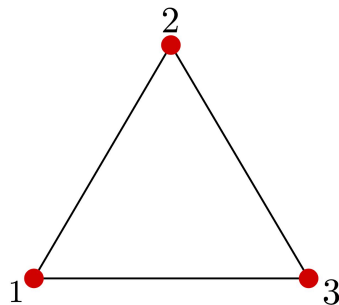


Universidad Técnica Federico Santa María
Departamento de Física

OTTO AND STIRLING ENGINES IN A SYSTEM OF THREE ENTANGLED QUBITS IN A RING TOPOLOGY

BASTIÁN ESTEBAN ALBERTO CASTORENE CASTORENE
ADVISOR PROFESSOR. DR. PATRICIO VARGAS



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Abstract

This study explores the thermodynamic behavior of a system comprising three spin- $\frac{1}{2}$ particles, modeled using a Heisenberg XXX-type arrangement in a ring topology. The system's performance as quantum Stirling, quasistatic Otto, and quantum Otto engines near two Quantum Critical Points (QCPs) is investigated, with an external magnetic field serving as the control parameter. The research focuses on the quantum phase transitions at $B = 0$ and $B = 3J$ in the antiferromagnetic system, examining their impact on engine efficiency through entanglement and spin correlation analyses. Results indicate that the Stirling engine performs optimally at low temperatures, achieving Carnot efficiency at the lower QCP, while the Otto engines are more efficient at higher temperatures, with the quasistatic engine reaching Carnot's efficiency at the higher QCP. The study also reveals a deep interrelationship between information theory and thermodynamics, demonstrating that thermodynamic functions in this tripartite system can be expressed through spin correlations. This highlights the intricate link between quantum information and thermodynamic performance, offering insights into the efficiency of quantum thermodynamic cycles near QCPs.

INTRODUCTION

1.1 ✂ Historical motivation

Richard Feynman pondered the nature of the computational machinery required to simulate physics, particularly the quantum mechanics of many particles [1, 2]. He elucidated that the computational challenges associated with these problems grow exponentially as more particles are introduced, owing to the exponential growth of Hilbert Space dimensions. Consequently, it was inferred that conventional computers would be ill-equipped to keep pace with quantum calculations. Professor Feynman then postulated a groundbreaking concept: Why not harness quantum mechanics to simulate quantum mechanics itself? In other words, why not employ quantum tools to devise a computer capable of simulating processes within this microcosm? This line of thought birthed the concept of quantum computers, bridging the realms of computer science and quantum physics.

Then, a significant development occurred: the affirmation of the EPR theorem, an acronym for the famous paradox formulated by Einstein, Podolsky, and Rosen [3]. The experimental refutation of Bell's inequalities, culminating in the Nobel Prize in Physics in 2022, confirmed the technological feasibility of quantum entanglement [4–6]. This breakthrough sparked a global surge in public interest and competition in these areas, with a notable increase in activity from 2015 to the present [7].

Prominent tech giants such as *Google* and *IBM* started a competitive race to establish quantum computing supremacy. The foundation of this technology hinges on the ability to harness artificial artifacts that exploit quantum properties. In classical computing, information is processed using binary digits, either 0 or 1, known as a *bit*. However, in quantum mechanics, the computational unit is a two-state system in superposition. Upon measurement, this system collapses to one of two distinguishable states, labeled as 0 or 1, defining what is termed a *qubit* short name for *Quantum Bit*. [8–13]

1.1.1 ✂ Quantum Entanglement

What and why is quantum entanglement so important in quantum computing?

