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Quantum antidot with Aharonov-Bohm flux as a Quantum Otto Engine

Benjamín Andrés Mimica Figari

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Advisor: Dr. Francisco Peña
Committee: Dr. Patricio Vargas
Dr. Vladimir Juricic

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Abstract

In this work, we propose a Quantum Otto Engine (QOE) made by a spinless electron trapped in a quantum dot, in addition to a quantum anti-dot (QAD) and an Aharonov-Bohm flux (AB-flux). We compare the quasistatic "usual" formulation of adiabatic and isochoric processes with their quantum definition. In contrast with the spineless quantum dot system, the addition of QAD and AB-flux produce zones in the parameter temperature vs external magnetic field diagram where a direct magnetocaloric effect (MCE) is found and thus gives us the freedom to work both on direct and inverse MCE regimes. It is found that working on either MCE zone, the cycle shows the behavior of a heat engine (heat applied results in positive work output). In every case analyzed, quasistatic work and efficiency are greater than their quantum counterpart as expected.

En este trabajo, proponemos un motor cuántico de Otto (QOE por sus siglas en inglés) que trabaja con un electrón sin spin en una trampa de punto cuántico, donde hemos añadido la influencia de un antidot cuántico (QAD) y flujo de Aharonov-Bohm (AB-flux). Comparamos la formulación quasi-estática "usual" de procesos adiabáticos e isocóricos con su formulación cuántica. En contraste con el sistema de punto cuántico sin spin, añadir QAD y AH-flux produce zonas en el diagrama temperatura vs campo magnético externo donde ocurre efecto magnetocalórico (MCE) directo. Encontramos que trabajando tanto en MCE directo o inverso, el ciclo se comporta como un motor (calor convertido en trabajo). En todos los casos analizados, el trabajo y eficiencia quasi-estático supera al cuántico como se espera.

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Chapter 1

Quantum Heat Engines

Quantum heat engines (QHEs) produce work using quantum substances [1]. In the search for QHEs, unusual properties appear because of the quantum behavior of these systems. For example, it has been found that under certain conditions QHEs could surpass work done by a classical efficiency [2]. Moreover, measurements have proven that these conditions can be achieved experimentally. For example, using an ensemble of nitrogen-vacancy centers in diamond in the regime of small engine action, researchers found that quantum effects can enable a QHE to produce more power than any equivalent classical heat engine [3].

In this work, we wish to make a theoretical description of a Quantum Otto engine (QOE) done with a quantum dot, in addition to a quantum antidot and an Aharonov-Bohm flux. For this, we need the quantum analog of isochoric and adiabatic processes which we will define now.

1.1 First Law

Let us consider a system described by a Hamiltonian that can be diagonalized in terms of discrete energy levels E_n and eigenfunctions $|n\rangle$. If we assume no degeneration in the energy levels, we can write,

$$\mathcal{H} = \sum_n E_n |n\rangle \langle n|. \quad (1.1)$$

At thermal equilibrium, internal energy can be calculated as the expected value of the Hamiltonian:

$$U = \langle H \rangle = \sum_n P_n E_n, \quad (1.2)$$

for a given occupation distribution. Here P_n denotes the probability of the state to be found in the n -th eigenstate. In analogy with classic thermodynamics, the quantum version of the first law can be defined in analogy with the first law of thermodynamics:

$$dU = \partial Q + \partial W \longrightarrow dU = \partial Q^q + \partial W^q \quad (1.3)$$

Where Q^q, W^q are quantum heat and work respectively to be defined. Applying to equation (1.2) yields:

$$dU = \sum_n (E_n dP_n + P_n dE_n). \quad (1.4)$$

Now we make the following identification:

$$\partial Q^q \equiv \sum E_n dP_n \quad (1.5)$$

$$\partial W^q \equiv \sum P_n dE_n. \quad (1.6)$$

Heuristically, the first equation can be identified via Boltzmann's definition of entropy $S = -k \sum P_n \ln P_n$ with quasistatic heat exchange $\partial Q = T dS$. On the other hand, the equation for quantum work is in accordance with the fact that work is done by a change in generalized coordinates of the system [4], thus resulting in changes in energy levels. For a more detailed and general derivation of this set of equations see for example [5]. These equations imply that the work performed on the system corresponds to a change in the eigenenergies of the system (E_n), while heat exchange with the system corresponds to a change in occupation probabilities (P_n).

1.2 Quantum isochoric process

Strictly speaking, an isochoric process is such that involves no change in the volume of the system. In this context though, we will call a process *isochoric* when no work is done on the system. In a quantum isochoric process, a working

substance is placed in contact with a heat bath. We see from equations (1.5) (1.6) that this requires invariance on the energy levels. Energy exchange with the heat bath will produce a change of the occupation probabilities P_n and thus the entropy S changes until the working substance reaches thermal equilibrium with the heat bath [4]. Consequently, at the end of the process, the system satisfies Boltzmann's distribution

$$P_n = \frac{e^{-\beta E_n}}{Z} \quad (1.7)$$

1.3 Quantum adiabatic process

An *adiabatic* process by definition has no heat exchange between the system and the heat bath. According to the adiabatic theorem, an adiabatic process is characterized by a gradual change in external conditions (slow change of control parameters). If the process occurs slowly enough, only energy levels will change but not their occupation probabilities ($dP_n = 0$).

Imposing this condition satisfies the classical definition of an adiabatic process, as no change of occupation probabilities implies $dS = 0$. On the other hand, in general, a classical adiabatic process is not necessarily adiabatic in the quantum sense. It does not necessarily leave occupation probabilities P_n unchanged. This means that quantum adiabatic processes are a subset of quasistatic adiabaticity defined via equation $dS = 0$.

Chapter 2

Otto Cycle: Quasistatic and quantum approach

The *Otto Cycle* has been widely studied in its classical formulation. It consists of two adiabatic and two isochoric processes. Theoretical quantum Otto engines (QOE) have been calculated [6] and experimental realization has been proposed [7, 8]. In a similar way, we suggest a QOE controlled by an external magnetic field to take advantage of the magnetocaloric effect (MCE).

2.1 Magnetocaloric effect

The MCE consists of a material's thermal response when subjected to a magnetic field change [9]. This effect can be quantified as a reversible change in temperature ΔT_{ad} if the process is *adiabatic* or as a reversible change in magnetic entropy ΔS_m if the process is *isothermal*.

Consider total entropy as

$$S_T(B, T) = S_m(B, T) + S_l(T) + S_e(T) \quad (2.1)$$

where S_m is the entropy of magnetization of the material, S_l is lattice entropy which characterizes the vibrations of the crystal lattice and S_e is the electronic entropy which describes the entropy of the material's free electrons. Notice that in equation 2.1, both lattice and electronic entropy are considered to depend only on temperature. In general, only magnetic entropy depends strongly on the external magnetic field, and thus we can make that approximation.

When an adiabatic change in the magnetic field is done, then by definition $\Delta S_T = 0$. Because S_m changes with magnetic field changes, the temperature must change an amount ΔT_{ad} to compensate for this change in entropy. On the other hand, when we quantify the thermal response with an isothermal process, it involves a change in total entropy. By definition, an isothermal process involves no change in temperature, and thus total entropy change can only change via magnetic entropy, so $\Delta S_T = \Delta S_m$.

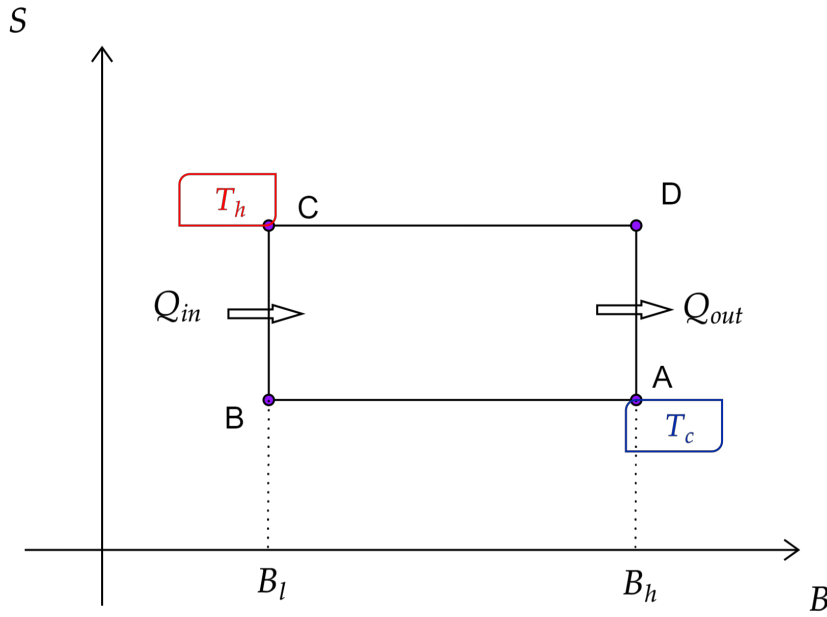


Figure 2.1: Otto Cycle on an Entropy vs Magnetic field graph. Cycle is done in order $A \rightarrow B \rightarrow C \rightarrow D \rightarrow A$.

