2.62), we find the temperatures at each point. and then we can replace the work and heat, so the thermodynamic quantities are functions of the external parameter λ . The efficiency of the engine is given by

$$\eta = -\frac{W_{\text{comp}} + W_{\text{exp}}}{Q_h} \quad (2.63)$$

while the power output is

$$P = -\frac{W_{\text{comp}} + W_{\text{exp}}}{\tau_{\text{cyc}}} \quad (2.64)$$

where $\tau_{\text{cyc}} \equiv \gamma(\tau_h + \tau_l)$ is the cycle duration. The efficiency at maximum power (EMP) can be obtained by maximizing the power output, and depending on the

working substance, it is expected to be limited by the CA efficiency. However, recently, Deffner showed that applying the endoreversible approach to the case of an Otto cycle with a single classical and quantum harmonic oscillator as the working medium yielded an efficiency at maximum power equal to CA for the classical working medium and an efficiency at maximum power greater than CA for the quantum working medium [8, 22].

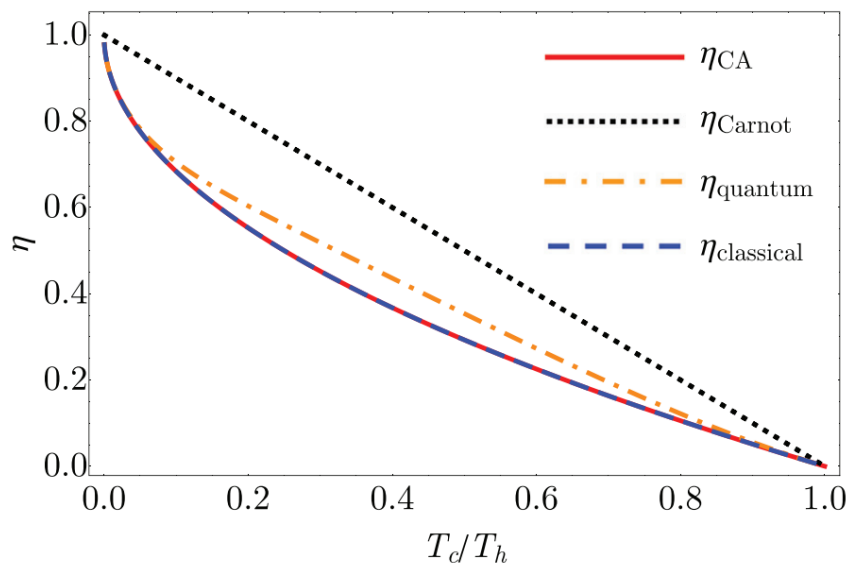


Figure 2.2.2: Comparison of the efficiency at maximum power between a classical harmonic oscillator (blue, dashed) and a quantum harmonic oscillator (yellow, dot-dashed) as a working substance. It includes the Carnot efficiency (black, dashed) and Curzon-Ahlborn efficiency (red, solid) [8, 22].

One of the main conclusions from this work is that, unlike the Carnot efficiency, the Curzon-Ahlborn efficiency is not a general upper bound on the efficiency at maximum power. It is possible to find working substances for which the efficiency at maximum power may exceed the CA efficiency, as is true for continuous engines operating outside the linear regime [49, 50].

Chapter 3

Enhanced Efficiency at Maximum Power in a Fock-Darwin Model Quantum Dot Engine

3.1 Quantum Dots

For a long time, scientific research on electronic systems was limited to studying naturally isolated atoms or particles and metallic and semiconductor crystals. Most of these systems are three-dimensional, except for electrons and atoms localized at crystal defects (e.g., impurities), which can effectively reduce their geometry [51].

The early 1970s marked a new era in studying two-dimensional electronic structures through devices known as quantum wells. A quantum well consists of a very thin, flat semiconductor layer placed between two layers of another semiconductor with a higher conduction band. The difference between the conduction bands traps the electron in the thin layer, allowing it to move in two dimensions, with excitations in the perpendicular direction being strongly quantized. These properties led to significant advancements in electronics, including the discovery of the integer quantum Hall effect, which earned a Nobel Prize in 1985 [52], and the fractional quantum Hall effect [53].

By the early 1980s, it became possible to confine electrons in one-dimensional quantum wires, with dimensions ranging from 10 to 500 nm. Complete quantization of electron motion was achieved by trapping electrons in zero-dimensional cavities known as quantum dots. This was first demonstrated in

1986 [54] with dimensions of 250 nm. Today, dimensions as small as 30-45 nm have been reported.

Some effects seen in two-dimensional electronic systems, such as the formation of composite fermions leading to the fractional quantum Hall effect, also occur in quantum dots, where solving the Schrödinger equation numerically can significantly aid understanding. Generally, the study of quantum dots has numerous applications in physics, including light emission and absorption in the visible or infrared spectrum, Raman scattering, optics, thermal machines, and more.

3.2 Model

The Fock-Darwin (FD) model describes our working substance. The FD Hamiltonian corresponds to a cylindrical quantum dot subject to an external magnetic field perpendicular to the plane in which the dot is present [55, 56],

$$\mathcal{H} = \frac{1}{2m^*} \left[\left(p_x - \frac{eyB}{2} \right) + \left(p_y + \frac{exB}{2} \right) \right] + \frac{1}{2}m^*\omega_0^2(x^2 + y^2), \quad (3.1)$$

where e is the electron charge, m^* is the effective mass of the electron (characteristic of each material), ω is an effective parameter for the strength of the harmonic trap, and B is the intensity of the magnetic field in the z direction. The problem has cylindrical symmetry and eigenenergies,

$$E_{nm}^{dot} = \hbar\Omega(2n + |m| + 1) + \frac{1}{2}\hbar\omega_c m, \quad (3.2)$$

where $\omega_c = eB/m^*$ is the cyclotron frequency, n and m are the radial and magnetic quantum numbers ($n = 0, 1, 2, \dots$ and $m = -\infty, \dots, +\infty$), respectively, and Ω is the effective frequency of the system,

$$\Omega = \omega_0 \left(1 + \left(\frac{\omega_c}{2\omega_0} \right)^2 \right)^{\frac{1}{2}}. \quad (3.3)$$

Notice that when the parameter $\omega_0 \rightarrow 0$, the energy levels of Equation (3.2) take the usual form of the Landau energy levels in cylindrical coordinates. For

high magnetic fields, $(\omega_c/2\omega_0 \gg 1)$, Equation (3.2) simplifies to,

$$E_{n,m} = \frac{\hbar\omega_c}{2}(n + 1/2 + |m| + m), \quad (3.4)$$

as $|m| + m = 0$ for $m < 0$. Each Landau level, labeled by n , is infinitely degenerate in this limit.

In this paper, we considered a low-frequency coupling for the parabolic trap given by $\omega_0 \sim 2.637$ THz, which in terms of energy units corresponds to a coupling of approximately 1.7 meV. This value is comparable to the typical energy of intraband optical transitions of quantum dots [57]. The order of this transition is approximately ~ 1 meV for cylindrical GaAs quantum dots with effective mass $m^* \sim 0.067m_e$ [57–59]. The quantum dot length can be calculated using $l_{dot} = \sqrt{\hbar/m^*\omega_0} \sim 25$ nm for the above values. The effective mass gives a cyclotron frequency of $\omega_c(B = 1) \sim 2.62$ THz for an intensity of $B = 1$ T. It is important to mention that we neglected the Zeeman splitting and the spin-orbit interaction, which is very small for GaAs systems [57, 58]. The partition function for our working substance can be written as [60],

$$\mathcal{Z}_d = \frac{\omega_+ \omega_-}{4\omega_0^2} \operatorname{csch}\left(\frac{\hbar\beta\omega_+}{2}\right) \operatorname{csch}\left(\frac{\hbar\beta\omega_-}{2}\right), \quad (3.5)$$

where $\beta = 1/k_B T$ is the inverse temperature and the frequencies $\omega_{\pm}$ are given by,

$$\omega_{\pm}^2 = \frac{1}{2} \left(\omega_c^2 + 2\omega_0^2 \pm \omega_c \sqrt{\omega_c^2 + \omega_0^2} \right). \quad (3.6)$$

Note that if $\omega_0 \rightarrow 0$, then $\omega_- \rightarrow 0$ and $\omega_+ \rightarrow \omega_c$, recovering the typical partition function for the Landau problem.

The entropy, $S(T, B)$, and internal energy, $U(T, B)$, are derived from the partition function using,

$$S(T, B) = k_B \ln \mathcal{Z}_d + k_B T \left(\frac{\partial \ln \mathcal{Z}_d}{\partial T} \right)_B, \quad (3.7)$$

and,

$$U(T, B) = k_B T^2 \left(\frac{\partial \ln \mathcal{Z}_d}{\partial T} \right)_B. \quad (3.8)$$

In particular, the internal energy is expressed entirely in terms of β , ω_+ , and

ω_- ,

$$U(T, B) = \frac{1}{2} \left[\hbar \omega_+ \coth \left(\frac{\hbar \beta \omega_+}{2} \right) + \hbar \omega_- \coth \left(\frac{\hbar \beta \omega_-}{2} \right) \right]. \quad (3.9)$$

Note that this expression is simply the sum of the internal energies of two oscillators, one with frequency ω_+ and the other with frequency ω_- . Conversely, the entropy cannot be decomposed in this manner due to the prefactor present in the partition function in Equation (3.5). This prefactor accounts for the degeneracy of the energy levels and depends on the external magnetic field. Only in the absence of this term can the entropy be expressed as the sum of the entropies of two independent oscillators with frequencies ω_+ and ω_- .

While these thermodynamic quantities are widely discussed in the literature, we pay special attention to the conditions under which the entropy remains constant, as this will prove an essential aspect of our analysis of the cycle performance. With this in mind, we seek a relationship between the temperature and the external magnetic field that holds the entropy constant. In Figure 3.2.1, we plotted the isentropic trajectories as a function of the temperature and magnetic field. From this plot, we see that the temperature and magnetic field are inversely related, i.e., when we increase the magnetic field, the temperature must decrease if we wish to hold the entropy constant. In Figure 3.2.2, we plotted the entropy as a function of temperature for a range of magnetic field strengths. From this plot, we observe that, at low temperatures, there is a large region where the entropy remains almost constant. In this region, the entropy depends only on the partition function degeneracy term, which is proportional to the value of the external field. Thus, to observe changes in entropy, a considerable increase in the temperature is required. This results in the near-vertical isentropic lines observed at low temperatures in Figure 3.2.1.

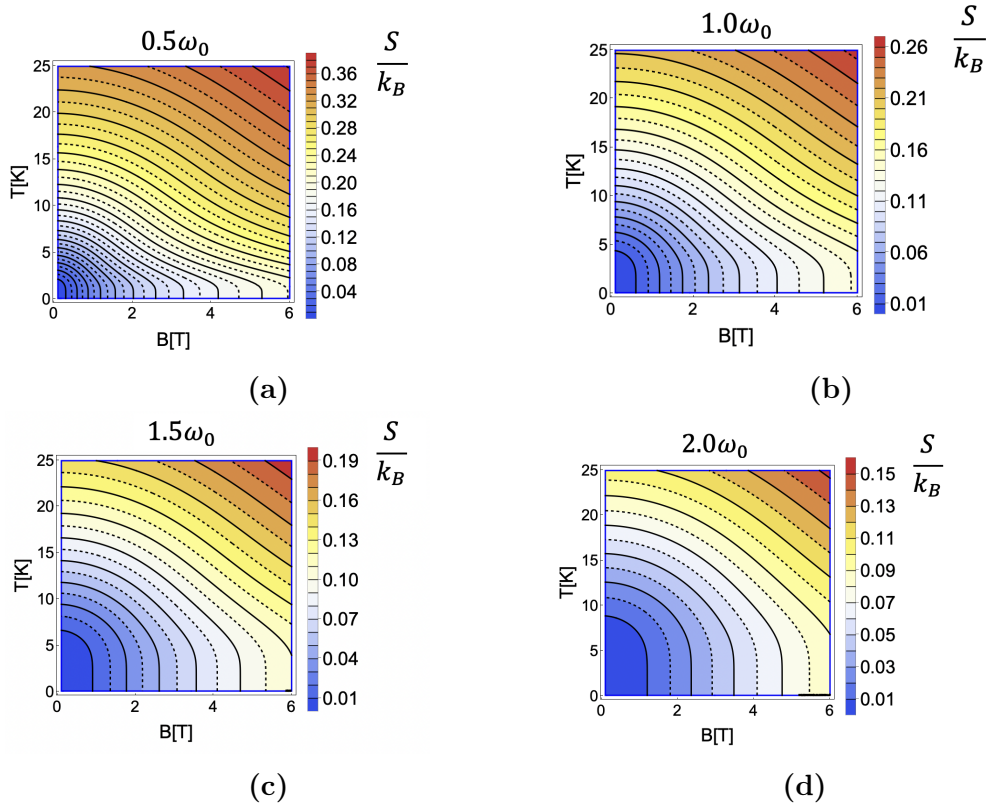


Figure 3.2.1: (a–d) Contour map showing constant entropy curves as a function of temperature, T , (in Kelvin) and the external magnetic field B (in Tesla) for different values of the geometric confinement with $\omega_0 = 2.67$ THz.