Entanglement is a characteristic trait of quantum physics that has no classical counterpart. It is considered counterintuitive and presents a radical departure from classical physics. Erwin Schrodinger believed that entanglement was the defining feature that differentiated quantum theory from classical mechanics [14, 15]. Quantum systems are described by what Schrodinger called 'catalogues of information' (ψ -wavefunctions). These catalogues contain the probabilities for all possible outcomes of the measurements we can make on the system. When two physical systems are entangled, their joint catalogue of information can be better specified than the catalogue of each individual system. This means the whole can be less uncertain than either of its parts, which is impossible in classical physics. Quantum Mechanics permits the superposition of wave-functions without any constraints, even if nature has a preferred basis for distinguishable scenarios. For example, it's possible to place an atom or a qubit in a superposition of its ground and excited states. A state involving two or more quantum systems is termed 'entangled' if it can't be represented as a simple tensor product of the states of its individual systems [16]. Mathematically, an

entangled state $|\psi\rangle^{[12]}$ is defined as:

$$|\psi\rangle^{[12]} \text{ is entangled if } \Leftrightarrow |\psi\rangle^{[12]} \neq |\psi\rangle^{[1]} \otimes |\psi\rangle^{[2]}.$$

In contrast, any two separable two-level systems may also get entangled because the common bath they are immersed in can serve as a medium to provide indirect interactions. Entanglement can be quantified using Entropy, correlations and concurrence among others. In this Thesis it will be shown how entanglement is degraded as the temperature increases [17, 18]. The significance of entanglement in quantum computing extends to various domains. It facilitates computational accelerations (both exponential and polynomial), tackles optimization challenges, guarantees secure communication across extensive distances, aids in the creation of robust and efficient quantum algorithms, propels advancements in quantum information processing, and paves the way for the evolution of the quantum internet [19, 20]. However, to achieve these notable results, qubits must be maintained near zero temperature, as entanglement is prone to vanishing due to finite temperature fluctuations [21, 22]. To entangle qubits, researchers employ various methods to enhance performance, such as utilizing the Hadamard gate to assure maximum entanglement [23, 24].

1.2 $\bowtie$ Measure entanglement

Given the significance of entanglement, the question arises: 'To what extent are two or more qubits entangled?' It is posited that particles with a higher degree of entanglement would be a more valuable resource than those less entangled. In light of this, researchers have endeavored to identify and categorize various forms of entanglement [25, 26]. This exploration has led to the development of various metrics to quantify entanglement as correlations and concurrences.

1.2.1 $\bowtie$ Concurrences and Quantum phase transitions

In thermal equilibrium, the system's state is described by the Gibbs density operator:

$$\rho = \frac{\exp\left\{-\frac{\hat{H}}{T}\right\}}{Z} = \sum_n P_n |\psi_n\rangle \langle \psi_n| \quad \sum_n P_n = 1 \quad (1.1)$$

For subsequent discussions, we assume $k_b = 1$ and consider $P_n = \exp\{-E_n/T\}/Z$ as the Boltzmann occupation probabilities of the eigenstates $|\psi_n\rangle$, where $Z = \sum_n \exp\{-E_n/T\} = \text{Tr}\{\exp\{-\hat{H}/T\}\}$ represents the partition function. Let ρ_{ij} represent the density matrix associated with two adjacent sites, i and j , on a qubit system. The density matrix's character may be either pure or mixed. This matrix finds one of its most critical uses in its capacity to depict subsystems within a more extensive, composite quantum system, a concept embodied by the reduced density operator. The importance of the reduced density operator is unequivocal. It transcends mere utility, becoming an essential cornerstone in the field [8]. Consider two physical systems, A and B , described by a density operator ρ^{AB} . The reduced density operator for system A is given by

$$\rho^A \equiv \text{tr}_B (\rho^{AB})$$

where tr_B represents a mapping of operators called the partial trace over system B . The partial trace is defined as follows:

$$\text{tr}_B (|a_1\rangle \langle a_2| \otimes |b_1\rangle \langle b_2|) \equiv |a_1\rangle \langle a_2| \text{tr} (|b_1\rangle \langle b_2|),$$

Here, $|a_1\rangle$ and $|a_2\rangle$ are arbitrary vectors in the state space of A , and $|b_1\rangle$ and $|b_2\rangle$ are arbitrary vectors in the state space of B . The trace operation on the right-hand side is the conventional trace operation for system B , meaning $\text{tr} (|b_1\rangle \langle b_2|) = \langle b_2 | b_1 \rangle$. We have thus far defined the partial trace operation solely for a specific subset of operators on AB .