To produce an otto cycle, only adiabatic changes in the magnetic field are considered as in diagram 2.1. When changing the external magnetic field, the system changes its temperature by the quantity ΔT_{ad} . Direct ($\Delta T_{ad} > 0$) or inverse ($\Delta T_{ad} < 0$) MCE can be found depending on the substance used. This will determine where the reservoirs are placed. In the example below (diagram 2.1) an inverse MCE is assumed so that reservoirs T_c at point A and T_h at point B are the coldest and hottest points in the cycle respectively.

2.2 Quasistatic Otto

For now, we will assume an inverse MCE and analyze the system as in figure (2.1). A quasistatic cycle is totally reversible. This means the system is in equilibrium at every point in the cycle. For this reason, internal energy and other thermodynamical quantities derived from the partition function are well-defined at every point in the cycle. Our Otto cycle is defined by the following steps:

1. System starts at thermal equilibrium at point A with a cold reservoir at temperature T_c and with an external magnetic field B_h . By changing the external magnetic field, the system heats up *adiabatically* to a magnetic field value of B_l . As $S \equiv S(T, B)$ we may find temperature T_B in point B using condition $S(T_c, B_h) = S(T_B, B_l)$. This process results in work applied to the system given by¹:

$$W_{AB} = \int_{B_h}^{B_l} -M(T, B)dB = U_B - U_A \quad (2.2)$$

2. At point B , the system is placed in contact with the hot reservoir of temperature T_h and heats up at a constant magnetic field value B_l until it gets to thermal equilibrium with the reservoir at point C . Here there is a positive heat applied to the system given by

$$Q_{in} = U_C - U_B \quad (2.3)$$

3. Points $C \rightarrow D$ and $D \rightarrow A$ follow the same logic: an adiabatic cooldown of the system followed by an isochoric curve given by putting the system into contact with the cold reservoir. The same equations may be found,

$$W_{CD} = \int_{B_l}^{B_h} -M(T, B)dB = U_D - U_C \quad (2.4)$$

$$Q_{out} = U_A - U_D \quad (2.5)$$

The net work of the complete cycle is given by $W_{tot} = W_{AB} + W_{CD}$. Thus, if

¹Note that the fact that work here is *applied to/extracted from* the system will be evident by the sign we obtain. In our convention, $W > 0$ is work applied to the system.

we know an expression for internal energy, we can calculate every work and heat applied to the system.

2.3 Quantum Otto

For illustration, we still use figure (2.1) for the quantum cycle. Nevertheless, the quantum formulation does not require thermodynamic equilibrium at every point in the cycle. This means that even though we expect the cycle to achieve points A, B, C, D in the cycle, it will not follow the same paths drawn in the figure. Only points mentioned will coincide in both quantum and quasistatic formulation. Additionally, we can not define temperature and internal energy everywhere, as these quantities are well-defined at equilibrium only. Instead, we use occupation probabilities and energy levels.

Let's call occupation probabilities in point X of the cycle $P_n(X)$ and energy levels will be $E_n(B_l) \equiv E_n^l, E_n(B_h) \equiv E_n^h$ ². Considering equation (1.6), heat absorbed in isochoric process $B \rightarrow C$ is

$$Q_{in}^q = \sum_n \int_B^C E_n dP_n = \sum_n E_n^l [P_n(C) - P_n(B)] \quad (2.6)$$

analogously,

$$Q_{out}^q = \sum_n \int_D^A E_n dP_n = \sum_n E_n^h [P_n(A) - P_n(D)] \quad (2.7)$$

To satisfy adiabatic condition we need $P_n(C) = P_n(D)$ and $P_n(A) = P_n(B)$. Quantum heat and work must satisfy the quantum version of the first law of thermodynamics. Using the first law leads to an expression for net work. From equation (1.3):

$$W^q = -(Q_{in}^q + Q_{out}^q) = \sum_n (E_n^l - E_n^h) [P_n(A) - P_n(C)] \quad (2.8)$$

²Here, summation has to be done on every quantum number. For simplicity, only one index n is used.

2.4 Classification of cycles and efficiency

Different kinds of thermal machines can be achieved by making an Otto cycle. This will depend on both heat flow from and to the reservoirs. The efficiency of the cycle will depend on what kind of thermal machine we have.

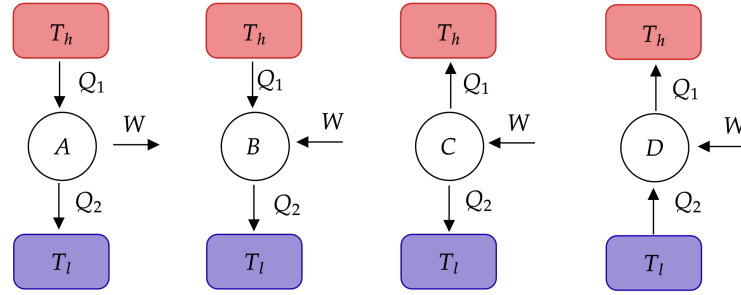


Figure 2.2: Four kinds of thermal machines can be achieved by an Otto cycle working between two heat reservoirs [10]. In our sign convention, arrows that go *into* the system denote positive heat or work, and arrows that go *outwards* are negative heat and work.

It is important to define the sign convention we are using. In this work, $dU = \partial W + \partial Q$, so that *positive* work (heat) is work (heat) applied *to the system*.

- (A) *Heat engines* take heat Q_1 from the hot bath, partially converts it in work W and supplies the rest in form of heat Q_2 to the cold bath.
- (B) *Heathers type II* take heat Q_1 from the hot reservoir, and with the aid of work W into the system, supply heat Q_2 into the cold reservoir. This type of thermal machine is not very convenient, we have to apply external work to make a process that would occur spontaneously (transferring heat from a hot reservoir to a cold one).
- (C) *Heathers type I* convert work W into heat Q_1, Q_2 applied to the hot and cold reservoir respectively.

- (D) *Refrigerators* take heat Q_2 from the cold reservoir, and with help of work W it supplies heat Q_1 into the hot reservoir.

Commonly we will deal with either an engine or a refrigerator. In fact, in the quasistatic formulation (reversible) the same cycle describes both behaviors: an engine running backward will result in a refrigerator. The efficiency of a thermal machine depends on what one wants to achieve. In an engine, we take heat from a hot reservoir to produce work, then the ratio *what you want to achieve/what you need to supply* is given by:

$$\eta = \frac{-W}{Q_1} = \frac{Q_1 + Q_2}{Q_1} = 1 + \frac{Q_2}{Q_1} \quad (2.9)$$

Note that, because it is an engine as defined before, Q_2 in the figure is *negative*, so efficiency takes values between 0 and 1. For a refrigerator, the quantity that measures the efficiency is called COP (coefficient of performance). If one wants to make a machine that cools down a cold reservoir then

$$COP = \frac{Q_2}{W} = \frac{Q_2}{Q_1 + Q_2} \quad (2.10)$$

Chapter 3

Working substance

General properties of QHEs have been discussed in this work in [chapter 2](#). A more general and detailed discussion can be found in references [\[1, 2, 4, 5\]](#). In particular, it is important to discuss the properties that the chosen substance of work has, as this will define what kind of MCE is found and also what kind of thermal machine we are dealing with. Our working substance consists of a quantum dot electronic trap, in addition to an antidot and an Aharonov-Bohm flux. In this chapter, we describe separately these systems and some of their properties. Finally, we give a description of the whole system based on the solution of Bogachev-Landman [\[11\]](#).

There is currently a strong interest in nanotechnology. Much of this is because many materials change their properties on a very small scale. Some interesting aspects of small-scale structures are[\[12\]](#):

- (a) Number of possible vibration or electronic states is drastically reduced with respect to infinite solids. As a consequence, the continuum of allowed energy states in a macroscopic solid is turned into a few discrete levels. This effect is known as **quantum confinement**.
- (b) Small objects necessarily have a large surface area. This is, a larger ratio of surface area to volume than macroscopic objects. Atoms on the surface find themselves in a different environment from those on that of the bulk atoms and thus have different properties.
- (c) Ferromagnetic ordering in a particle is affected by the structure size. For very small particles, the magnetization of the particle can be rotated by thermal fluctuations at lower temperatures.

3.1 Quantum dot

A *quantum dot* (QD) is a semiconductor cluster with a radius of less than $\approx 100nm$. It is often described as a 0-dimensional structure, as it confines electrons in all 3 space directions. For this reason, possible energies of electrons are quantized, just as the quantization of real-life atoms.

Electrons can be effectively confined in two dimensions by incorporating a flat layer of semiconductor material between two layers of another semiconductor. The differences in the band structure between these layers create a binding effect on the electrons, resulting in their confinement within the two-dimensional space. From this configuration, Lithography techniques, for instance, are often utilized to restrict the remaining two dimensions of electron movement. By carefully patterning the semiconductor layers, the electrons can be confined in every direction, thus achieving confinement in all three dimensions.

The first quantum dot was proposed and done in 1986 by M.A. Reed [13], who reported the creation of a square QD with a side length of 250nm. More advanced techniques allow the construction of smaller QDs of $\approx 1nm$ [14]. Nowadays, QDs are made with such precision that some call them artificial atoms, as their confinement properties resemble that of atomic levels with the advantage that it is controllable experimentally.