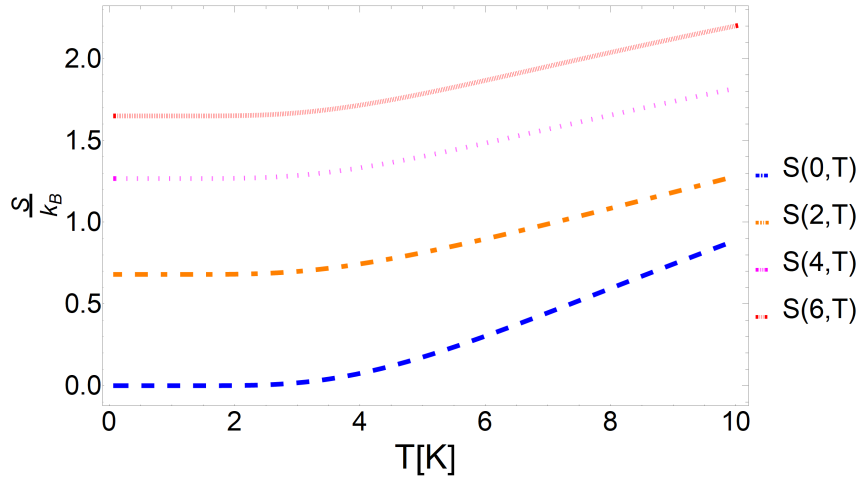


Figure 3.2.2: Entropy as a function of temperature for magnetic field strengths of $B = 0$ T (blue), $B = 2$ T (orange), $B = 4$ T (magenta), and $B = 6$ T (red).

3.3 The Endoreversible Otto Cycle

The Otto cycle, sketched on an entropy-magnetic field diagram in Figure 3.3.1, consists of four strokes: two isentropic (horizontal lines) processes and two isochoric processes (vertical lines). During the first process ($1 \rightarrow 2$), the working substance is disconnected from the thermal reservoir, and the external magnetic field is changed adiabatically from B_1 to B_2 . Since $B_1 > B_2$, the internal energy of the working medium decreases during this process while the working medium temperature increases. Thus, this stroke is correctly classified as an isentropic compression in which the magnetic field is analogous to the volume. The following process ($2 \rightarrow 3$) is an isochoric heating stroke during which the working substance is in contact with a thermal reservoir at temperature T_h and allowed to exchange heat while the magnetic field remains constant. The next stroke ($3 \rightarrow 4$) is accomplished by disconnecting the working substance from the thermal reservoir and changing the magnetic field adiabatically from B_2 back to B_1 . As the internal energy of the working medium increases during this stroke while decreasing in temperature, it corresponds to an isentropic expansion. Finally, the last process ($4 \rightarrow 1$) is an isochoric cooling stroke, during which the working substance is put in thermal contact with a reservoir at temperature $T_c < T_h$ and allowed to exchange heat. At the same time, the magnetic field is again held constant. We note that the inverted behavior of the temperature during the compression and expansion strokes (in comparison to the typical Otto cycle) arises due to the inverse relationship between the temperature and magnetic field necessary to maintain a constant entropy, as observed in the negative slope of the isentropic curves in Figure 3.2.1.

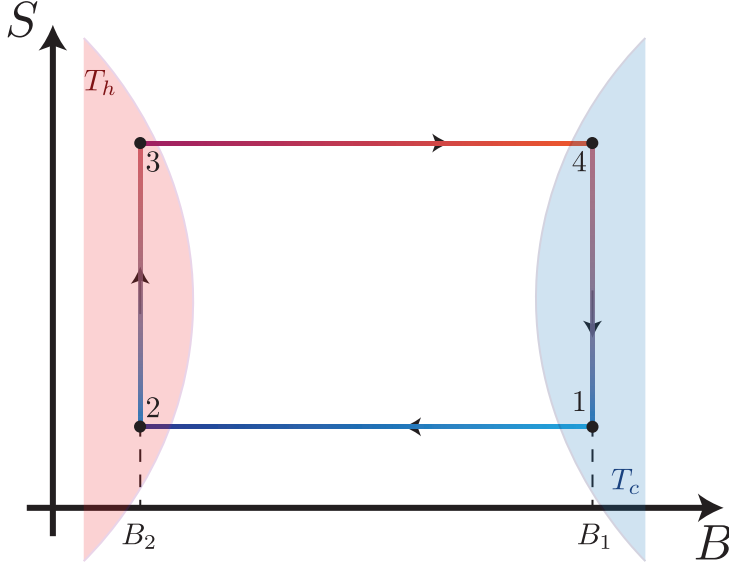


Figure 3.3.1: Entropy versus external field diagram for the endoreversible Otto Cycle. Note that the system is only in contact with the thermal reservoirs during the isochoric (vertical) strokes. Under the assumptions of endoreversibility, the working substance does not fully thermalize to the temperatures of the hot and cold reservoirs, T_h and T_c , at points 3 and 1.

Thermodynamically, the cycle is characterized by the temperatures of the two thermal reservoirs (T_h and T_c) and by the initial and final values of the magnetic field (B_1 and B_2). Under the assumption of endoreversibility, we note that the working medium is always assumed to be in a state of local equilibrium with a well-defined temperature but never fully thermalizes with the reservoirs. Following the analysis established in [22], we determine the heat exchanged with the reservoirs during the isochoric heating stroke ($2 \rightarrow 3$) using,

$$Q_{\text{in}} = U_3(T_3, B_2) - U_2(T_2, B_2), \quad (3.10)$$

where we note $T_3, T_2 \neq T_h$. The temperatures T_2 and T_3 satisfy the following conditions,

$$T(0) = T_2 \quad \text{and} \quad T(\tau_h) = T_3 \quad \text{with} \quad T_2 < T_3 \leq T_h, \quad (3.11)$$

where τ_h is the duration of the heating stroke. We can explicitly model the temperature change from T_2 to T_3 by applying Fourier's law of heat conduction,

$$\frac{dT}{dt} = -\alpha_h (T(t) - T_h), \quad (3.12)$$

where α_h is a constant that depends on the working medium's thermal conductivity and heat capacity. Solving Equation (3.12) results in

$$T_3 - T_h = (T_2 - T_h)e^{-\alpha_h \tau_h}. \quad (3.13)$$

The isentropic expansion stroke (from $3 \rightarrow 4$) is performed identically to the case of a quasi-static cycle. Since the working medium is decoupled from the thermal reservoirs during this stroke, the work is determined entirely from the change in internal energy,

$$W_{\text{exp}} = U_4(T_4, B_1) - U_3(T_3, B_2). \quad (3.14)$$

The isochoric cooling stroke ($4 \rightarrow 1$) can be modeled identically to the heating stroke. The heat exchanged with the cold reservoir is

$$Q_{\text{out}} = U_1(T_1, B_1) - U_4(T_4, B_1), \quad (3.15)$$

where T_1 and T_4 satisfy the conditions

$$T(0) = T_4 \quad \text{and} \quad T(\tau_c) = T_1 \quad \text{with} \quad T_4 > T_1 \geq T_c. \quad (3.16)$$

As in the heating stroke, the temperature change can be modeled by Fourier's law,

$$\frac{dT}{dt} = -\alpha_c (T(t) - T_c), \quad (3.17)$$

By solving Equation (3.17), we obtain

$$T_1 - T_c = (T_4 - T_c) e^{-\alpha_c \tau_c}. \quad (3.18)$$

Finally, the work done during the adiabatic compression stroke ($1 \rightarrow 2$) can be found from the change in internal energy,

$$W_{\text{comp}} = U_2(T_2, B_2) - U_1(T_1, B_1). \quad (3.19)$$

The efficiency of the engine can then be found from the ratio of the total

work and the heat exchanged with the hot reservoir,

$$\eta = -\frac{W_{\text{comp}} + W_{\text{exp}}}{Q_{\text{in}}}. \quad (3.20)$$

The power output is given by the ratio of the total work to the cycle duration,

$$P = -\frac{W_{\text{comp}} + W_{\text{exp}}}{\gamma(\tau_h + \tau_c)}, \quad (3.21)$$

where $\gamma > 1$ is a multiplicative factor that incorporates the duration of the isentropic strokes [22].

As the entropy remains constant during the isentropic process, we can obtain a relationship between T and B from the condition $dS(T, B) = 0$. This first-order differential equation is given by,

$$\frac{dB}{dT} = -\frac{\left(\frac{\partial S}{\partial T}\right)_B}{\left(\frac{\partial S}{\partial B}\right)_T}. \quad (3.22)$$

For the case of a Fock–Darwin model quantum dot, even though the analytic form of the partition function is known, as given in Equation (3.5), this equation does not yield a straightforward analytical solution. Nevertheless, it can be solved numerically, as was done to determine the constant entropy curves in Figure 3.2.1. In addition, it is useful to define the “magnetic length” as

$$l_B = \sqrt{\frac{\hbar}{eB}}. \quad (3.23)$$

By taking the ratio of the magnetic lengths,

$$r = \frac{l_{B_2}}{l_{B_1}} = \sqrt{\frac{B_1}{B_2}}, \quad (3.24)$$

we obtain a quantity analogous to the compression ratio for the classical Otto cycle.

In the limit of $\tau_h, \tau_c \rightarrow \infty$, the working medium will fully thermalize and we expect to recover the quasi-static cycle behavior. We see that in this limit,

$$\begin{aligned} \lim_{\tau_h \rightarrow \infty} (T_3 - T_h = (T_2 - T_h)e^{-\alpha_h \tau_h}) &\rightarrow T_3 = T_h, \\ \lim_{\tau_c \rightarrow \infty} (T_1 - T_c = (T_4 - T_c)e^{-\alpha_c \tau_c}) &\rightarrow T_1 = T_c. \end{aligned} \quad (3.25)$$

However, this limit also results in a vanishing power output, as seen from Equation (3.21).

3.4 Results and Discussions

We began by considering a specific example with bath temperatures of $T_c = 13$ K and $T_h = 25$ K in order to illustrate the cycle performance. These results are presented in Figure 3.4.1, for the work extracted and in Figure 3.4.2 for the efficiency. In Figure 3.4.1, we observe that as the parabolic trap parameter ω_0 decreases, the amount of work extracted increases. Conversely, the efficiency presented in Figure 3.4.2 follows the opposite behavior, growing as ω_0 increases. This comparison demonstrates a clear trade-off between work and efficiency. In addition, we observe in Figure 3.4.1 that there exists a region in which the total work becomes negative for the case of $2\omega_0$, indicating that our cycle is no longer behaving as an engine in this regime. With this in mind, we next explored the parameter regimes where the cycle functioned as different types of thermal machines.