The concurrence associated with the reduced density matrix [27–30], defined for two m -distant sites i and $j = i + m$, can be computed from ρ_{ij} as:

$$c_{ij} = \max \{ \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0 \} \quad (1.2)$$

On this case, λ_i are the square roots of the eigenvalues of $\rho\tilde{\rho}$, arranged in descending order. where Let $\tilde{\rho}$ be the spin-reversed density matrix, $\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^\dagger (\sigma_y \otimes \sigma_y)$, $\rho^\dagger$ indicates conjugate transpose, note that these eigenvalues are guaranteed to be real and nonnegative, even though $\rho\tilde{\rho}$ is not necessarily Hermitian. The values of concurrence span from zero, representing an unentangled state ($c_{ij} = 0$), to one, indicative of a fully entangled state such as the Bell state ($c_{ij} = 1$). Another quantum property intimately related to concurrence is the Quantum Phase Transition (QPT). A QPT represents a transition from one phase of matter to another, driven by quantum fluctuations and entailing macroscopic changes. This is propelled by alterations in the ground state of a many-body system at zero temperature. Such transitions can be induced by varying an external parameter as an external magnetic field. Understanding a QPT requires insight into the global entanglement of the entire state, as no local order parameter can distinguish between the ordered and disordered topological phases. Entanglement can serve as an order parameter, characterizing quantum phase transitions. There is mounting evidence that quantum topological phase transitions can be understood solely in terms of entanglement [31, 32]. More precisely, a discontinuity in the first-order derivative of the concurrence, as described in Eq. (1.2), corresponds to a first-order quantum phase transition. The point where this non-analytic behavior occurs is known as a Quantum Critical Point (QCP).

Methods for determining concurrences have been studied [33–37]. Observations indicate that when a Hamiltonian exhibits multiple symmetries, it can facilitate a reduction in the number of non-zero elements in the reduced density matrix. Specifically, the principle of translation invariance dictates that $\rho_{i,i+m} = \rho_{i+m,i}$, thereby ensuring that $\rho_{\alpha\beta} = \rho_{\beta\alpha}$. Additionally, the global phase-flip symmetry necessitates that the commutator $[\sigma_i^z \sigma_{i+m}^z, \rho_{i,i+m}]$ is zero, which mandates that the coefficients $\rho_{12} = \rho_{21}, \rho_{13} = \rho_{31}, \rho_{24} = \rho_{42}$, and $\rho_{34} = \rho_{43}$ are nullified. Furthermore, the z -component of the total magnetization, which commutes with the Hamiltonian $\mathcal{H}$ as $[\sum_i \sigma_i^z, \mathcal{H}] = 0$, precludes the possibility of a coherent superposition of the basis states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ for any pair of spins. Consequently, the coefficients ρ_{41} and ρ_{14} , corresponding to the matrix elements $|\uparrow\uparrow\rangle\langle\downarrow\downarrow|$ and $|\downarrow\downarrow\rangle\langle\uparrow\uparrow|$ respectively, are null.

Furthermore, if the 4x4 reduced density matrix of a physical system, namely a ring of N spin- $\frac{1}{2}$ particles interacting via the Heisenberg antiferromagnetic Hamiltonian has the following block-diagonal form [27]:

$$\rho^{ij|k} = \frac{1}{Z} \begin{pmatrix} v & 0 & 0 & 0 \\ 0 & w & z & 0 \\ 0 & \bar{z} & x & 0 \\ 0 & 0 & 0 & y \end{pmatrix} \quad (1.3)$$

One can show by direct calculation that the concurrence associated to this density matrix is:

$$c = \frac{2}{Z} \max \{ |z| - \sqrt{vy}, 0 \} \quad (1.4)$$

1.2.2 $\bowtie$ Correlations

Another way to identify a QPT is analyzing the two-point correlation function when the entanglement ground states changes to partially entanglement [38–42]:

$$C_{ij}^{\alpha\beta} = \langle \sigma_i^\alpha \sigma_j^\beta \rangle - \langle \sigma_i^\alpha \rangle \langle \sigma_j^\beta \rangle \quad (1.5)$$