To give a theoretical description, an effective mass approximation is made to consider the effects of crystalline structure over electrons. Also one assumes that there is a strong binding in the z direction. This allows us to represent the system as a periodic potential over a plane array. This results in solving the eigenfunctions for the Fock-Darwin Hamiltonian for a symmetric gauge $\mathbf{A} = B/2(-y, x, 0)$ [15]:

$$H = \frac{1}{2m^*}(\mathbf{p} + e\mathbf{A})^2 + \frac{1}{2}m^*\omega_0^2 r^2 \quad (3.1)$$

characterized by the length $l_{dot} = \sqrt{\hbar/m^*\omega_0}$. Its corresponding energy eigenvalues are

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

where $n = 0, 1, \dots$ and $m = -n, -n+2, \dots, n$. Effective frequency is defined $\Omega = \sqrt{\omega_0^2 + \omega_c^2/4}$.

3.2 Quantum antidot

Fundamentally, a *quantum antidot* (QAD) is the opposite of a quantum dot. It describes forbidden regions of two-dimensional electron systems. While the quantum dot system is described as an effective attractive potential, antidot is proposed as a repulsive potential. In this work we use

$$U_{AD} = \frac{\mathcal{A}}{r^2} \quad (3.3)$$

One thing to note is that this potential on its own does not confine electrons. In the presence of an external magnetic field, bound states appear due to Landau levels quantization. We generally add a uniform magnetic field $\mathbf{B} = \text{const}$ for this purpose. When adding a QD and a QAD together, we have an additional controlling parameter: confinement and a repulsive potential both acting on the same system and thus changing both electronic properties and energy spectrum.

3.3 Aharonov Bohm effect

We know that electrodynamical systems are (classically) described by Maxwell equations. These equations are written in terms of electric and magnetic fields, and electromagnetic potentials are introduced as a convenient mathematical aid for calculating fields. On the other hand, the quantum mechanical description of a system requires canonical formalisms, so it contains explicit dependence on these potentials. The *Aharonov-Bohm* effect describes the physical consequences of the electromagnetic potentials in the behavior of quantum systems.

3.3.1 Statement of the problem

Consider an very large cylindrical solenoid of radius R . When you let current pass through an infinite solenoid, a constant magnetic field passes through the center as a consequence and no magnetic field appears on the outside. In cylindrical coordinates,

$$\mathbf{B} = \begin{cases} B\hat{\mathbf{z}} & r \leq R \\ 0 & r > R \end{cases} \quad (3.4)$$

For the region inside the solenoid ($r \leq R$), the magnetic field only has $\hat{z}$ component so vector field $\mathbf{A}$ must have only an azimuthal coordinate, i.e $\mathbf{A} = A\hat{\phi}$. We can use Stokes' theorem

$$\oint_{\partial S} \mathbf{A} \cdot d\mathbf{l} = \int_S \mathbf{B} \cdot d\mathbf{a} = \Phi(r) \quad (3.5)$$

Where S is the circumference of radius r centered at the symmetry axis of the solenoid, so line integral on equation (3.5) yields

$$\Phi = A \cdot 2\pi r \implies A = \frac{\Phi}{2\pi r} \quad (3.6)$$

Outside the solenoid ($r > R$), Φ represents the total magnetic flux through the loop. Because of the continuity of the vector field, again it has only an azimuthal component at every point in space.

Now, the electromagnetic Hamiltonian of an electron is given by (in CGS units):

$$H = \frac{1}{2m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + qV \quad (3.7)$$

Where $\mathbf{p} = m\mathbf{v} + \frac{e}{c} \mathbf{A}$ is the canonical momentum.

3.3.2 Energy levels and its dependence on flux

Consider a system that has only the Aharonov-Bohm flux. This allows us to take $V = 0$ and $\mathbf{A} = A_\phi$ as in equation (3.6). Then Hamiltonian may be written as:

$$\begin{aligned} H &= \frac{1}{2m} \left(-\frac{i\hbar}{r} \partial_\phi - \frac{e}{c} A_\phi \right)^2 \\ &= \frac{1}{2mr^2} \left(-i\hbar \partial_\phi - \frac{e}{c} \frac{\Phi}{2\pi} \right)^2 \end{aligned} \quad (3.8)$$

using $\psi = \frac{1}{\sqrt{2\pi r}} e^{in\phi}$ results in energy levels given by

$$E_n = \frac{\hbar^2}{2mr^2} \left(n - \frac{\Phi}{\Phi_0} \right)^2 \quad (3.9)$$

where $n = 0, 1, 2, \dots$ and $\Phi_0 = 2\pi\hbar c/e$ is the quantum of flux. Even when is natural from the classical perspective to conclude that physical behavior, and

consequently observables, remain invariant, quantum formulation shows an explicit dependence of the energy levels and wave functions on Aharonov-Bohm flux *even when the particle is in a region with $\mathbf{B} = 0$* . This was discovered by Aharonov and Bohm [16] in 1959, where they show that vector potential *can* affect the quantum behavior of a charged particle moving in space with no electromagnetic field.

3.4 Description of the working substance

To make a cycle, we use the model proposed and solved by Bogachev and Landmann [11] of a spinless electron in the presence of a quantum antidot in addition to a quantum dot and an Aharonov-Bohm flux. As before, repulsive potential is modeled as $qV(r) = \mathcal{A}r^{-2}$, where the constant $\mathcal{A}$ is related to chemical potential μ and to the antidot radius r_0 by equation

$$\mu = \frac{\mathcal{A}}{r_0^2} \quad (3.10)$$

The vector potential can be written as $\mathbf{A} = \mathbf{A}_1 + \mathbf{A}_2$ where $\mathbf{A}_1$ corresponds to external magnetic field $\mathbf{B}_{ext} = \nabla \times \mathbf{A}_1 = B\hat{\mathbf{z}}$ and $\mathbf{A}_2$ describes the additional contribution of magnetic Aharonov-Bohm flux inside the solenoid Φ_{AB} . This system's Hamiltonian is

$$H = \frac{1}{2m^*} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + \frac{\mathcal{A}}{r^2} \quad (3.11)$$

And its energy levels are given by [17]:

$$E_{nm} = \hbar\omega_B \left[n + \frac{[(m + \alpha)^2 + a^2]^2 + (m + \alpha) + 1}{2} \right] \quad (3.12)$$

where $\omega_B = eB/m^*$ is the cyclotron frequency, e is the electron charge and m^* is the effective mass. Also, we define the constant $a^2 = 2m^*\mathcal{A}/\hbar^2 = 2m^*\mu r_0^2/\hbar^2$ and $\alpha = \Phi_{AB}/\Phi_0$ where $\Phi_0 = h/2e$ is the magnetic flux quantum. If we include in addition a parabolic confining potential of the form

$$U = \frac{1}{2}m^*\omega_0^2 r^2 \quad (3.13)$$

energy levels become

$$E_{nm}^{ad} = \hbar\Omega \left[2n + \sqrt{(m + \alpha)^2 + a^2} + 1 \right] + \frac{1}{2}\hbar\omega_B(m + \alpha), \quad (3.14)$$

where $\Omega = \omega_0 \left[1 + \left(\frac{\omega_B}{2\omega_0} \right)^2 \right]^{1/2}$. This last equation is what we will use to model the quantum antidot system. An important thing to note is that when $\alpha \in \mathbb{N}$, the partition function will be the same as in case $\alpha = 0$. Then we have an oscillatory behavior of MCE in this case: $Z(\alpha = n) = Z(\alpha = n + 1)$. This allows us to take only values in the range $\alpha \in [0, 1]$.

Chapter 4

Results

4.1 Thermodynamical Quantities

Thermodynamical quantities are calculated using partition function. Summation on quantum number n is straightforward, but we do not have an analytic solution for summation on m . Partition function then has the following form:

$$\begin{aligned} Z^{ad} &= \sum_n \sum_m e^{-\beta E_{nm}^{ad}} \\ &= \frac{1}{2} \operatorname{csch}(\beta \hbar \Omega) \sum_m \exp \left(-\beta \hbar \left[\Omega \sqrt{(m + \alpha)^2 + a^2} \right] - \frac{\beta \hbar \omega_B}{2} (m + \alpha) \right) \end{aligned} \quad (4.1)$$

Where sum goes over $n = 0, 1, 2, \dots$ and $m = 0, \pm 1, \pm 2, \dots$. From partition function, all thermodynamic quantities can be calculated. We will list now thermodynamical quantities that will be used in the analysis. A detailed

derivation of these quantities is made in Appendix A.

$$U = kT^2 \left(\frac{\partial \ln Z}{\partial T} \right)_B \quad (4.2)$$

$$S = kT \left(\frac{\partial \ln Z}{\partial T} \right)_B + k \ln Z \quad (4.3)$$

$$\Delta S_{isothermal} = \int_{B_0}^{B_f} \left(\frac{\partial M}{\partial T} \right)_B dB \quad (4.4)$$

$$\Delta T_{adiabatic} = - \int_{B_0}^{B_f} \frac{T}{C_B} \left(\frac{\partial S}{\partial B} \right)_T dB \quad (4.5)$$

$$M = kT \left(\frac{\partial \ln Z}{\partial B} \right)_T \quad (4.6)$$

4.2 Cycle construction

MCE has been widely studied using these quantities [17]. Magnetic Otto engine has been made for an electron trapped in a quantum dot [6]. We would like to see how the engine behavior changes when Antidot and Aharonov-Bohm flux is added. As mentioned, there is no analytic solution for partition function Z^{ad} so numerical methods were used here. For the confining potential, we used a frequency $\omega_0 = 4.4 \cdot 10^{12} Hz$ which means an energy of $\hbar\omega_0 \approx 2.896 meV$. We took m to be in the range $m = -300 \rightarrow 300$.