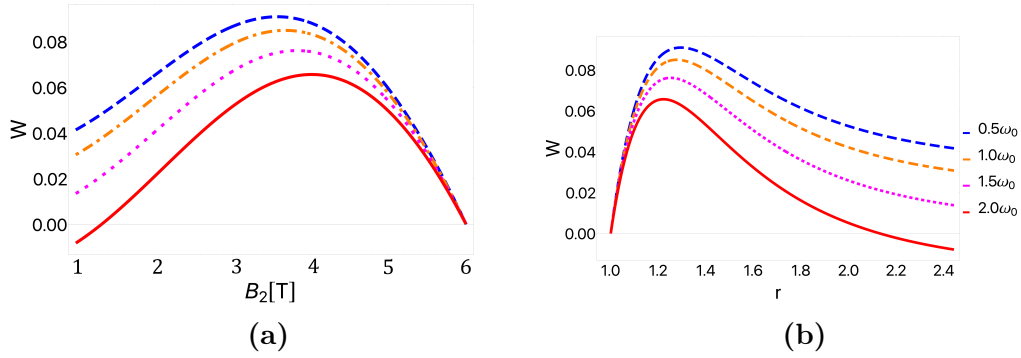


Figure 3.4.1: Total work as a function of (a) the external field and (b) the compression ratio for geometric confinement frequencies of $0.5\omega_0$ (blue), ω_0 (orange), $1.5\omega_0$ (magenta), and $2\omega_0$ (red). We used $T_c = 13$ K, $T_h = 25$ K, and $B_h = 6$ T. Note the clear decrease in the net work with increasing values of the dot confinement. In particular, for these values, a transition to negative net work is observed for the case of $2\omega_0$ (red curve). At this transition point, the cycle switches from behaving as an engine to behaving as a refrigerator.

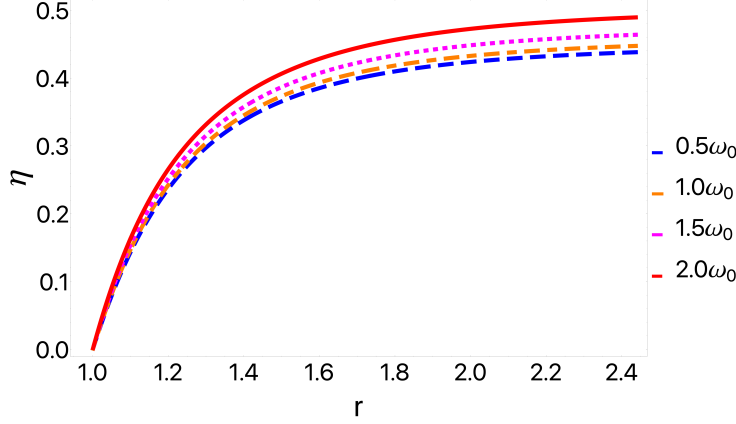


Figure 3.4.2: Efficiency as a function of r for geometric confinement frequencies of $0.5\omega_0$ (blue), ω_0 (orange), $1.5\omega_0$ (magenta), and $2\omega_0$ (red). We used $T_c = 13$ K and $T_h = 25$ K. We observe that the system's efficiency increases as we increase the geometric confinement.

In general, four possible types of thermal machines exist, corresponding to all possible combinations of heat and work flow consistent with the first and second laws of thermodynamics. An engine corresponds to a positive work output, along with a heat flow from the hot bath into the working medium and from the working medium into the cold bath. A refrigerator corresponds to a negative work output, along with a heat flow from the cold bath into the working medium and from the working medium into the hot bath. A heater corresponds to a negative work output and a heat flow from the working medium into both baths. Finally, an accelerator corresponds to a negative work output and a heat flow from the hot bath into the working medium and from the working medium into the cold bath. The heater and accelerator regimes generally emerge due to nonequilibrium behavior. Thus, we do not expect a cycle operating endoreversibly to act as either of these types of thermal machines.

By numerical calculation, we determined the results of Equations (3.10), (3.14), (3.15), and (3.19) across the parameter space. By comparing the signs of the resulting heat and work flows, we determined the regions where the cycle behaved as an engine, refrigerator, heater, or accelerator.

Figure 3.4.3 shows the regions where the cycle operates as an engine or as a refrigerator as a function of the cold bath temperature and the external magnetic field for two different values of ω_0 while holding the temperature of

the hot reservoir constant at $T_h = 25$ K. We observe that by increasing the frequency of geometric confinement, the region in which the cycle operates as an engine is reduced. This behavior can be understood from Figure 3.4.1, where it is observed that as the trap frequency increases, the extracted work decreases, resulting in a transition into the regime of negative work. From Figure 3.4.3, we see that increasing the value of T_c increases the value of the magnetic field at which the transition to the refrigerator regime occurs. Recalling Figure 3.4.1b, increasing T_c corresponds to shifting the peak to the left, and thus also shifting to the left the critical point at which the transition to the negative work regime occurs while maintaining the same qualitative behavior.

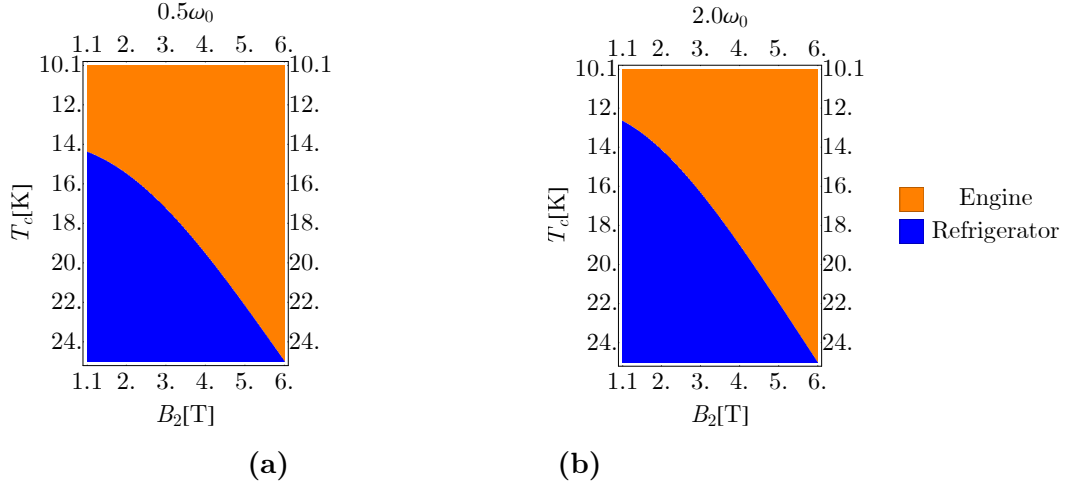


Figure 3.4.3: Cycle behavior as a function of the external magnetic field strength and cold bath temperature for a geometric confinement of (a) $0.5\omega_0$ and (b) $2\omega_0$. Note the increased size of the refrigerator region as the value of the parabolic trap frequency increases.

To numerically determine the EMP, we fixed the temperature of the hot bath at $T_h = 25$ K and the high magnetic field value at $B_h = 12$ T. We then varied the cold bath temperature across the range $T_c \in [0 \text{ K}, 25 \text{ K}]$ and the low magnetic field value from $B_l \in [0 \text{ T}, 12 \text{ T}]$. This range of parameter space was selected to ensure that the peak in the work as a function of the compression ratio (see Figure 3.4.1b) was captured for all combinations of bath temperatures. For each bath temperature ratio, we scanned the parameter space to determine the magnetic field strengths that produced the maximum power output and then determined the efficiency at that maximum power. In Figure 3.4.4, we plotted the EMP as a function of the bath temperature ratio T_c/T_h for different values of ω_0 . These EMPs were then compared with the CA efficiency.

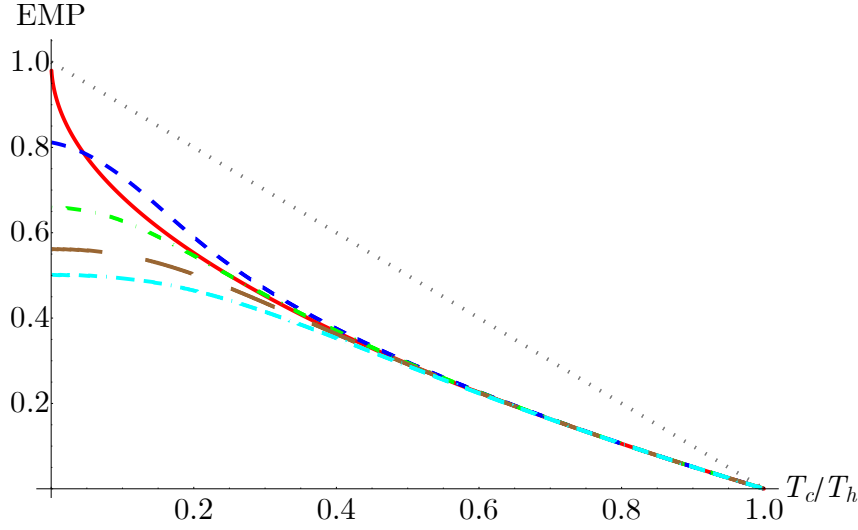


Figure 3.4.4: Efficiency at maximum power as a function of the bath temperature ratio for $0.5\omega_0$ (blue, short dashed), $1.0\omega_0$ (green, dot-dashed), $1.5\omega_0$ (brown, long dashed), and $2.0\omega_0$ (cyan, dot-dash-dashed). The Carnot (black, dotted) and Curzon-Ahlborn (red, solid) efficiencies are provided for comparison. We observe that the efficiency at maximum power exceeds CA for lower values of dot confinement frequency at low bath temperature ratios. Parameters are $T_h=25$ K and magnetic field $B_h = 12$ T.

From Figure 3.4.4, we can see that the geometric confinement frequency significantly impacts the EMP at low bath temperature ratios. Lower values of the confinement frequency yield higher EMPs. In particular, for the case of $\omega_0 = 0.5$, we see a range of bath temperatures where the EMP exceeds the CA efficiency. At higher bath temperatures, we see the EMP converge towards the CA efficiency for all values of the confinement frequency, as is expected in the high-temperature classical limit.

Previous results have shown that the EMP of an endoreversible quantum Otto engine with a pure harmonic oscillator as the working medium exceeds the CA efficiency [22]. As the partition function in Equation (3.5) simplifies to that of a two-dimensional isotropic harmonic oscillator in the limit $\omega_0 \rightarrow 0$ [60], finding that a low ω_0 leads to a region where the CA efficiency can exceed is consistent. Here, we further demonstrated that adding geometric confinement had a strictly detrimental impact on the engine performance.

An additional feature of note is the asymptotic flattening of the EMP as the bath temperature ratio approaches zero. This behavior again arises from the structure of the isentropic curves seen in Figure 3.2.1. As the entropy is

nearly independent of temperature in the low-temperature regime, the value of the compression ratio that maximizes the power output (and thus the value of the EMP) does not change significantly until the system moves out of this regime. This explains why the asymptotic behavior is especially pronounced at high values of the confinement frequency, which display larger ranges of temperatures under which the isentropic curves are nearly vertical with respect to the magnetic field.

3.5 Conclusions

In this work, we analyzed the performance of an endoreversible Otto cycle using a quantum-dot-trapped electron in the presence of an external magnetic field as a working substance. Modeling our working substance using the Fock–Darwin Hamiltonian, we found that the net work, power, and efficiency depended strongly on the intensity of the parabolic trapping frequency, as well as influencing whether the cycle behaved as either an engine or a refrigerator. In particular, we found that larger values of the trapping frequency led to increased efficiency but reduced work, power, and EMP. Despite this, we demonstrated that there existed a parameter regime in which the cycle EMP exceeded the Curzon–Ahlborn efficiency for small values of the trapping frequency. Furthermore, we found that the strongly nonlinear temperature dependence of the entropy for the Fock–Darwin model quantum dot had distinct signatures in the engine performance, namely an asymptotic behavior of the EMP at low temperatures.