The spin correlation function delineated above is computed utilizing the density matrix at thermal equilibrium, expressed as the expectation value of an arbitrary operator $\hat{\mathbf{A}}$ is defined, utilizing Eq. (1.1), as:

$$\langle \hat{\mathbf{A}} \rangle = \text{Tr}\{\rho \hat{\mathbf{A}}\}$$

In a 3-qubit context, $\{i, j\}$ represent site labels within the set $\{1, 2, 3\}$, while $\{\alpha, \beta\}$ denote spin components within the set $\{x, y, z\}$. Assuming that the three-qubit system is characterized by the product (uncorrelated) state $\rho = \rho_1 \otimes \rho_2 \otimes \rho_3$, a straightforward calculation reveals that $C_{ij}^{\alpha\beta} = 0$ for all $\alpha \neq \beta$, indicating the absence of correlations along any different axis. Consequently, any value $C_{12}^{\alpha\beta} \neq 0$ signifies the presence of spin correlations within the system. A similar pattern in concurrence is observed in the behavior of correlations, where, far from the thermodynamic limit and as one approaches absolute zero temperature, long-range and sharp features in the correlations emerge at the Quantum Critical Points (QCPs). Investigating this sharp, non-analytic behavior occurring in the first-order derivative of the correlation with respect to the control parameter reveals a first-order transition, indicative of a first-order Quantum Critical Point.

1.3 $\otimes$ Heisenberg Model

1.3.1 $\otimes$ General Heisenberg XYZ Model

The Hamiltonian of a general Heisenberg XYZ model in a non-uniform magnetic field B is given by [43]:

$$H = H_{XYZ} + H_{\text{mag}}$$

where those Hamiltonians are respectively:

$$H_{XYZ} = \sum_{n=1}^N \left(\frac{J_1}{2} \sigma_n^x \sigma_{n+1}^x + \frac{J_2}{2} \sigma_n^y \sigma_{n+1}^y + \frac{J_3}{2} \sigma_n^z \sigma_{n+1}^z \right) \quad (1.6)$$

$$H_{\text{mag}} = \sum_{n=1}^N B_n \sigma_n^z \quad (1.7)$$

In this case, σ_n^i (where $i = \{x, y, z\}$) represents the Pauli operators in the σ_z eigenbasis of the n -th qubit. Assuming boundary conditions similar to a ring [27], so that $\sigma_{N+1}^i = \sigma_1^i$ ($i \in \{x, y, z\}$). The set $\{J_1, J_2, J_3\}$ represents the exchange constants in the x, y, and z directions, respectively. These constants can adopt positive values in antiferromagnetic scenarios and negative values in ferromagnetic contexts [44]. Reflecting this distinction, the Curie-Weiss temperature is used to characterize the magnetic properties of ferromagnetic systems, while the Néel temperature is used for antiferromagnetic systems. The relationship between these temperatures and their respective systems becomes clear when analyzing the linear dependence of the inverse of the magnetic susceptibility at high temperatures [45]. Additionally, B_n denotes the site dependent external magnetic field applied to the n -th qubit in the z direction. Emphasizing that Pauli matrices carry significant weight in forming the matrix representation of the Hamiltonian, it becomes imperative to establish a method to generate them quickly and efficiently.

1.3.2 $\otimes$ Matricial Pauli Operators for n-Qubits

If $|0\rangle$ and $|1\rangle$ represent the states of the spin aligned and anti-aligned with the direction of the magnetic field, the Pauli matrices $\sigma_i^{x,y,z}$ can be constructed using quantum logic gates [8]:

$$\left. \begin{aligned} \alpha |0\rangle + \beta |1\rangle &\xrightarrow{\sigma_z} \alpha |0\rangle - \beta |1\rangle \\ \alpha |0\rangle + \beta |1\rangle &\xrightarrow{\sigma_x} \beta |0\rangle + \alpha |1\rangle \\ [\sigma_i, \sigma_j] &= 2i\epsilon_{ijk}\sigma_k \end{aligned} \right\} \quad (1.8)$$