We would like to construct an Otto engine using both Aharonov Bohm and antidot effects. In terms of the MCE, interesting zones (quantum effects) are at small values of the quantum antidot radius (according to literature, $a < 5$). On the other hand, as we mentioned, AB-flux can be taken to be in the values $0 \leq \alpha < 1$. In what follows, temperature and magnetic field are presented in canonical units, while work output is given in meV. A more detailed discussion is given in appendix B.

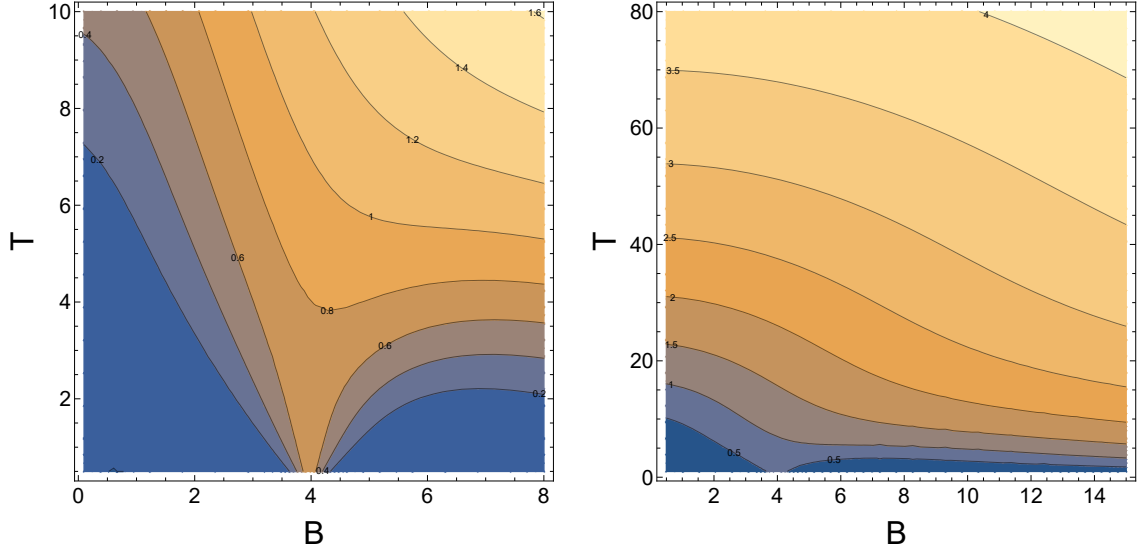


Figure 4.1: Adiabatic level surfaces with $a = \alpha = 0.1$.

We see that in comparison with a (spinless) quantum dot in which only an inverse MCE is present [6], a direct MCE appears at low temperatures, approximately in the range $4 < B < 6$. This will be very important in the construction of the cycle because it depends on how our machine will behave. By choosing an isentropic line ($S = S_0$) in the former graph, we can obtain the first process $A \rightarrow B$. We now choose to work only at zones where there is an inverse MCE, that is: going from a high value of the magnetic field to a low value heats up the system.

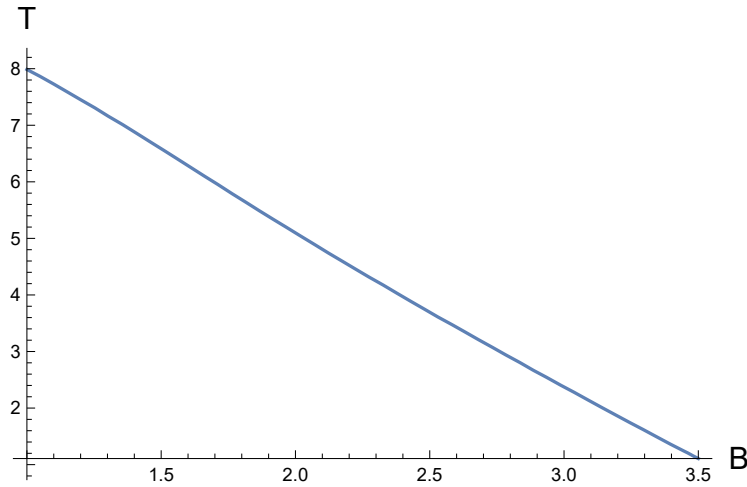


Figure 4.2: On the graph the case of $\alpha = a = 0.1$ as before. We can see how temperature (Kelvin) behaves with respect to the external magnetic field (Tesla) for an entropy value of $S/k = 0.4$.

To use the adiabat chosen in figure 4.2, a low-temperature heat bath must correspond to high magnetic field values. At the start of the adiabatic process ($B = B_h = 3.5\text{T}$) the system is in equilibrium with the low-temperature reservoir, so we set $T_l \approx 1.1\text{K}$ to agree with our T vs B curve.

At the end of the adiabatic $A \rightarrow B$, the system is put in contact with a hot reservoir, so this reservoir has to be chosen to have a temperature higher than the higher achieved by the MCE, this is $T(B_l^{min}) \approx 8\text{K}$. We don't want to get the temperature of the system too high because quantum effects might be lost. For this purpose, we set $T_h = 10\text{K}$. Now that we have set the values for low and high-temperature heat reservoirs, we leave B_h fixed and vary the low magnetic field value B_l . This will allow us to compute work and efficiency of a continuum of different otto cycles between these two reservoirs.

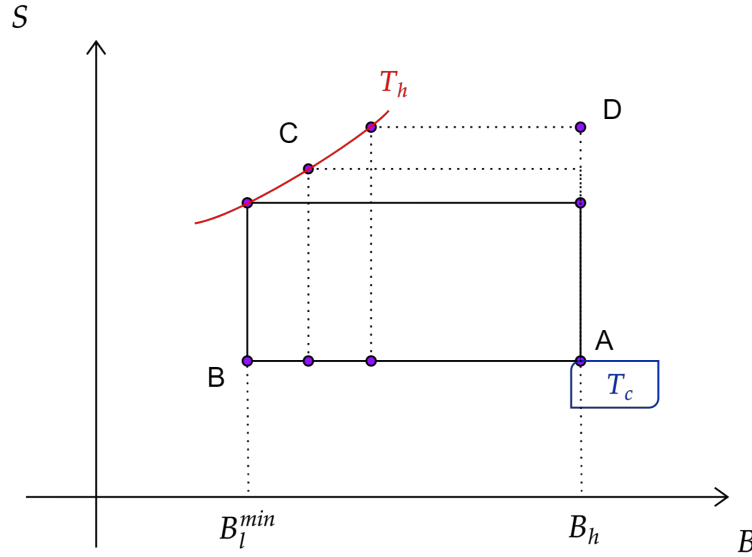


Figure 4.3: Schematic procedure of varying low magnetic field value. Point A is now the only point fixed in the cycle.

In figure 4.3 we can see a schematic explanation of what we are calculating. When we fix T_h, T_l and let B_l take values between $B_l^{min} < B_l < B_h$ we get an (infinite) set of cycles. Point A is fixed by fixing B_h, T_l . Point B is obtained by imposing the adiabatic condition as a function of B_l . In a similar way, point C is obtained as a function of B_l, T_h . This way, point C always lies in the $T \equiv T_h$ isotherm. Finally, point D is obtained through C by the adiabatic condition again. Under this procedure we've made different cycles for different values of

a, α as shown in the figure below:

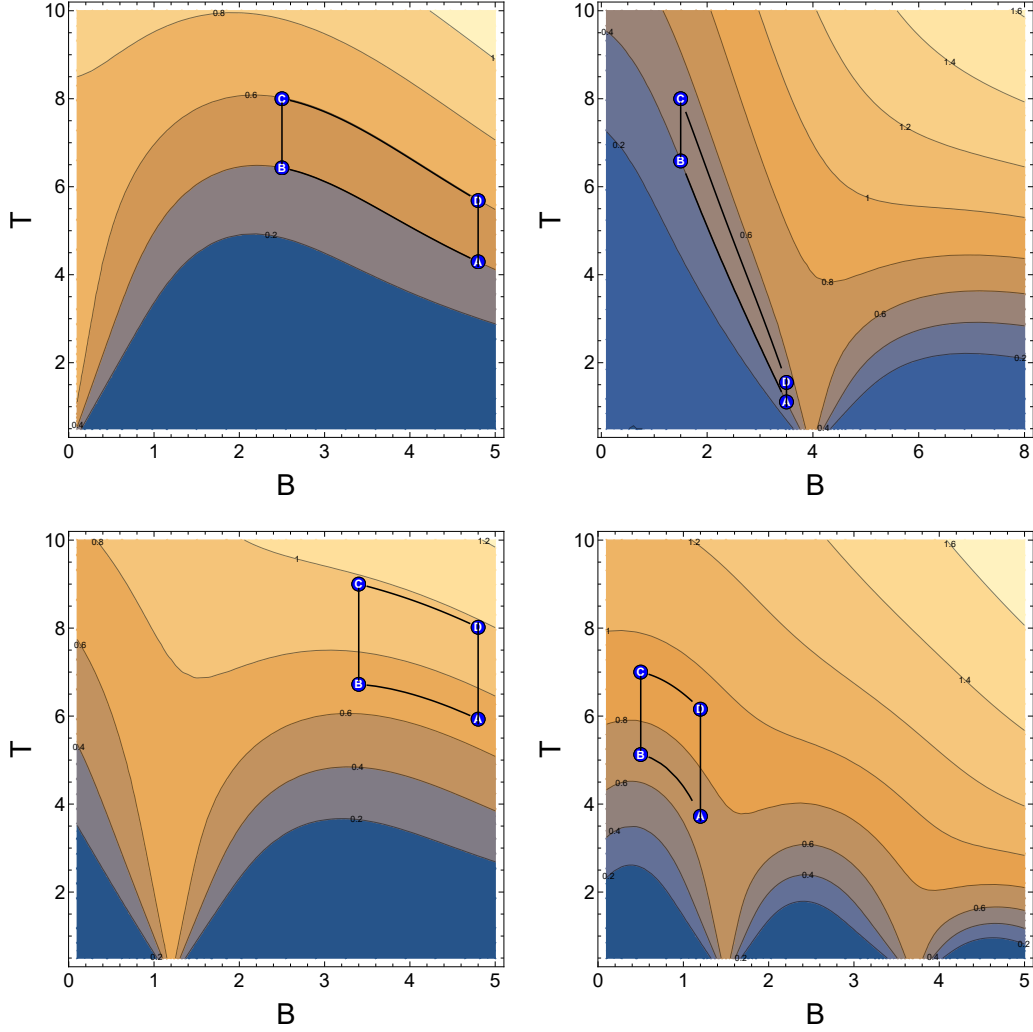


Figure 4.4: Cycles drawn in the entropy level curves. Point B has been chosen to be in the minimum value of the low magnetic field value. Values of (α, a) are the following: *Top left:* Cycle $\mathcal{A} \rightarrow (0.5, 0.2)$. *Top right:* Cycle $\mathcal{B} \rightarrow (0.1, 0.1)$. *Bottom left:* Cycle $\mathcal{C} \rightarrow (0.3, 0.3)$. *Bottom right:* Cycle $\mathcal{D} \rightarrow (0.8, 1.5)$.

Values of B_l are changed between values shown from point B up to point A in the figure. Doing this moves *every point in the cycle* except A which is fixed.

Cycle	(α, a)	High reservoir T_h (K)	Low reservoir T_l (K)	B_h (T)	B_l^{min} (T)
$\mathcal{A}$	(0.5, 0.2)	8	4.29	4.8	2.5
$\mathcal{B}$	(0.1, 0.1)	8	1.11	3.5	1.5
$\mathcal{C}$	(0.3, 0.3)	9	5.93	4.8	3.4
$\mathcal{D}$	(0.8, 1.5)	7	3.72	1.2	0.5

4.3 Results

Quasistatically, analyzing how magnetization behaves with respect to the magnetic field is important to obtain the sign of the work obtained, and thus to define what kind of machine we get. For example, taking the first cycle, magnetization as a function of the magnetic field provided by equation (4.6) is plotted below.

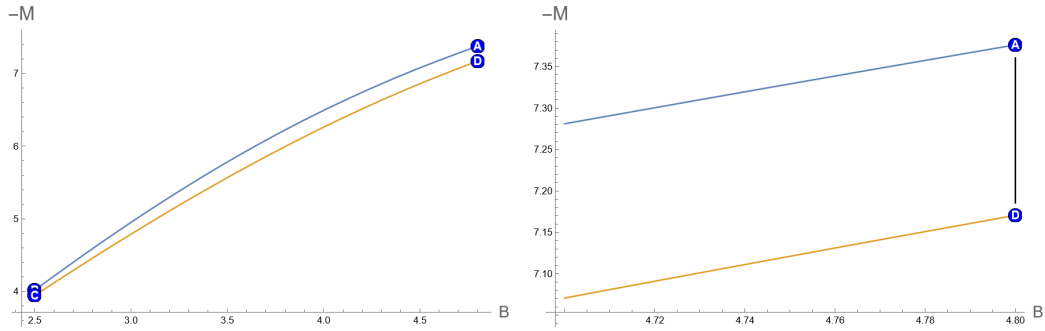


Figure 4.5: Magnetization as a function of external magnetic field for cycle $\mathcal{A}$. Note that magnetization $A \rightarrow B$ is greater at any point than $C \rightarrow D$. *Left:* Cycle drawn on the magnetization curve. *Right:* A zoom into the curve close to see more clearly the difference between the curves.

Since work is defined as equation (2.2), figure 4.5 shows that cycles on an inverse Magnetocaloric effect have a negative net work. This is in accordance with the fact that the quantity $Q_{in} + Q_{out} = -W$ is *positive* when calculated as the difference on internal energy (2.3),(2.5). This means the cycle works as an *engine*, as in every case we have work extracted from the system ($W < 0$), and heat flow from the heat reservoir to the system ($Q_{in} > 0$) and from the system to the cold reservoir ($Q_{out} < 0$).

The net work of the quasistatic cycle is calculated with equations (2.2),(2.4). Then, the total work *extracted from the system* is $W_{tot} = -(W_{AB} + W_{CD}) = Q_{in} + Q_{out}$. Quantum work extracted can be calculated also as $W_{tot}^q = Q_{in}^q + Q_{out}^q$ as equation (2.8). A comparison between these quantities is given in the figure below,

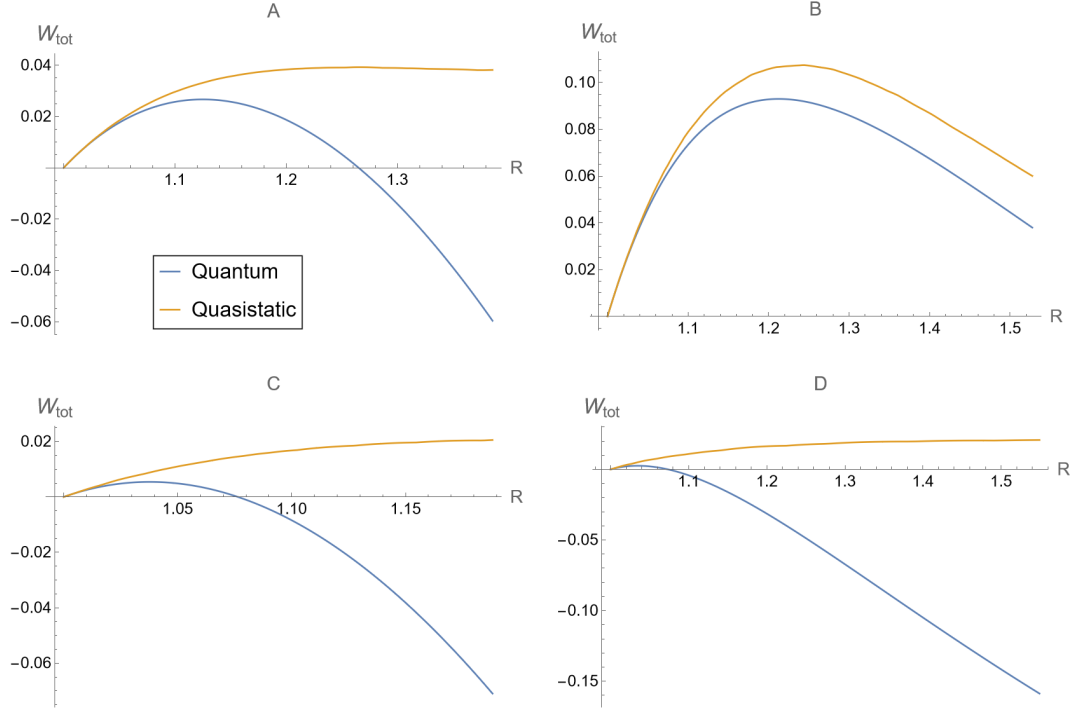


Figure 4.6: Quantum and quasistatic net work extracted from the system as a function of $R(B_l) = \sqrt{B_h/B_l}$ for every cycle $\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}$. In every case, we see that quasistatic net work is greater than quantum.

We can see that for low values of $R(B_l)$ (or equivalently $B_l \approx B_h$) quantum and quasistatic work are almost the same. On higher values of R differences become more evident. From the quantum net work curve, we see that the regime of validity of the cycle defined as we did is only insured for values of R such that $W_{\text{tot}}^q \geq 0$, as from quasistatic formulation there is no transition to negative values. Even though it could be of theoretical interest to analyze the cycle in the regime where $W_{\text{tot}}^q < 0$, to compare the cycles here quantum cycle has to be redefined, and it is out of the scope of this work.