Chapter 4

Magnetic Otto Engine for an Antidot System with Aharonov-Bohm flux

4.1 Quantum Antidots

Antidots are structures introduced in two-dimensional electron gas (2DEG) systems within semiconductors like GaAs/AlGaAs. Unlike quantum dots, which confine electrons in potential wells, antidots create regions that repel electrons, forming a periodic pattern of barriers. This arrangement influences electron transport and allows quantum interference to be studied in mesoscopic systems.

Early research into antidot lattices provided insights into how these structures affect electron paths and conductance. For instance, Beenakker and van Houten [61] discussed how periodic potentials in structures like antidots impact quantum transport properties, emphasizing the influence of phase coherence on electron behavior in these materials. Under magnetic fields, antidots exhibit phase coherence effects, as demonstrated by Aquino et al. [62], who observed how the Aharonov-Bohm effect causes phase shifts in electron paths around antidots, altering conductance. The work of Ley-Koo et al. [63] further explored this by studying annular cylindrical systems, showing how antidot geometry impacts phase coherence and interference in electron behavior.

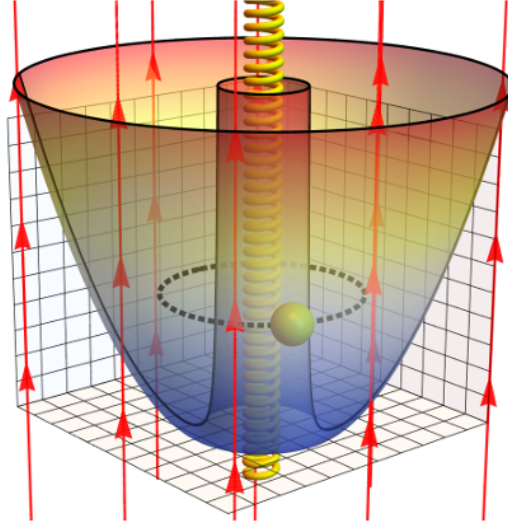


Figure 4.1.1: Pictorial representation of an antidot, with an electron trapped in a ring structure subjected to an uniform magnetic field, plus an Aharonov-Bohm flux in the middle on the ring, depicted as an infinite solenoid producing a magnetic field confined inside it [64].

The structured paths created by antidots have applications beyond quantum interference studies. Tan and Inkson [65] modeled electron states in ring-shaped antidot structures, showing how these configurations stabilize electron trajectories with coherent transport properties. This capability to control electron flow and maintain phase coherence is particularly promising for quantum thermal machines, where quantum dots and antidots can manipulate energy levels and transport properties at the nanoscale. These structures are thus valuable for advancing quantum thermodynamics and designing efficient quantum heat engines, helping optimize energy conversion in quantum devices.

4.2 Aharonov-Bohm Effect

The Aharonov-Bohm effect is an essential phenomenon in quantum mechanics that demonstrates how magnetic potentials can influence the phase of a charged particle, even in regions where fields are absent. In classical physics, it is well established that a charged particle is affected by the electric field $\mathbf{E}$ and the magnetic field $\mathbf{B}$ in the region it travels. However, Aharonov and Bohm proposed in 1959 that even in regions where these fields are zero, the electromagnetic potentials—the vector potential $\mathbf{A}$ and the scalar potential

V —can influence the particle’s phase, provided that the region encircles a magnetic flux [66]. This implies a new level of non-locality in quantum mechanics, where particles can be affected by field configurations in regions where the field does not exist [67].

The essence of the AB effect is that if a charged particle, such as an electron, moves in a closed path around a region with magnetic flux (such as inside a solenoid), its wave function acquires a phase shift proportional to the flux, even if the particle never encounters the magnetic field directly. One of the first experimental validations of the AB effect came in 1960 when R. G. Chambers observed shifts in electron interference patterns caused by magnetic flux within a solenoid without the electrons passing through the magnetic field [68]. This was later confirmed with even greater precision by Tonomura et al. [69], who used electron holography to measure the phase shift caused by a confined magnetic field. Their results provided compelling evidence for the AB effect and reinforced the idea that potentials are physically significant.

Over the years, the AB effect has become critical in understanding quantum phenomena in mesoscopic systems, where coherence lengths are large enough for quantum interference effects to be observed. For instance, in ring-like structures where electrons move along closed paths, periodic oscillations in conductance are observed due to the magnetic flux, a phenomenon known as AB oscillations. This behavior has been detected in metals, semiconductors, and, more recently, graphene [70–76], where high electron mobility and two-dimensional geometry allow for more precise observation of the phase coherence. The AB effect has also had significant practical implications. In technologies that rely on quantum interference, such as SQUIDs (Superconducting Quantum Interference Devices), which are used to measure small magnetic fields, the phase coherence demonstrated by the AB effect is central. Similarly, controlling the electron phase through magnetic flux is crucial in designing quantum circuits and quantum computing systems, where precise control over quantum states is necessary for robust performance [77]. These technologies underscore the importance of phase coherence in quantum systems and the AB effect’s role in modern quantum devices.

4.3 Model

The Bogachek-Landman model [78] consists of an electron confined by two potentials, one attractive ($U_D(r) \propto r^2$), and a repulsive one ($U_{AD}(r) \propto r^{-2}$). In addition, we have an external magnetic field $\mathbf{B}$ perpendicular to the plane of potentials. In the center of this system, a current passes through a solenoid, generating an Aharonov-Bohm flux Φ_{AB} . The Hamiltonian of the system is given by

$$\hat{\mathcal{H}} = \frac{1}{2m^*}(\mathbf{p} + e\mathbf{A})^2 + U_{AD}(r) + U_D(r) \quad (4.1)$$

where m^* is the effective electron mass, $\mathbf{A} = \mathbf{A}_1 + \mathbf{A}_2$ is the total vector potential, which considers the effect of $\mathbf{A}_1$, related to the external magnetic field $\mathbf{B} = \nabla \times \mathbf{A}_1$, and $\mathbf{A}_2$, related to the additional magnetic flux Φ_{AB} inside the antidot. The potentials $U_{AD}(r)$ and $U_D(r)$ are given by

$$U_{AD}(r) = \frac{\zeta}{r^2}, \quad U_D(r) = \frac{1}{2}m^*\omega_0^2r^2 \quad (4.2)$$

here, the constant ζ is related to the chemical potential μ and the effective radius of the antidot r_0 given by the relation

$$\mu = \frac{\zeta}{r_0^2} \quad (4.3)$$

The external magnetic is oriented along the z direction, $\mathbf{B} = B\hat{\mathbf{z}}$, so we can solve the Schrödinger equation in cylindrical coordinates using the Coulomb (or symmetric) gauge to obtain energy levels

$$E_{nm} = \hbar\Omega(2n + [(m + \alpha)^2 + a^2]^{1/2} + 1) + \frac{1}{2}\hbar\omega_c(m + \alpha) \quad (4.4)$$

where $\omega_c = \frac{eB}{m^*}$ is the cyclotron frequency, $\Omega = \omega_0(1 + \left(\frac{\omega_c}{2\omega_0}\right)^2)^{1/2}$ is the effective frequency of the trap, and ω_0 indicates the frequency of the parabolic potential; n and m are the radial and magnetic quantum numbers; $a^2 = \frac{2m^*\zeta}{\hbar^2} = \frac{2m^*\mu}{\hbar^2}r_0^2 = k_F^2r_0^2$ is a constant proportional to the antidot radius r_0 , in which k_F is the Fermi wave vector of the electron, and $\alpha = \frac{\Phi_{AB}}{\Phi_0}$ is an adimensional constant related to the AB-flux $\Phi_{AB} = AH = \pi r_s^2 H$, where $\Phi_0 = \frac{h}{2e}$ is the magnetic flux quantum, r_s is the radius of the solenoid and H is the magnetic field generated by it. Because this model incorporates a combination of quantum

dot, antidot, external magnetic field, and AB-flux, we can identify different cases in Equation (4.4):

1. When $a = 0$ and $\alpha = 0$, we eliminate the effect of the antidot and the AB-flux, so we have the case of a quantum dot system, i. e., we recover the energy levels for the Fock-Darwin model

$$E_{nm}^{\text{dot}} = \hbar\Omega(2n + |m| + 1) + \frac{1}{2}\hbar\omega_c m \quad (4.5)$$

discussed in the previous section.

2. Now if $\omega_0 \rightarrow 0$, from Equation (4.4), we have the energy spectrum of a pure antidot with AB-flux system,

$$E_{nm}^{\text{antidot}} = \hbar\omega_c \left[n + \frac{[(m + \alpha)^2 + a^2]^{1/2} + (m + \alpha) + 1}{2} \right] \quad (4.6)$$

3. Finally, when applying $a = 0$ and $\alpha = 0$ to Equation (4.6), we find the Landau levels in cylindrical coordinates

$$E_{nm}^{\text{Landau}} = \frac{\hbar\omega_c}{2}(2n + 1 + |m| + m) \quad (4.7)$$

Again, it is important to mention that for $m < 0$, we have $|m| + m = 0$, so the Landau levels are infinitely degenerate.

We can calculate the partition function $\mathcal{Z}$, using the general solution of Equation (4.4) and summing over n ($n = 0, 1, 2, \dots$) and m ($m = 0, \pm 1, \pm 2, \dots$)

$$\mathcal{Z} = \sum_{m,n} e^{-\beta E_{mn}} \quad (4.8)$$

Unlike the Fock-Darwin case in which the partition function has a full analytical solution, the structure of Equation (4.4) does not allow for an exact solution, so we use numerical calculations to obtain the canonical partition function of Equation (4.8). We separate the contributions of antidot energy (E_{mn}^{ad}) in the

form

$$\begin{aligned}\mathcal{Z} &= \sum_n e^{-2\beta\hbar\Omega(n+\frac{1}{2})} \sum_m e^{-\beta\hbar\Omega[(m+\alpha)^2+a^2]^{1/2} - \frac{\beta\hbar\omega_c}{2}(m+\alpha)} \\ &= \frac{1}{2} \operatorname{csch}(\beta\hbar\Omega) \sum_m e^{-\beta\hbar\Omega[(m+\alpha)^2+a^2]^{1/2} - \frac{\beta\hbar\omega_c}{2}(m+\alpha)}\end{aligned}\quad (4.9)$$

Given the form of Equation (4.8), we can notice that if $\alpha \in \mathbb{N}$, the partition function is the same as if $\alpha = 0$. This is because we can always define a new quantum number such that $\bar{m} = m + \alpha$ and make the sum over $\bar{m}$; therefore, the recursions for the partition function repeat in the thermodynamic quantities. In this work, we consider a temperature range between 0.2 K and 25 K, so we will use a quantum number $m = -70$ to $m = 30$ to ensure a good convergence in the thermodynamic calculations. From the partition function, we can calculate the entropy and internal energy that we require to perform the Otto cycle:

$$S(T, B, \alpha, a) = k_B \ln \mathcal{Z}_d + k_B T \left(\frac{\partial \ln \mathcal{Z}_d}{\partial T} \right)_B, \quad (4.10)$$

and,

$$U(T, B, \alpha, a) = k_B T^2 \left(\frac{\partial \ln \mathcal{Z}_d}{\partial T} \right)_B. \quad (4.11)$$

This study examined a low-frequency coupling in the parabolic trap, with a frequency of $\omega_0 \sim 4.4$ THz, corresponding to a coupling energy of around ~ 2.896 meV. This energy level is similar to the typical energy of intraband optical transitions in quantum dots [57]. The transition order is about ~ 1 meV for cylindrical GaAs quantum dots with an effective mass of $m^* \sim 0.067m_e$ [57–59]. Again, it is important to note that we did not consider the Zeeman splitting and the spin-orbit interaction, which are negligible for GaAs systems [57, 58].