Using the natural basis $|0\rangle, |1\rangle$ and this logic gates (1.8) we can construct entirely the matrix representation for the 2×2 Pauli matrices

$$\begin{aligned} \sigma_1 = \sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & \sigma_2 = \sigma_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma_3 = \sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & \sigma_4 = \mathbb{I} &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned} \quad (1.9)$$

These matrices, given in Eq. (1.9), are Hermitian, unitary, traceless, and trace-wise orthogonal. We can extend these 2×2 matrices to define a unitary basis for the complex algebra of $2^n \times 2^n$ matrices by considering a Kronecker tensor product of i th Pauli matrices, whose elements are referred to as Pauli strings. Consequently, the unitary basis for an i -qubit system is termed Pauli strings [46, 47]:

$$\sigma_{\vec{i}} := \bigotimes_{n=1}^N \sigma_{i_n}^{(n)} = \sigma_{i_1}^{(1)} \otimes \cdots \otimes \sigma_{i_N}^{(N)}, \quad \vec{i} = (i_1, \dots, i_N) \in \{0, 1, 2, 3\}^{\times N}$$

or

$$\sigma_a^{(n)} = \mathbb{I}^{(1)} \otimes \cdots \otimes \mathbb{I}^{(n-1)} \otimes \sigma_a \otimes \mathbb{I}^{(n+1)} \otimes \cdots \otimes \mathbb{I}^{(N)}, \quad a = 1, 2, 3 \quad (1.10)$$

MODEL

2.1 ⋈ Isotropic Heisenberg XXX Model in a ring topology

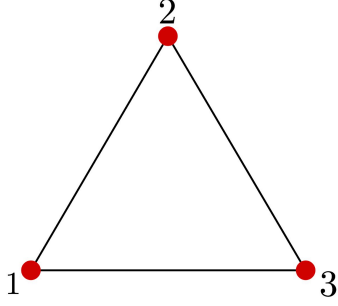


Figure 2.1: Triangle for tripartite system.

In the case of a three-qubit system, even the most intricate scenario is susceptible to numerical scrutiny. However, this thesis primarily concentrates on the isotropic scenario where $J_1 = J_2 = J_3 = 2J$ and $J = \pm 1$, with a particular emphasis on the antiferromagnetic system. By setting $B_n = B$, we transition from the non-uniform magnetic field, as described by (1.7), to a homogenous magnetic field in the z direction. This constraints transforms the Hamiltonian, as given by equation (1.6), into a Hamiltonian H_{XXX} representing the isotropic Heisenberg XXX spins that describes 3 sites of spin- $\frac{1}{2}$ entities in a ring topology as shown in Fig. 2.1 [30]:

$$H_{XXX} = J \sum_{i=1}^3 \hat{\mathbf{g}}_i \cdot \hat{\mathbf{g}}_{i+1} + B \sum_{i=1}^3 \hat{\mathbf{g}}_i^z \quad (2.1)$$

where $\hat{\mathbf{g}}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$, and assuming boundary ring conditions $\sigma_{3+1}^i = \sigma_1^i$ ($i \in \{x, y, z\}$). By employing (1.10) in conjunction with (1.9), we explicitly construct the $\sigma_i^{x,y,z}$ for the i th qubit in this tripartite system (2.1):

$$\left. \begin{aligned} \sigma_1^x &= \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} & \sigma_2^x &= \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} & \sigma_3^x &= \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \\ \sigma_1^y &= \begin{pmatrix} 0 & 0 & 0 & 0 & -i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & i & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i & 0 & 0 & 0 & 0 \end{pmatrix} & \sigma_2^y &= \begin{pmatrix} 0 & 0 & -i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i & 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & i & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 & i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & i & 0 & 0 \end{pmatrix} & \sigma_3^y &= \begin{pmatrix} 0 & -i & 0 & 0 & 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i & 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 0 & i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 & 0 & 0 & i & 0 \end{pmatrix} \\ \sigma_1^z &= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} & \sigma_2^z &= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} & \sigma_3^z &= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \end{aligned} \right\} \quad (2.2)$$