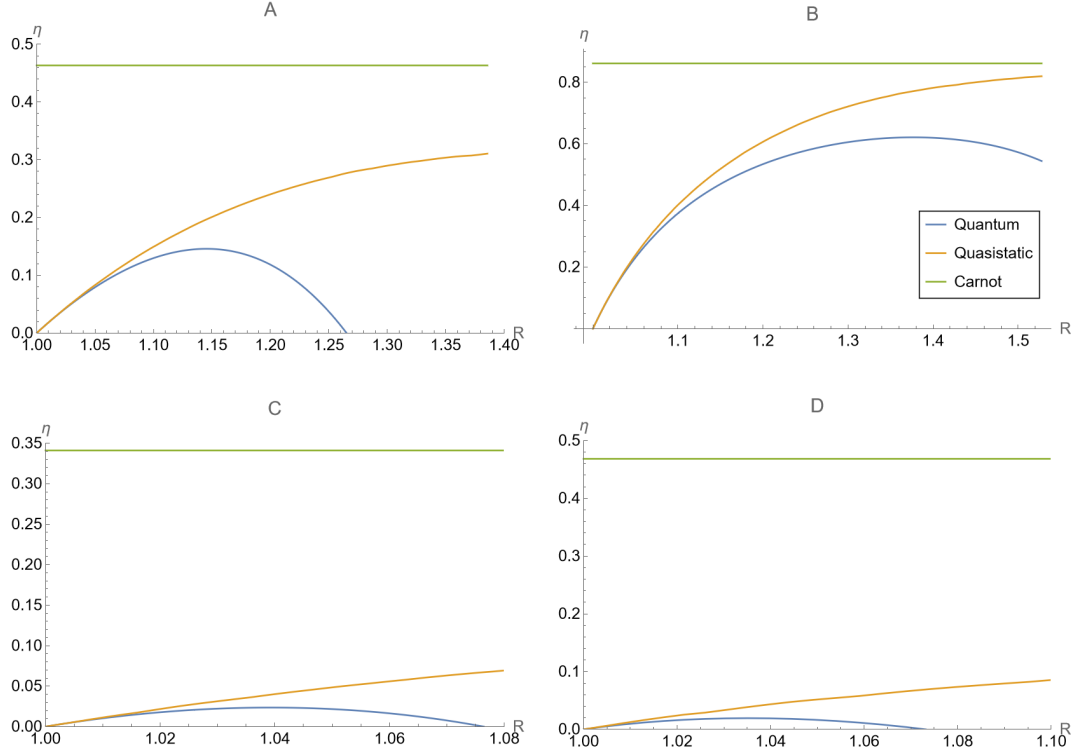


Figure 4.7: Quantum and quasistatic efficiency for every cycle. As mentioned, the validity of the quantum cycle is only for $\eta > 0$. Also plotted in green the Carnot efficiency defined as $\eta_{carnot} = 1 - \frac{T_l}{T_h}$.

Efficiency for both quasistatic and quantum formulation is calculated using equation (2.9). In every case, quasistatic efficiency is greater than quantum efficiency. In reference [18], it has been discussed that quantum and quasistatic efficiency will be the same when temperature relates linearly to the magnetic field: $T = CB$. In the same manner, we see that cycle $\mathcal{A}$ and especially cycle $\mathcal{B}$ show almost a linear behavior in figure 4.4. Then it is not surprising to see that quantum and quasistatic cycles behave similarly. In addition, these two cycles show efficiencies much closer to Carnot's, which is our limit imposed by the second law of thermodynamics.

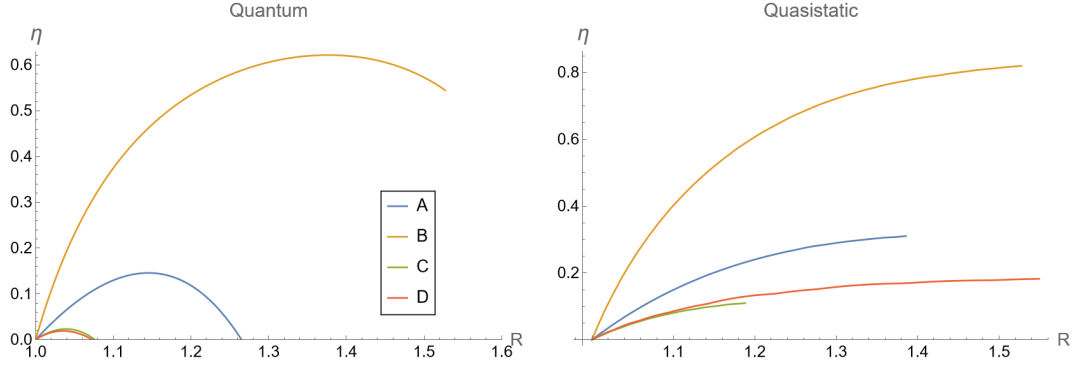


Figure 4.8: Quantum efficiency comparison for every cycle in terms of R .

We can see in the figure that cycles $\mathcal{A}, \mathcal{B}$ have validity in a much broader range of magnetic field values. Cycles $\mathcal{C}, \mathcal{D}$ are valid upon $R \approx 1.1$ while in the figure we see that cycle $\mathcal{B}$ is valid at least up to $R = 1.6$, but since we have not calculated the cycle further we could expect to lower even more the low magnetic field value B_l .

4.3.1 Change on the high-temperature reservoir

In deciding the high-temperature reservoir value, one makes a somewhat arbitrary decision. To illustrate how this parameter affects the cycle, we vary its value in cycle $\mathcal{B}$, which is the most efficient cycle as mentioned before.

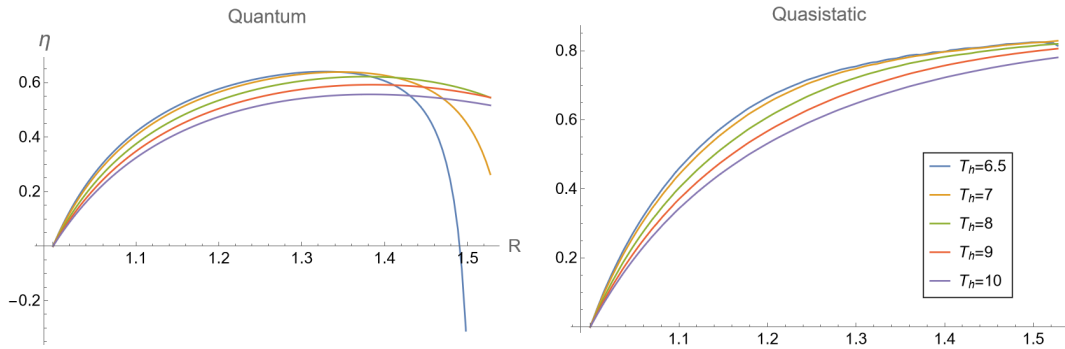


Figure 4.9: Quantum and quasistatic efficiencies in the left and right figure respectively. The inset has the temperature listed with its corresponding color in the graph.

We can see that lower temperatures of the hot reservoir do a "smaller cycle". This results in better quasistatic efficiency for every value of R . One thing to

have in mind is that the cycle has an upper bound of R , which corresponds to the value where the temperature at point B is exactly T_h . For higher values of R , temperature $T(B)$ will be higher than T_h . This is not convenient, as higher temperatures than the hot reservoir in the adiabatic stroke would mean that the reservoir acts as a *cold reservoir* when connected to the system in the isochoric process.

For quantum efficiency, we have also a more efficient cycle for lower temperatures for low values of R . We see in figure 4.9 that efficiency for the lower temperature reservoirs has a lower range of validity, and becomes less efficient at high values of R . For example, at $T_h = 6.5$ the cycle has the higher quantum efficiency, and from $R \approx 1.4$ it quickly falls and becomes the less efficient cycle.

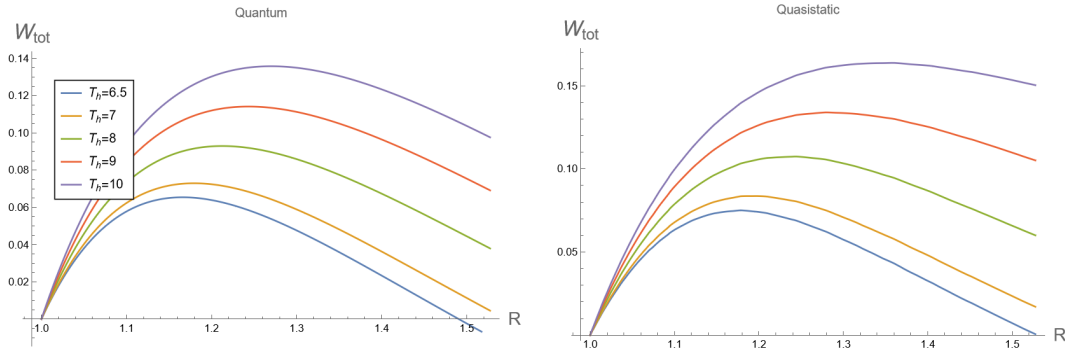


Figure 4.10: Total work extracted from the cycle for quantum and quasistatic cycle. Again, the inset shows the same temperatures calculated before.