Entropy has a fundamental role in the Otto cycle since, in the adiabatic strokes, we can find a relationship between temperature and magnetic field and thus calculate heat, work, and the cycle's efficiency. From equation (4.10), we note that the entropy also depends on parameters α and a , related to the AB-flux and the radius of the antidot, so we will first analyze the entropy in terms of its variables before performing the cycle.

In Figure 4.3.1, we have plotted the entropy as a temperature function for various magnetic field values and the antidot radius size (denoted as a). Figure

4.3.1a depicts the configurations for $a = 0$ and $a = 0$, corresponding to the Fock-Darwin model without AB flux and antidot. Like the previous chapter, we observe that the entropy increases with temperature and magnetic field and then rapidly drops to zero for temperatures below 1 K. Upon introducing the antidot, we notice a behavior change. Although the entropy still increases with temperature and field, we observe crosses for different magnetic fields and temperature values, which are associated with direct or inverse magnetocaloric effects depending on the chosen values of B_i and B_f .

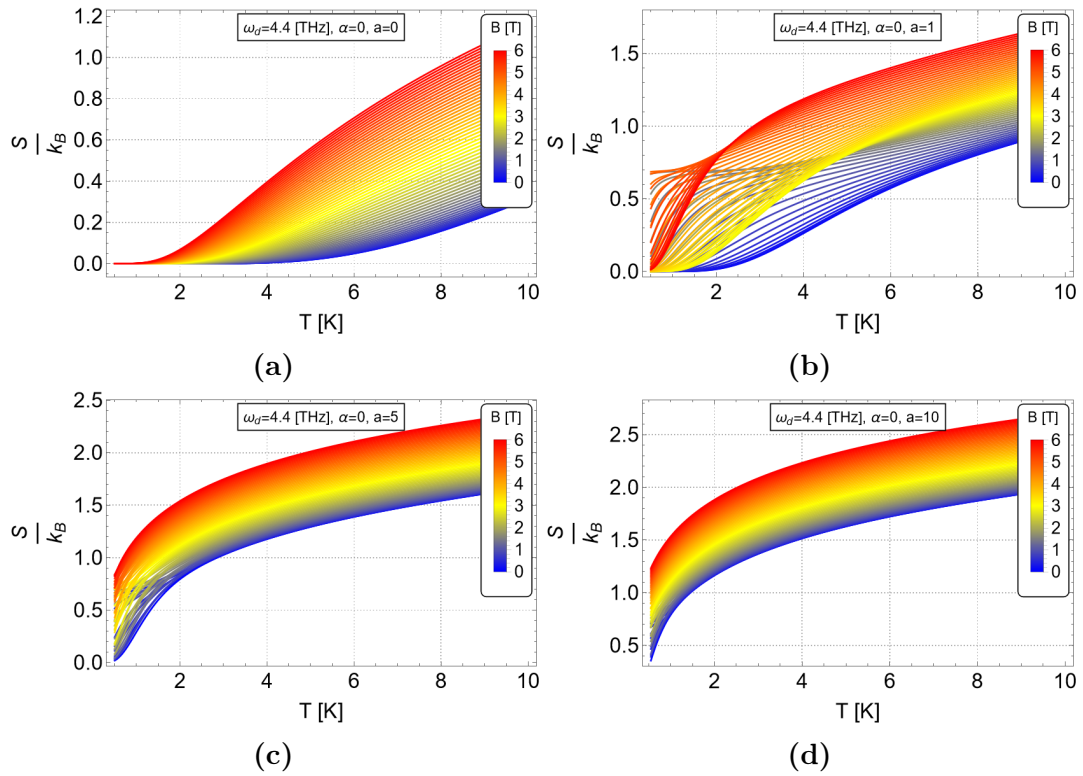


Figure 4.3.1: Entropy as a temperature function for different external magnetic field values between 0 T and 6 T. In all cases, we consider $\alpha = 0$ (absence of AB-flux) and a frequency of 4.4 THz for the quantum dot while varying the antidot radius with values of $a = 0$ for (a), $a = 1$ for (b), $a = 5$ for (c) and $a = 10$ for (d).

When we plot entropy against the magnetic field for different temperature values, we see in Figure 4.3.2 that the points where the entropy values intersect correspond to oscillatory behavior when we introduce the antidot.

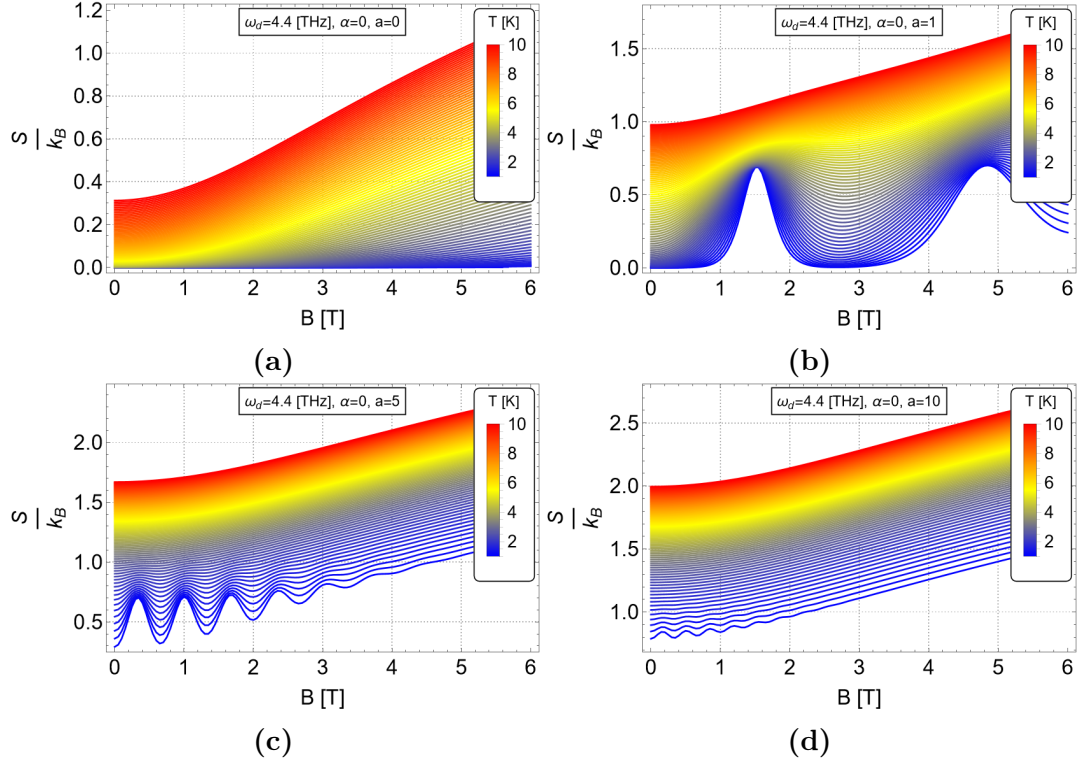


Figure 4.3.2: Entropy as a function of the magnetic field, for different values of temperature between 1 K and 10 K. We maintain the same configurations as above.

In Figure 4.3.2b, we observe two distinct peaks at around $B = 1.5$ T and $B = 4.8$ T for low temperatures. As the value of a increases, we see more oscillation of the entropy but it decreases in intensity. By comparing this with the contour plots generated by the condition $S(T, B, \alpha, a) = \text{const}$ in Figure 4.3.3, we can see that these oscillations align with those shown in the contour maps. In cases **(b-d)**, we note that to maintain constant entropy, there are regions where the relationship between temperature and field is direct, while in others, it is inverse. However, in the entropy peaks, such as in case **(b)**, we find that this relationship between temperature and field breaks down for specific temperature values, reaching zero and causing entropy to increase unavoidably. Conversely, at higher temperatures and values of a , we observe that the oscillation in the entropy decreases, and we regain a behavior similar to that of the Fock-Darwin model, as we can observe comparing to the case in **(a)**.

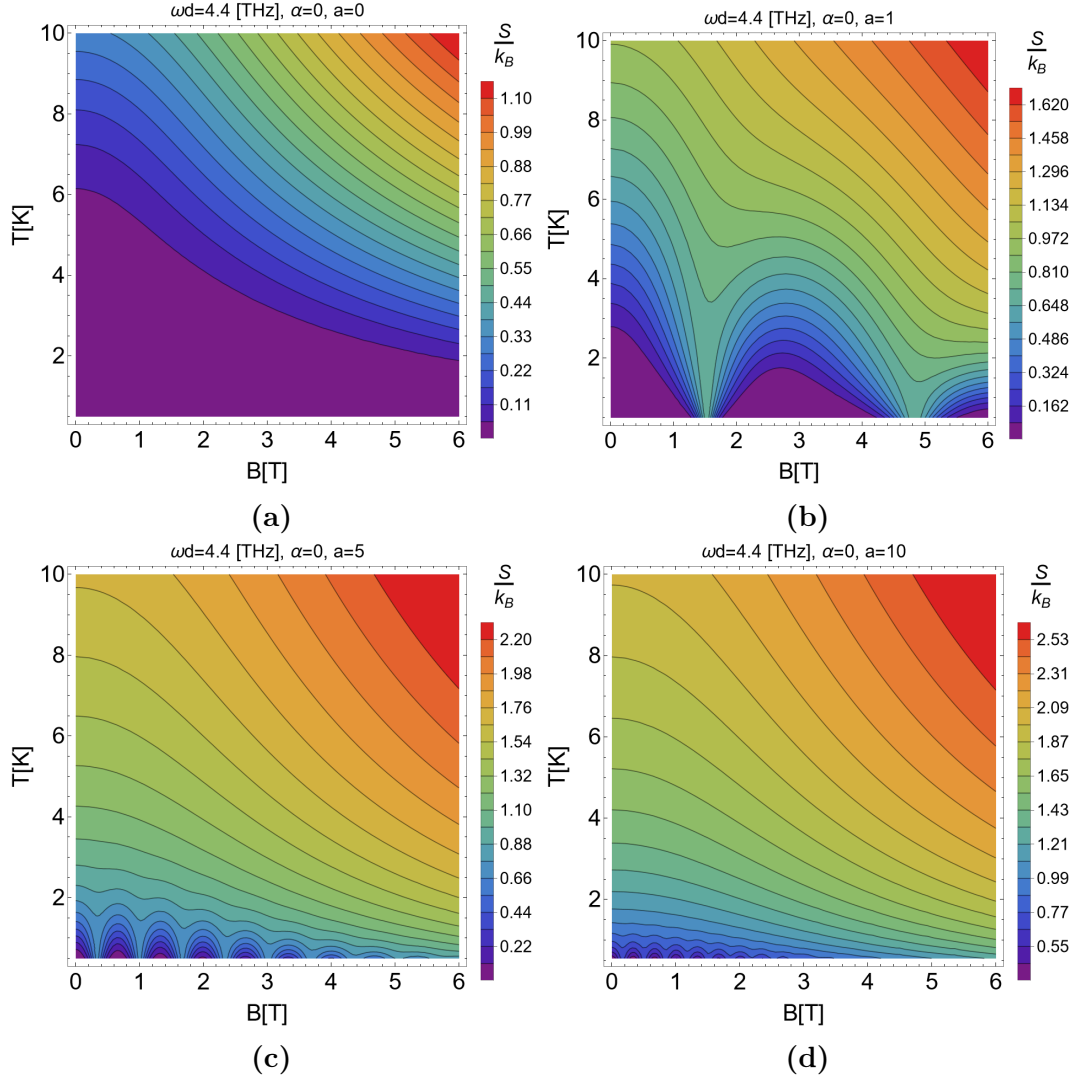


Figure 4.3.3: Contour maps for constant entropy curves as a function of temperature and magnetic field, for different values of a

The AB-flux also causes oscillations in entropy, as observed in Figure 4.3.4. This figure shows entropy as a function of α for different configurations of external magnetic field and antidot radius. An analysis of the left column reveals that without an external magnetic field, there is a maximum at $\alpha = 0.5$ for any value of a and T , indicating symmetric behavior in the change of entropy, which is maintained across different temperatures, besides with reduced intensity as temperature increases. In the central and right columns, where external magnetic fields of 2 T and 4 T are introduced, respectively, the peak in entropy no longer occurs at $\alpha = 0.5$, and the symmetry is lost for different temperatures. This effect is consistent for different external field strengths. Additionally, as

we increase the parameter a , the oscillatory effect in entropy diminishes.