2.2 ✂ Hamiltonian and Eigenenergies

The Matricial representation of Hamiltonian (2.1) can be constructed using the i th qubit Pauli matrices (2.2) obtaining:

$$\tilde{\mathcal{H}} = \begin{pmatrix} 3B+3J & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & B-J & 2J & 0 & 2J & 0 & 0 & 0 \\ 0 & 2J & B-J & 0 & 2J & 0 & 0 & 0 \\ 0 & 0 & 0 & -B-J & 0 & 2J & 2J & 0 \\ 0 & 2J & 2J & 0 & B-J & 0 & 0 & 0 \\ 0 & 0 & 0 & 2J & 0 & -B-J & 2J & 0 \\ 0 & 0 & 0 & 2J & 0 & 2J & -B-J & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3B+3J \end{pmatrix} \quad (2.3)$$

respectively, then in the natural basis $\{|111\rangle, |110\rangle, |101\rangle, |100\rangle, |011\rangle, |010\rangle, |001\rangle, |000\rangle\}$ the eigenvectors and eigenvalues from Hamiltonian (2.3) are respectively:

$$\begin{aligned} E_1^{\text{tot}} &= -\chi_+ & |\psi_1\rangle &= \frac{1}{\sqrt{2}}(|001\rangle - |100\rangle) \\ E_2^{\text{tot}} &= -\chi_+ & |\psi_2\rangle &= \sqrt{\frac{2}{3}}|010\rangle - \frac{1}{\sqrt{6}}|100\rangle - \sqrt{\frac{1}{6}}|001\rangle \\ E_3^{\text{tot}} &= \chi_- & |\psi_3\rangle &= \frac{1}{\sqrt{2}}(|011\rangle - |110\rangle) \\ E_4^{\text{tot}} &= \chi_- & |\psi_4\rangle &= \sqrt{\frac{2}{3}}|101\rangle - \sqrt{\frac{1}{6}}(|110\rangle + |011\rangle) \\ E_5^{\text{tot}} &= -3(B-J) & |\psi_5\rangle &= |000\rangle \\ E_6^{\text{tot}} &= 3(B+J) & |\psi_6\rangle &= |111\rangle \\ E_7^{\text{tot}} &= -\chi_- & |\psi_7\rangle &= \frac{1}{\sqrt{3}}(|001\rangle + |100\rangle + |010\rangle) \\ E_8^{\text{tot}} &= \chi_+ & |\psi_8\rangle &= \frac{1}{\sqrt{3}}(|011\rangle + |110\rangle + |101\rangle) \end{aligned}$$

Using $\chi_{\pm} = B \pm 3J$.

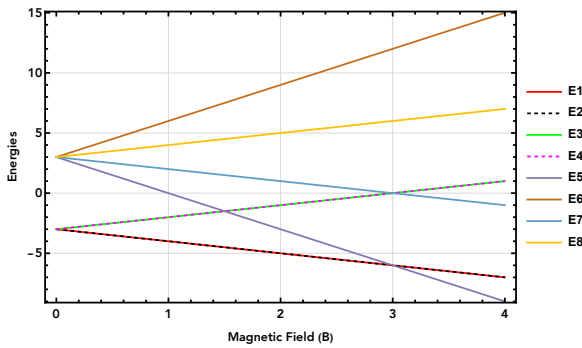


Figure 2.2: Variation of eigenenergies at $T = 0$ as a function of magnetic field B . With a chosen value of $J = 1$ for the antiferromagnetic system.

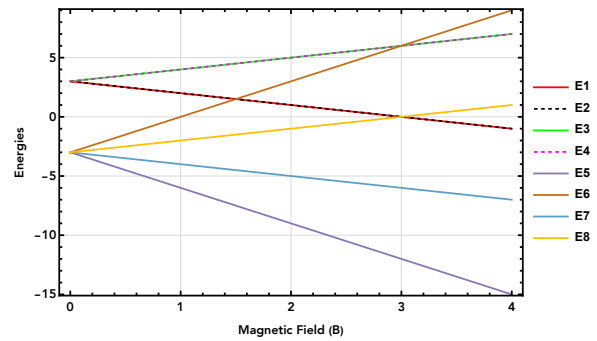


Figure 2.3: Variation of eigenenergies at $T = 0$ as a function of magnetic field B . With a chosen value of $J = -1$ for the ferromagnetic system.