Even though lower temperatures on the high reservoir do more efficient cycles, this is in exchange for a lower extracted work. But one has to take into account the fact that quasistatic formulation is an ideal cycle where every point is in equilibrium. Real thermal machines may have losses due to repetition of the cycle, so not only efficiency but net work produced has to be considered.

4.3.2 Direct MCE cycle

Because of the change in the behavior of adiabatic curve levels on 4.4, we can make a cycle either on the inverse (already discussed) or direct MCE zone.

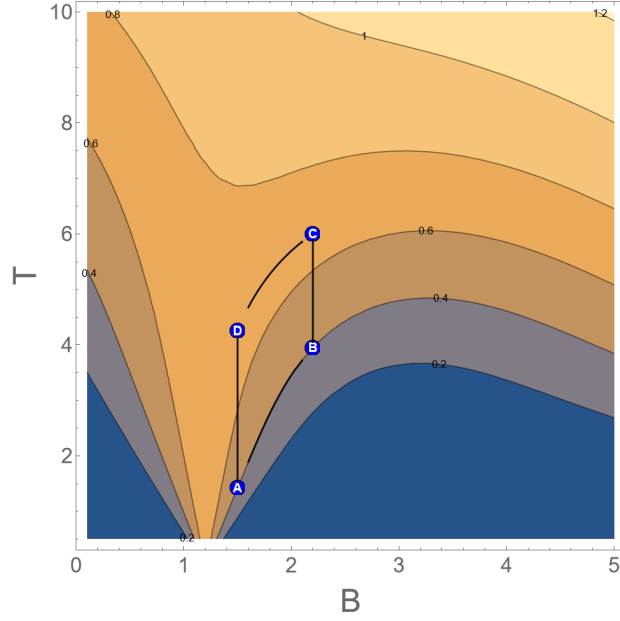


Figure 4.11: Cycle constructed for $\alpha = a = 0.3$ in a direct MCE zone.

Direct MCE on adiabatic strokes only occurs on low-temperature values and in specific values of the magnetic field. For example, for $\alpha = a = 0.1$ this occurs approximately in the range $1 < B < 3$. Construction of this cycle works similarly: we choose point A and set it to be in thermal equilibrium with the cold reservoir. Then our adjustment parameter is the high magnetic field value B_h . Defining $R = \sqrt{B_h/B_l}$ as before, we can plot the work extracted and the efficiency of the cycle.

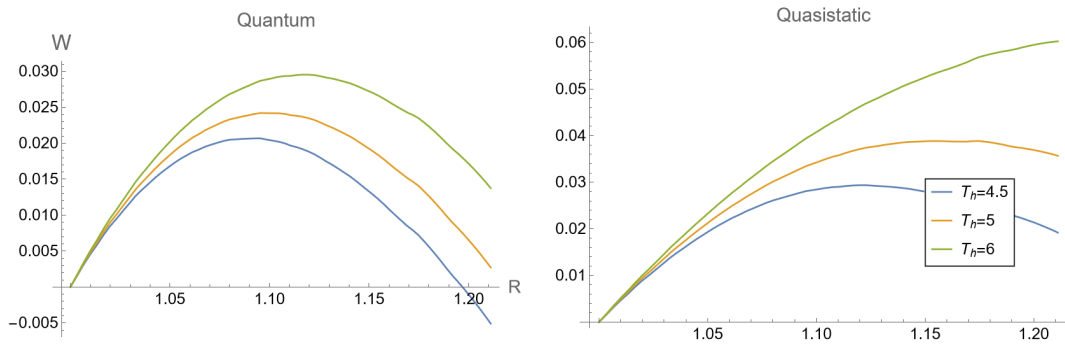


Figure 4.12: Quantum and quasistatic work extracted from the cycle for different values of the hot reservoir. Again, more work is found as we set the hot temperature higher.

We obtain *positive extracted work*, which means that in this regime, the

cycle behaves as an engine as well. In terms of the quasistatic definition of work $dW = -MdB$ again this makes no contradiction. Take for example curves in figure 4.4. The first figure (cycle $\mathcal{A}$) has only one transition.

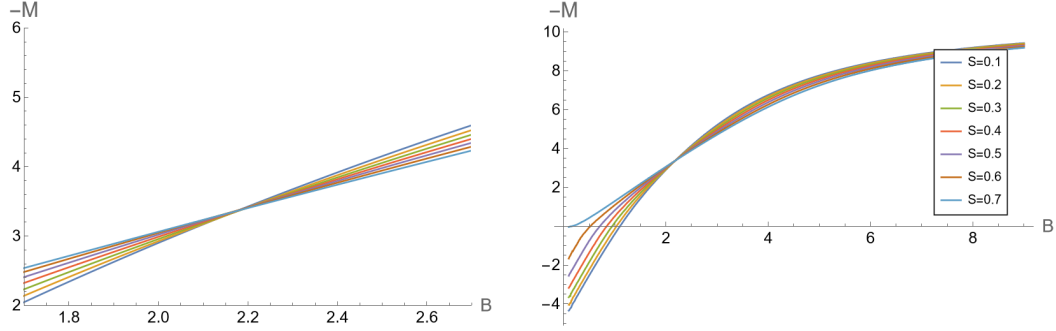


Figure 4.13: Magnetization for different values of entropy. The Left and right graphics are the same systems, but the left is a zoom-in into the critical point.

The critical point in figure 4.4 occurs at $B \approx 2.2$. When plotting the magnetization we see that this point results in the magnetization curves crossing, thus resulting in positive extracted work for either inverse or direct MCE. This can be demonstrated using values of internal energy U^1 . This also results in a positive work extracted from a quantum formulation on either zone. Efficiency is again calculated as equations (4.7)(4.8).

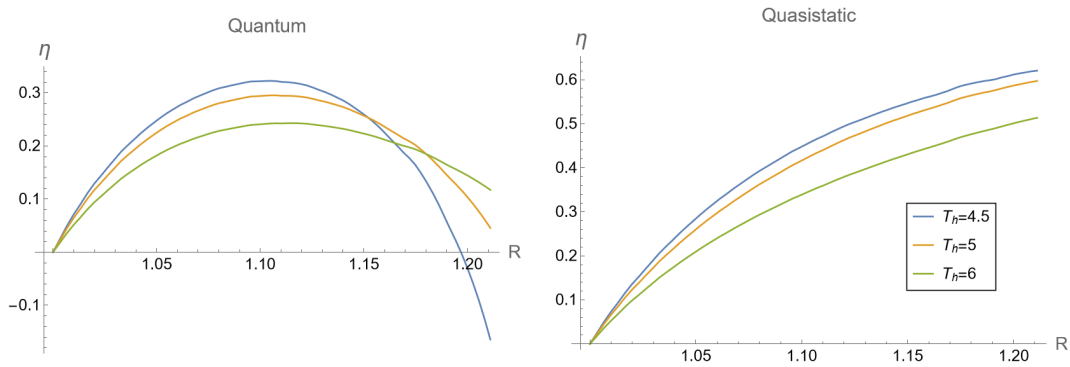


Figure 4.14: Quantum and quasistatic work extracted from the cycle for different values of the hot reservoir. Again, more work is found as we set the hot temperature higher.

Again, similar behavior is found: lower hot reservoir results in higher

¹In fact remember that work and heat are calculated using equations from section 2.2 and never using magnetization directly.

efficiency in exchange for a lower value of work extracted.

Chapter 5

Conclusions

The addition of AB-flux and AD potential produces a change in the MCE of the system. AD results in points at $T = 0$ where inverse and direct MCE converge to a certain value of external magnetic field (see figure 4.4). By setting higher values of a (more AD potential) more of these points appear. On the other hand, AB-flux also makes these points appear, but it is important to notice the periodic behavior of α values, as augmenting its value produces cyclic changes on the MCE. Using the fact that both inverse and direct MCE are found, an Otto engine can be made on either zone. This could be useful as it gives additional freedom when constructing the QOE.

A comparison between quasistatic and quantum formulation shows that quasistatic is more efficient and gives more amount of work in every case. This was both expected and already proven. However, it is crucial to acknowledge that the quasistatic engine presented here represents a theoretical limit, assuming infinite time cycles with thermodynamic equilibrium at each point. Therefore, while the quasistatic Otto engine serves as a useful benchmark, it is essential to consider its practical limitations

It is interesting to notice the asymptotic behavior of the efficiency curve as R grows (fig. 4.7). Even though cycle $\mathcal{B}$ shows a higher efficiency for higher values of R , one must notice that work output tends to 0. So not only the efficiency of the cycle has to be taken into account but also finding an equilibrium point where both efficiency and work output are maximized if one wants to scope for potential practical applications. In this regard, cycle $\mathcal{A}$ shows a better response in the limit of high values of R , as work output tends to a constant value. On the other hand, quantum work output achieves a maximum value in every

case and then tends to negative values. As we were interested in evaluating the engine performance, negative work output (or work input) was discarded, but as a scope for future works, it would be interesting to evaluate what this negative work output means in the context of machine functioning, what its causes are and how could it be taken advantage of.