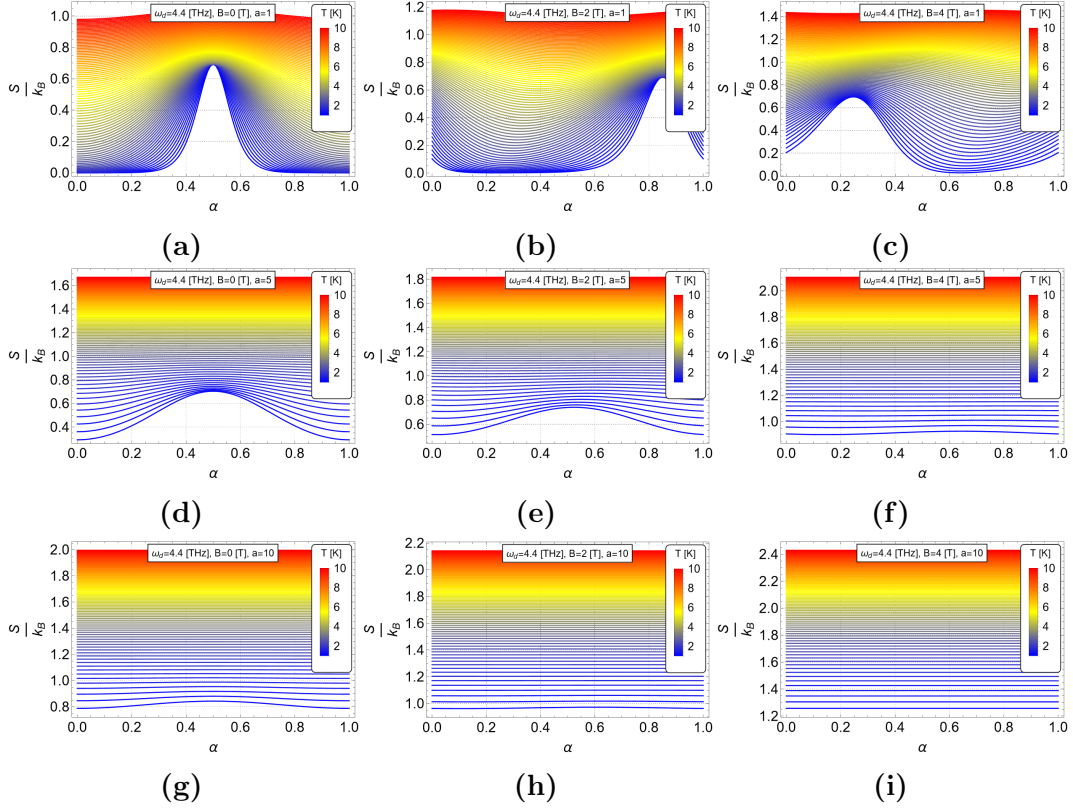


Figure 4.3.4: Entropy as a function of α , for various values of temperature between 1 K and 10 K. Each row has a different value of a , with $a = 1$ for the upper row, $a = 5$ for the middle row and $a = 10$ for the lower row. On the other hand, the columns have different magnetic field values, with $B = 0$ T for the left column, $B = 2$ for the central column, and $B = 4$ in the right column.

In the Otto cycle, work and heat can be calculated from the first law of thermodynamics, so understanding the behavior of internal energy is important and can give us an idea of how these quantities vary with parameters α and a . In Figure 4.3.5, we have the internal energy as a function of the temperature for different external magnetic field values and different antidot radius cases. Like the entropy plots, internal energy increases with temperature and magnetic field. When adding the antidot, crosses appear at low temperatures and low magnetic field values.

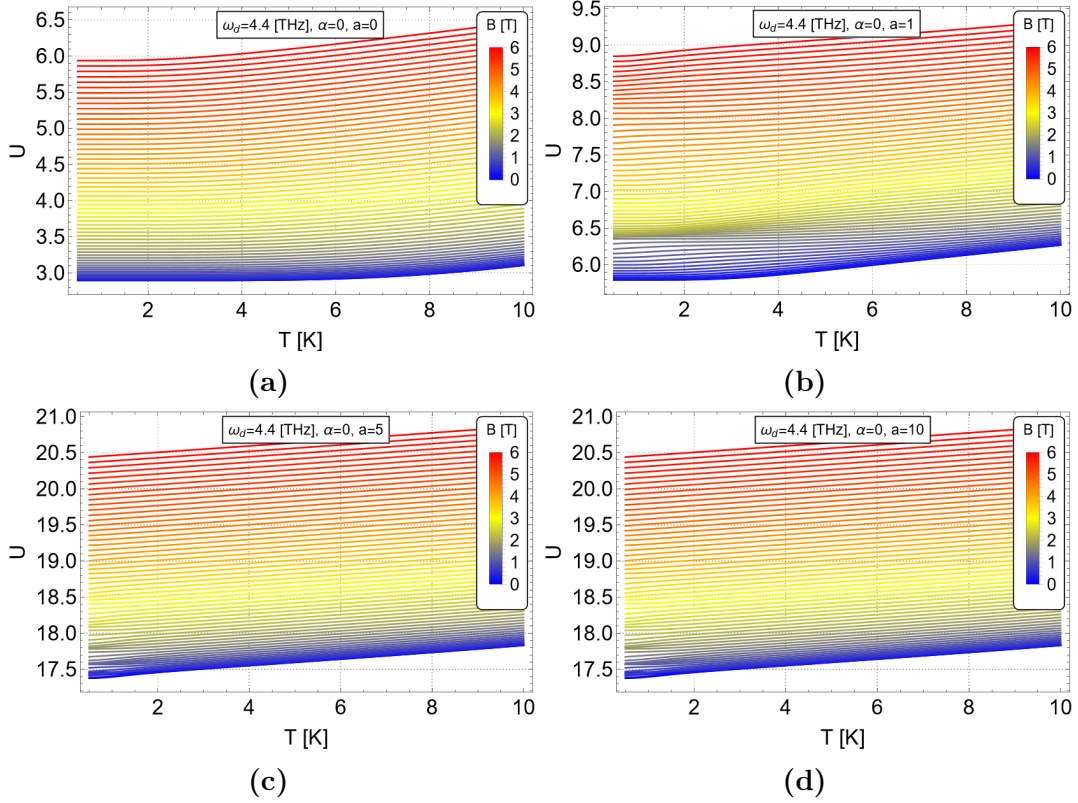


Figure 4.3.5: Internal energy as a function of temperature, for different values of the external magnetic field between 0 T and 6 T. In all cases, we consider $\alpha = 0$ (absence of AB-flux) and a frequency of 4.4 THz for the quantum dot, while varying the antidot radius with values of $a = 0$ for (a), $a = 1$ for (b), $a = 5$ for (c) and $a = 10$ for (d).

These crosses at low values of T and B can be seen when plotting the internal energy as a function of the magnetic field, just as in Figure 4.3.6. Here, oscillations appear similar to Figure 4.3.2, and the addition of the antidot creates more oscillations but with lower intensity. When performing the cycle, we report that increasing the value of the antidot parameter a leads to regions where heat and work changes sign, thus the system can behave like an engine or a refrigerator.

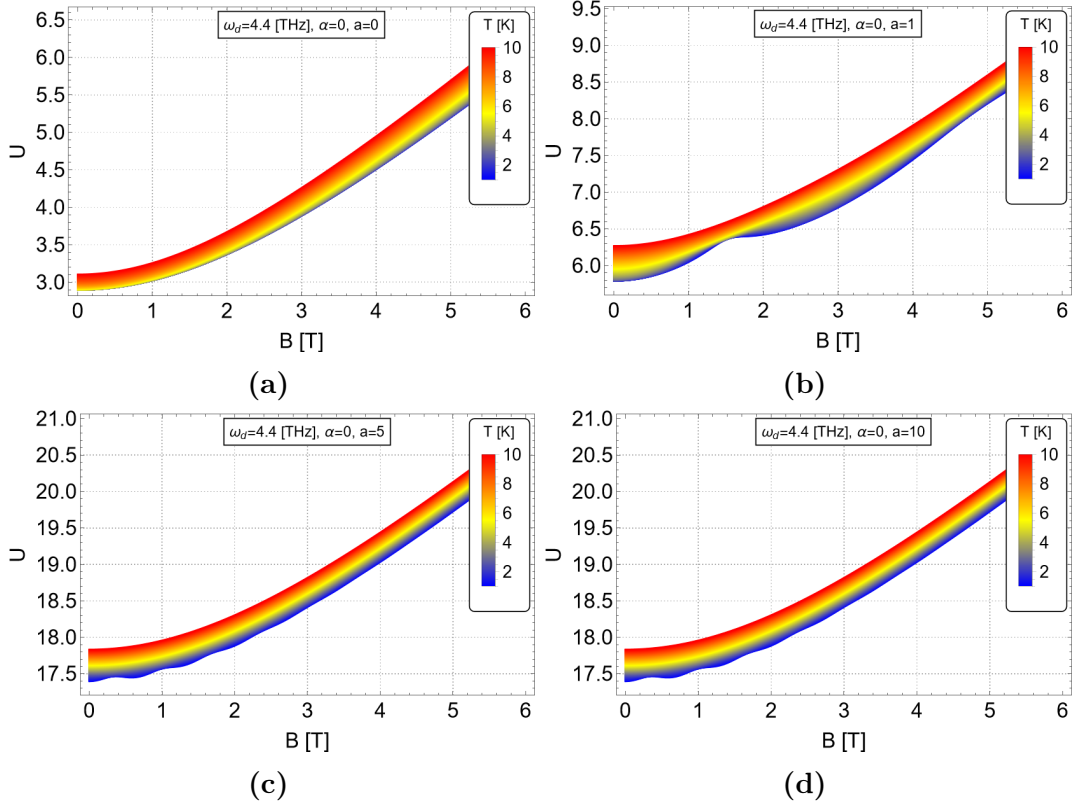


Figure 4.3.6: Internal energy as a function of magnetic field, for different values of temperature between 1 K and 10 K. We maintain the same configurations as above.

The addition of the AB-flux in Figure 4.3.7 also gives a similar behavior comparing to the entropy, here, the we observe an oscillation to the internal energy that has a maximum depending on the fixed value of the external magnetic field. In case (a) (d) and (g) corresponding to the left column, we have zero magnetic fields. Thus the maximum point in the oscillation is maintained at $\alpha = 0.5$ for any value of a and T , while in the central and right column, we check that the symmetry is broken. Then a change in the internal energy behavior is now at different points for any combination of a and T . In addition, increasing the value of a for a fixed α reduces the oscillation effect.