Cycle $\mathcal{B}$ shows significantly higher efficiency, being the closest to Carnot efficiency of all cycles evaluated, and higher work output (fig. 4.6). This might be attributed to the linear behavior of temperature as a function of the external magnetic field as well as its high slope: small changes in the magnetic field results in great changes in temperature. It is not a coincidence then that this is also the closest the quantum efficiency gets to quasistatic, as quantum efficiency tends to quasistatic efficiency in zones where MCE is linear [18].

We examined the influence of altering the high-temperature reservoir (T_h) on the cycle, observing that decreasing the temperature (resulting in smaller cycles) leads to higher quasistatic efficiency. Again, do not forget this gain in efficiency comes at the cost of reduced work output, necessitating multiple cycles to achieve the same work. In real engine design, these ideal cycles must be carefully considered, as energy losses resulting from cycle repetition could render the slight efficiency gain negligible. Additionally, future investigations could explore alternative models beyond the quasistatic approach, aiming to uncover potential improvements in quantum efficiency compared to classical cycle formulations.

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Appendix A

Calculation of Thermodynamical Quantities of a MCE

A1 First law of thermodynamics for paramagnetic systems

When matter is influenced by magnetic fields, it generally develops a magnetic moment. A description of this phenomenon and its interaction with thermal properties requires an extensive parameter. We expect that

$$dU = \partial Q + \partial W_M + \partial W_{mag} \quad (\text{A.1})$$

where $\partial W_M = -pdV$ is the usual mechanic work and

$$\partial W_{mag} = PdX \quad (\text{A.2})$$

is magnetic work. In this section, we expect to derive a form of both the extensive parameter X and its corresponding intensive parameter P . We will analyze the contributions to the change of energy made by a change in an external magnetic field, and by magnetization.

Consider a N -particle paramagnetic system. We have two possible states of magnetic moment for each particle: spin up ($E_1 = -mB$) and spin down ($E_2 = mB$). For a single particle system, partition function is given by the expression:

$$z = e^{-\beta E_1} + e^{-\beta E_2} = e^{-\beta mB} + e^{\beta mB} \quad (\text{A.3})$$

so probabilities of eigenstates are $p = \mathcal{P}(E_1) = \frac{1}{z}e^{\beta m B}$, $q = \mathcal{P}(E_2) = \frac{1}{z}e^{-\beta m B}$. Then mean total magnetic moment of the system is given by

$$M = Nm(p - q) = Nm(2p - 1) \tanh \beta m B \quad (\text{A.4})$$

Note that from equation (A.4) we get relations

$$p = 1 - q = \frac{1}{2} + \frac{M}{2mN} \quad (\text{A.5})$$

so that, from the statistical definition of entropy for one subsystem $s = \frac{S}{N} = -k \sum_p p \ln p$.

$$S = Ns = -Nk \left[\left(\frac{1}{2} + \frac{M}{2mN} \right) \ln \left(\frac{1}{2} + \frac{M}{2mN} \right) + \left(\frac{1}{2} - \frac{M}{2mN} \right) \ln \left(\frac{1}{2} - \frac{M}{2mN} \right) \right] \quad (\text{A.6})$$

Finally, note that

$$\ln q - \ln p = \ln \frac{q}{p} = \ln e^{-2\beta m B} = -2\beta m B \quad (\text{A.7})$$

Now we can relate differentials of these quantities, using $\beta = \frac{1}{kT}$:

$$\begin{aligned} dS &= -Nk d[p \ln p + q \ln q] \\ &= -Nk [dp(1 + \ln p) - dp(1 + \ln q)] \\ &= Nk dp [\ln q - \ln p] = -2Nm \frac{B}{T} dp \\ dM &= 2Nm dp \end{aligned}$$

thus $-TdS = BdM$. Now for total internal energy, we use the mean magnetization of the moment, such that $U = -MB$, concluding

$$dU = -BdM - MdB = TdS - MdB \quad (\text{A.8})$$

Identifying $\partial Q = TdS$ we then identify magnetic work $\partial W_{mag} = -MdB$.

A2 Helmholtz free energy

Consider a system of N magnetic dipoles, each having a magnetic moment $\boldsymbol{\mu}$ [19]. We may add an external magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$. The energy of each dipole is given by:

$$E_i = -\boldsymbol{\mu}_i \cdot \mathbf{B} = -\mu B \cos \theta \quad (\text{A.9})$$

then partition function for each particle is given by

$$z = \sum_i e^{E_i} = \sum_{\theta} e^{\beta \mu B \cos \theta} \quad (\text{A.10})$$

Then, total partition function is given by $Z = z^N$ because every subsystem is independent. Mean magnetic moment will have a tendency to align with $\hat{\mathbf{z}}$ direction (of the field). Its magnitude can be calculated as

$$\begin{aligned} M &= N \langle \mu \cos \theta \rangle \\ &= N \frac{\sum_{\theta} \mu \cos \theta e^{\beta \mu B \cos \theta}}{\sum_{\theta} e^{\beta \mu B \cos \theta}} \\ &= \frac{N}{\beta} \left(\frac{\partial \ln z}{\partial B} \right)_T \\ &= kT \left(\frac{\partial \ln Z}{\partial B} \right)_T = - \left(\frac{\partial F}{\partial B} \right)_T \end{aligned}$$

So we can characterize Helmholtz free energy as a function of T, B , i.e. $F \equiv F(B, T) = -kT \ln Z$. From this function, we derive thermodynamic quantities

$$dF = -MdB - SdT \quad (\text{A.11})$$

from which we deduce maxwell equations:

$$\left(\frac{\partial M}{\partial T} \right)_B = \left(\frac{\partial S}{\partial B} \right)_T \quad (\text{A.12})$$

And an expression for the entropy of the system

$$S = - \left(\frac{\partial F}{\partial T} \right)_B = kT \left(\frac{\partial \ln Z}{\partial T} \right)_B + k \ln Z \quad (\text{A.13})$$

Then an isothermal change in entropy is given by integrating the former

equation.

$$\Delta S_{isothermal} = \int_{B_0}^{B_f} \left(\frac{\partial S}{\partial B} \right)_T dB = \int_{B_0}^{B_f} \left(\frac{\partial M}{\partial T} \right)_B dB \quad (\text{A.14})$$

Now, consider $S \equiv S(B, T)$ so that

$$dS = \left(\frac{\partial S}{\partial B} \right)_T dB + \left(\frac{\partial S}{\partial T} \right)_B dT \quad (\text{A.15})$$

so that an adiabatic change of temperature ($dS = 0$) is given by

$$\Delta T_{adiabatic} = - \int_{B_0}^{B_f} \left[\left(\frac{\partial S}{\partial T} \right)_B \right]^{-1} \left(\frac{\partial S}{\partial B} \right)_T dB = - \int_{B_0}^{B_f} \frac{T}{C_B} \left(\frac{\partial S}{\partial B} \right)_T dB \quad (\text{A.16})$$

where C_B is heat capacity at constant B field for definition. On the other hand, we will need to calculate internal energy U as

$$\begin{aligned} U &= N \langle E \rangle = N \langle -\mu B \cos \theta \rangle \\ &= N \frac{\sum_{\theta} -\mu B \cos \theta e^{\beta \mu B \cos \theta}}{\sum_{\theta} e^{\beta \mu B \cos \theta}} \\ &= -N \frac{\partial}{\partial \beta} \ln z \\ &= - \left(\frac{\partial}{\partial \beta} \right)_B \ln Z \\ &= kT^2 \left(\frac{\partial \ln Z}{\partial T} \right)_B \end{aligned}$$

Also note that using equation (A.13) this agrees with the Legendre transformation between U and F :

$$F = U - TS \quad (\text{A.17})$$

Appendix B

Unit analysis

Here we want to give an explanation of the units used in this work. It was already mentioned in section 4.2 that the quantum dot frequency is given by $\omega_0 = 4.4 \cdot 10^{12} Hz$. In terms of energy, this corresponds to $\hbar\omega_0 \approx 2.896 meV$. The characteristic length of this QD is given by

$$l_{dot} = \sqrt{\frac{\hbar}{m^*\omega_0}} \quad (B.1)$$

for the effective $m^* = 0.067$ associated with GaAs structures. Then we get a characteristic length of the quantum dot used here is $l_{dot} \approx 20 nm$. On the other hand, the external magnetic field used here appears on the cyclotron frequency 3.4. Here canonical units are being used for e (Coulomb) and m^* (kg). Thus, graphics on 4.4 have magnetic field B in Tesla, for example, cycle $\mathcal{C}$ works in the range $3 < B < 5$ Tesla. Finally, work obtained in every graphic derives from ponderations of level energies (quasistatic is obtained from $U = \sum E_n P_n$ and quantum is from equation (2.8) which has the exact same units). Now, occupation probabilities are dimensionless, and energy levels are proportional to $\hbar$ which is represented in meV. Thus, for example, cycle $\mathcal{B}$ which has the greatest work output has about $W = 0.1 meV$ in its peak 4.6.