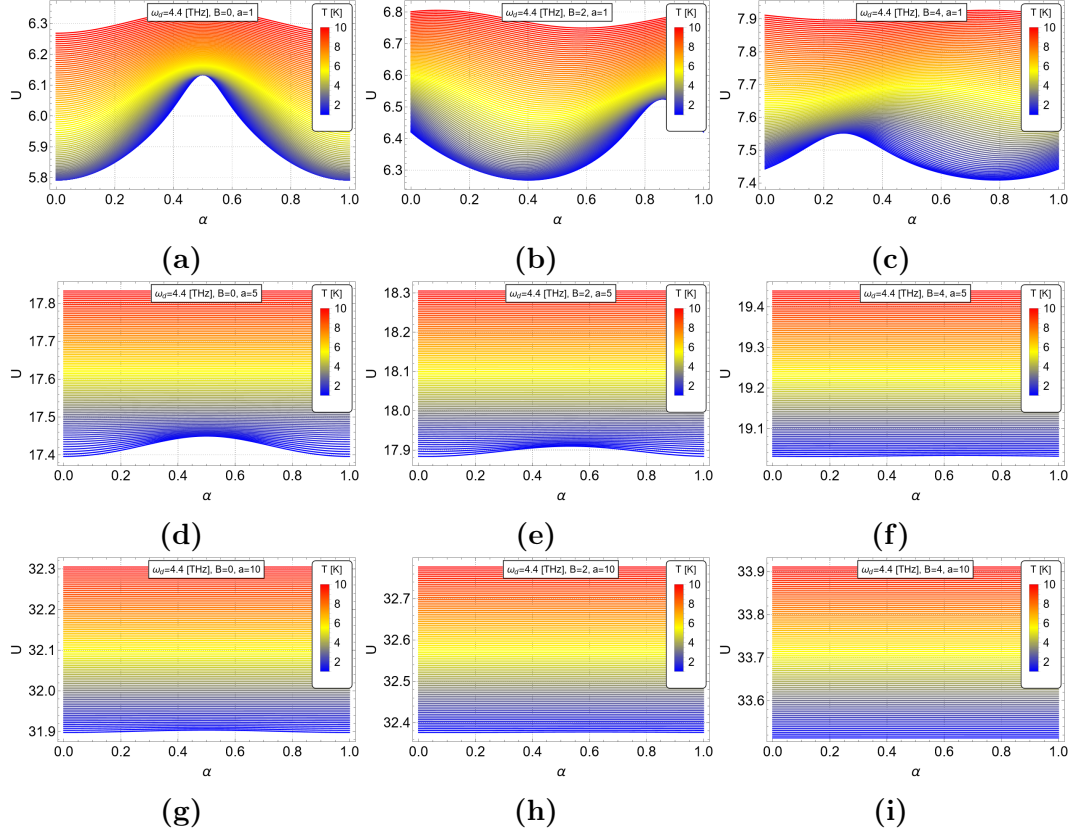


Figure 4.3.7: Internal energy as a function of α , for various values of temperature between 1 K and 10 K. Each row has a different value of a , with $a = 1$ for the upper row, $a = 5$ for the middle row and $a = 10$ for the lower row. On the other hand, the columns have different magnetic field values, with $B = 0$ T for the left column, $B = 2$ for the central column, and $B = 4$ in the right column.

4.4 Quasi-static Otto cycle

As discussed in this work, the Otto cycle consists of four strokes: two adiabatic, two isentropic processes with no heat exchange, and typically two isochoric processes, which can be generalized to a process with a constant external parameter. We can represent this in Figure 4.4.1, and during each stroke, we can make the next analysis

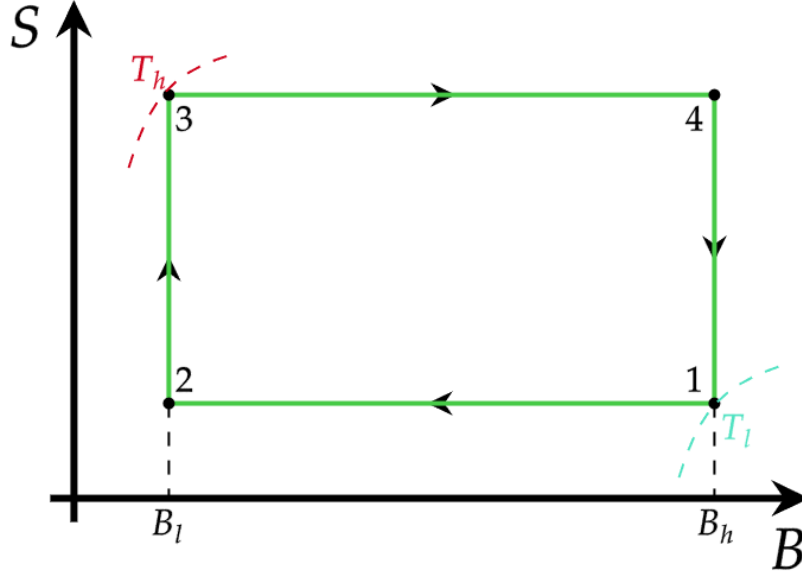


Figure 4.4.1: Entropy and external magnetic field diagram for the Otto cycle.

- Isentropic compression from 1→2: Starting at temperature T_l from the cold heat bath, we disconnect the working substance from the reservoir and decrease the external magnetic field from B_h to B_l , while maintaining a constant entropy defined by point 1 in the cycle. The temperature increases to an intermediate temperature T_2 , which can be obtained from the isentropic condition

$$S(T_2, B_l) = S(T_l, B_h) \quad (4.12)$$

Since there is no heat exchanged during this process, the work done by this "compression" can be expressed in terms of the internal energy by the first law of thermodynamics

$$W_{\text{comp}} = U(T_2, B_l) - U(T_l, B_h) \quad (4.13)$$

- Isomagnetic (or isochoric) heating from 2→3: The working substance is connected to the hot reservoir, thus the temperature rises up to T_h by exchanging heat at constant magnetic field B_l . The heat exchanged can be written as

$$Q_{\text{in}} = U(T_h, B_l) - U(T_2, B_l) \quad (4.14)$$

- Isentropic expansion from 3→4: Starting at temperature T_h from the hot heat bath, we disconnect the working substance from the reservoir and increase the external magnetic field from B_l to B_h , while maintaining a constant entropy defined by point 3 in the cycle. The temperature decreases to an intermediate temperature T_4 , which can be obtained from the isentropic condition

$$S(T_4, B_h) = S(T_h, B_l) \quad (4.15)$$

Since there is no heat exchanged during this process, the work done by this "expansion" can be expressed in terms of the internal energy

$$W_{\text{exp}} = U(T_4, B_h) - U(T_h, B_l) \quad (4.16)$$

- Isomagnetic (or isochoric) cooling from 5→1: We finish the cycle by connecting the working substance to the cold reservoir, thus the temperature decreases to T_l by exchanging heat at constant magnetic field B_h . The amount of heat exchanged is

$$Q_{\text{out}} = U(T_l, B_h) - U(T_4, B_h) \quad (4.17)$$

It is important to note that the relation between heat and magnetic field in the isentropic curves can show the direction of the cycle. In case $\alpha = 0$ and $a = 0$ we see that the temperature and magnetic field have an inverse relation, but when $\alpha \neq 0$ and $a \neq 0$ we see that there are regions with inverse and direct relations between T and B , thus we can have a negative impact on the cycle performance, but regardless of this it is necessary that during the isentropic compression and isomagnetic heating we always satisfy the conditions $T_l < T_2 < T_h$ and during the isentropic expansion and isomagnetic cooling we satisfy $T_h > T_4 > T_l$.

Once work and heat is calculated, we can find the efficiency of the cycle by the ratio of work and heat input in the isomagnetic heating stroke

$$\eta = -\frac{W_{\text{comp}} + W_{\text{exp}}}{Q_{\text{in}}} \quad (4.18)$$

In addition, we defined the "magnetic length" as

$$l_B = \sqrt{\frac{\hbar}{eB}} \quad (4.19)$$

By taking the ratio of the magnetic lengths,

$$r = \frac{l_{B_l}}{l_{B_h}} = \sqrt{\frac{B_h}{B_l}} \quad (4.20)$$

we obtain a quantity analogous to the compression ratio for the classical Otto cycle.

4.5 Results and Discussions

To calculate work, heat, and efficiency, we consider a cycle working between temperatures of $T_l = 5$ K and $T_h = 15$ K given by the heat baths and $B_h = 6$ T for the fixed high magnetic field while moving the low magnetic field B_l between 1 T and 6 T. We start comparing the effect of the antidot in the cycle by fixing the α parameter at $\alpha = 0.5$. In Figure 4.5.1, we have the heat input and output as a function of B_l and r along with Figure 4.5.2 for the total work and efficiency of the cycle for different values of a between 1 and 10. From Figure 4.5.1, we observe that the heat flowing from the hot bath decreases when a increases while the heat flowing into the cold bath increases with a . This is consistent with previous results, in particular with Figure 4.3.5, because for higher values of a , the curves have a lower slope.

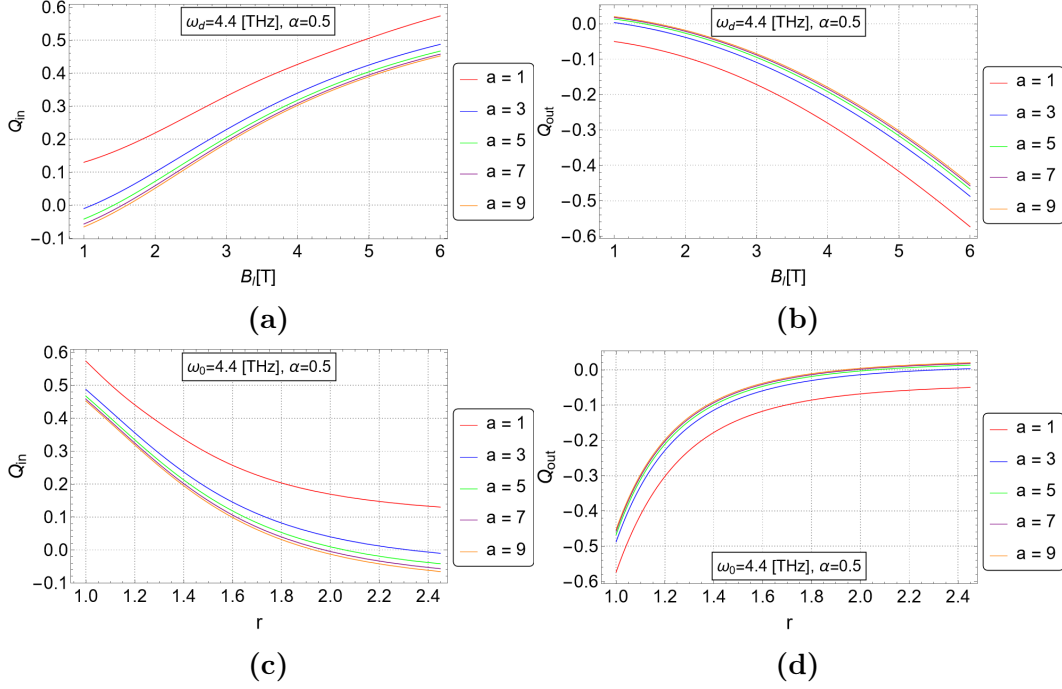


Figure 4.5.1: Heat plots for the proposed cycle for different values of a . (a) and (b) represents Q_{in} and Q_{out} exchanged during the isomagnetic strokes as function of B_l . (c) and (d) represents Q_{in} and Q_{out} exchanged during the isomagnetic strokes as a function of the compression ratio r . Fixed parameters for the cycle are $T_h = 15$ K, $T_l = 5$ K, $B_h = 6$ T and $\alpha = 0.5$.

In Figure 4.5.2, we see a similar trend in work output, but the efficiency behaves oppositely, increasing with a . This comparison highlights a clear trade-off between work and efficiency. We can also note that when increasing a , at low magnetic field values, the heat and work change signs, and thus, we have a refrigerator. It is important to mention that the cycle is not well defined at those values, so if we plotted the efficiency we will find that the Carnot efficiency is surpassed. To show the limit for the efficiency, we have added the Carnot efficiency at Figures 4.5.2b and 4.5.2d.

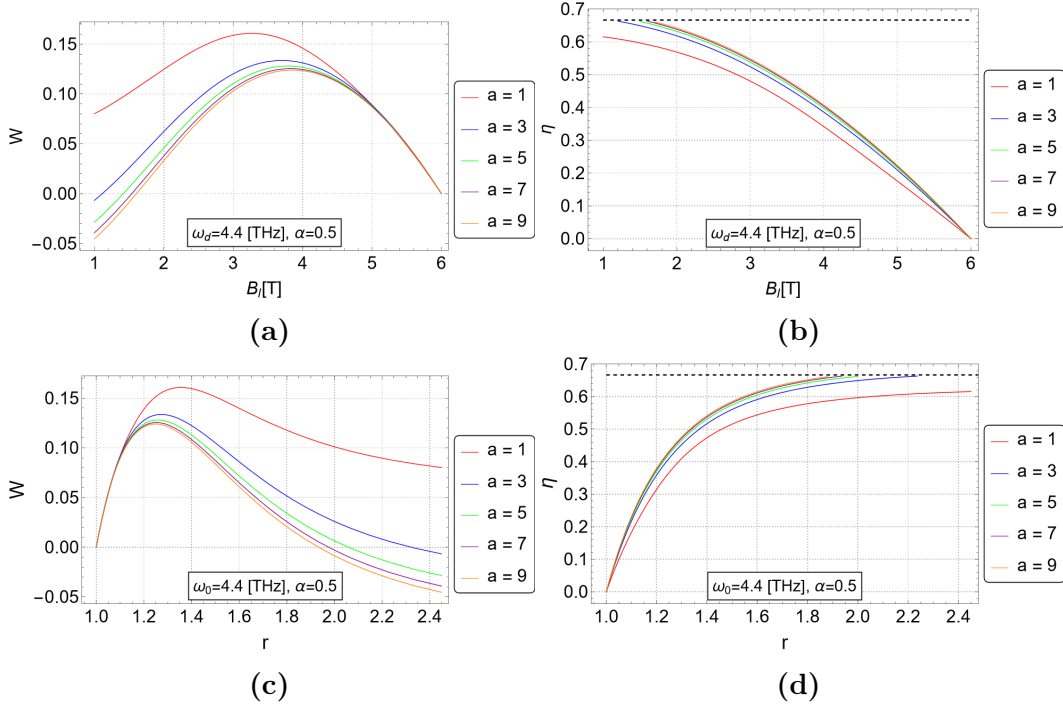


Figure 4.5.2: Work and Efficiency plots for the proposed cycle for different values of a . (a) represents W output during the isentropic strokes and (b) is the efficiency η of the cycle, both as functions of B_l , while in (c) and (d) are functions of the compression ratio r . In the efficiency plots we included the Carnot efficiency $\eta_{\text{Carnot}} \approx 0.67$ represented by the black dashed line. Fixed parameters for the cycle are $T_h = 15$ K, $T_l = 5$ K, $B_h = 6$ T and $\alpha = 0.5$.

For the second case, we fix the antidot parameter to be $a = 1$ and plotted curves for different α between 0 and 1. These results are shown in Figures 4.5.3 and 4.5.4, where we observe an interesting feature, the oscillatory behavior reported for the internal energy at Figure 4.3.6 and 4.3.7 is also displayed here, since increasing the value of α generates an increment in the heat input up and work up to $\alpha \approx 0.5$, but then it decreases for higher values of α . On the other hand, heat output and efficiency have the opposite behavior, first decreasing for values up to $\alpha \approx 0.5$ and then increasing for higher values of α . We need to mention that the symmetry in the oscillatory effect for the internal energy only appears for $B = 0$, having a maximum at $\alpha = 0.5$ for any temperature and a values, but for the Otto cycle we work with an external magnetic field between 1 T and 6 T, and thus the symmetry disappears. The maximum or minimum heat, work, and efficiency are not exactly at $\alpha = 0.5$.

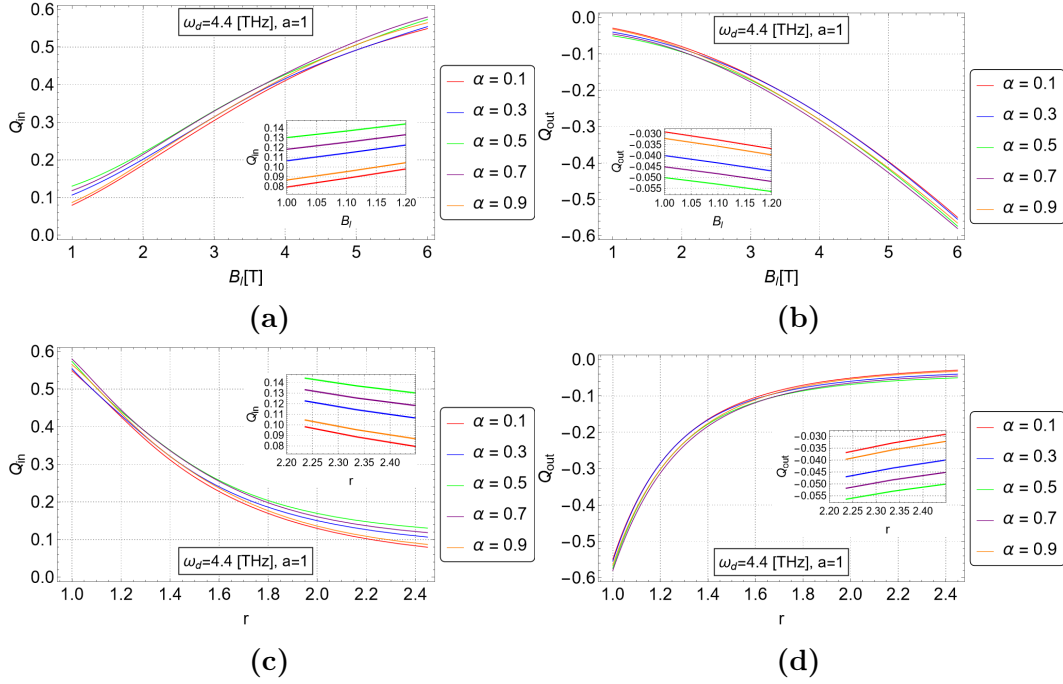


Figure 4.5.3: Heat plots for the proposed cycle for different values of α . (a) and (b) represents Q_{in} and Q_{out} exchanged during the isomagnetic strokes as function of B_l . (c) and (d) represents Q_{in} and Q_{out} exchanged during the isomagnetic strokes as a function of the compression ratio r . Fixed parameters for the cycle are $T_h = 15$ K, $T_l = 5$ K, $B_h = 6$ T, and $a = 1$.

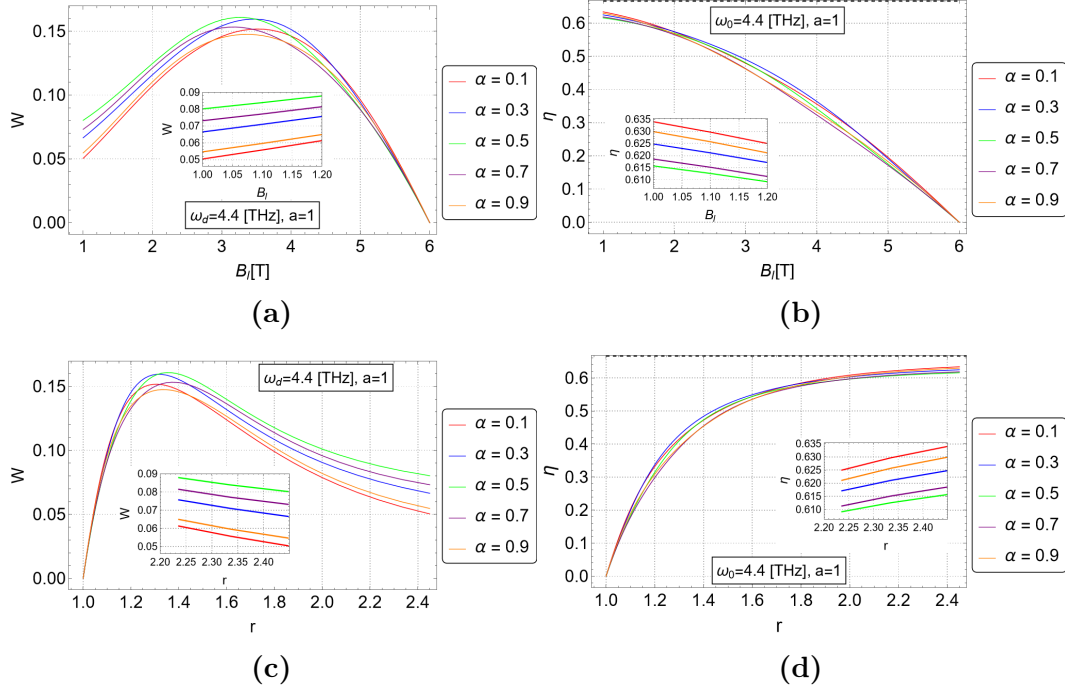


Figure 4.5.4: Work and Efficiency plots for the proposed cycle for different values of α . (a) represents W output during the isentropic strokes and (b) is the efficiency η of the cycle, both as functions of B_l , while in (c) and (d) are functions of the compression ratio r . In the efficiency plots, we included the Carnot efficiency $\eta_{\text{Carnot}} \approx 0.67$ represented by the black dashed line. Fixed parameters for the cycle are $T_h = 15$ K, $T_l = 5$ K, $B_h = 6$ T, and $a = 1$.

4.6 Conclusions

Our study examined the thermodynamics and performance of an Otto cycle for a working substance made up of an electron under the influence of both quantum dot and antidot potentials, along with an Aharonov-Bohm flux and an external magnetic field. We show that when we introduced the antidot and the Aharonov-Bohm flux, the entropy and internal energy displayed oscillatory behavior, resulting in regions where the relationship between the magnetic field and the temperature could be either direct or inverse, impacting the cycle's behavior.

We observed that heat, work, and efficiency are significantly influenced by the antidot and Aharonov-Bohm flux. Increasing the parameter a led to decreased heat input and work while heat output and efficiency increased. Furthermore, we found a region where the cycle stops operating as an engine, as evidenced by a change in the signs of heat and work, turning it into a

refrigerator instead. For the α parameter, we noticed similar heat, work, and efficiency oscillations. Heat input and total work increased until reaching a maximum value and then decreased, while the output heat and efficiency displayed the opposite behavior. The point where this quantity behavior is reversed is around $\alpha \approx 0.5$. Still, this value depends on the external field and the system's temperature due to the asymmetrical oscillation caused by the external magnetic field.

Chapter 5

Conclusions and Future Work

In this thesis, we explored the Otto cycle using two models as working substances: the Fock-Darwin and Bogachek-Landman models. Each reveals unique thermodynamic properties and responses to external magnetic fields and quantum interference effects.

Chapter 3 discusses the Fock-Darwin model, composed of an electron confined in a quantum dot under an external magnetic field, and shows how variations in the trapping frequency significantly influence work and efficiency. When considering endoreversibility, we identified regimes where efficiency at maximum power (EMP) exceeds the Curzon-Ahlborn efficiency, with larger trapping frequencies enhancing efficiency but reducing work, power, and EMP. This result illustrates that quantum properties can be tuned to enhance efficiency depending on specific operating conditions.

Chapter 4 analyzes the Bogachek-Landman model, which introduces both quantum dot and antidot and an Aharonov-Bohm flux, expanding the versatility of quantum-dot-based engines. We found that the antidot and magnetic flux induces oscillatory behavior in internal energy and entropy. This results in regions where magnetic field and temperature have direct or inverse relations, impacting the cycle's behavior. Parameter a , related to the antidot potential, and parameter α , related to the Aharonov-Bohm flux, modify the relationship between heat, work, and efficiency, obtaining oscillations in these quantities and operating regimes where the system may function as an engine or a refrigerator.

These findings show that quantum dots and antidots are promising working substances for nanoscale thermal machines. By comparing endoreversible and quasi-static cycles, we gain insight into how quantum confinement and the

Aharonov-Bohm effect can be harnessed to modulate heat and work production. Future research can build on these results by exploring more working substances and alternative confinement geometries to uncover additional methods for controlling heat and work. In addition, research in non-equilibrium effects may reveal new thermodynamic behavior. However, it is essential to mention that experimental validation of these theoretical models is a step towards understanding practical implementation and limitations.

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