For an antiferromagnetic system with $J = 1$ (Fig. 2.2), the ground state at $B = 0$ is four-fold degenerate, represented as a linear superposition of $|\psi_i\rangle$ states, where $i \in \{1, 2, 3, 4\}$. With a slight increase in the magnetic field ($0 < B < 3J$), the previous ground state splits on the states $|\psi_1\rangle$ and $|\psi_2\rangle$ forming a doubly degenerate ground state. In contrast, for $B > 3J$, the disentangled state $|000\rangle$ becomes the ground state. This demonstrates that the ground state properties can be manipulated through external magnetic field adjustments. At two critical points $\{B = 0, B = 3J\}$, a ground state energy level crossing occurs, leading to a discontinuity in the first-order derivative of the ground state energy. This phenomenon is indicative of a first-order *Quantum Phase Transition (QPT)*.

In a ferromagnetic system characterized by $J = -1$ as depicted in Fig. 2.3, the ground state exhibits four-fold degeneracy at $B = 0$, represented as a linear superposition of $|\psi_j\rangle$ with $j = \{5, 6, 7, 8\}$. However, upon the application of a slight magnetic field, the system consistently transitions to $|000\rangle$, a non-entangled state. This highlights a key difference: while entanglement in the antiferromagnetic XXX system can be induced by applying a magnetic field, the ferromagnetic system remains non-entangled regardless of the magnetic field strength [44].

2.3 Density Matrix

Thermal equilibrium with a heat bath at temperature T , the state of the system can be represented by the Gibbs State (1.1) using the eigenvectors:

$$P_i = \frac{1}{Z} \exp\{-E_i^{tot}\}/T \quad \text{with } i = \{1, \dots, 8\}$$

$$\rho = \sum_{i=1}^8 P_i |\psi_i\rangle \langle \psi_i|$$

$$\rho = \frac{1}{Z} \begin{pmatrix} e^{-\frac{3(B+J)}{T}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3}e^{-\frac{B+3J}{T}}(1+2e^{\frac{6J}{T}}) & -\frac{2}{3}e^{-\frac{B}{T}}\sinh\left(\frac{3J}{T}\right) & 0 & -\frac{2}{3}e^{-\frac{B}{T}}\sinh\left(\frac{3J}{T}\right) & 0 & 0 & 0 \\ 0 & -\frac{2}{3}e^{-\frac{B}{T}}\sinh\left(\frac{3J}{T}\right) & \frac{1}{3}e^{-\frac{B+3J}{T}}(1+2e^{\frac{6J}{T}}) & 0 & -\frac{2}{3}e^{-\frac{B}{T}}\sinh\left(\frac{3J}{T}\right) & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{3}e^{-\frac{B-3J}{T}}(1+2e^{\frac{6J}{T}}) & 0 & -\frac{2}{3}e^{-\frac{B}{T}}\sinh\left(\frac{3J}{T}\right) & -\frac{2}{3}e^{-\frac{B}{T}}\sinh\left(\frac{3J}{T}\right) & 0 \\ 0 & -\frac{2}{3}e^{-\frac{B}{T}}\sinh\left(\frac{3J}{T}\right) & -\frac{2}{3}e^{-\frac{B}{T}}\sinh\left(\frac{3J}{T}\right) & 0 & \frac{1}{3}e^{-\frac{B-3J}{T}}(1+2e^{\frac{6J}{T}}) & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{2}{3}e^{-\frac{B}{T}}\sinh\left(\frac{3J}{T}\right) & 0 & \frac{1}{3}e^{-\frac{B-3J}{T}}(1+2e^{\frac{6J}{T}}) & -\frac{2}{3}e^{-\frac{B}{T}}\sinh\left(\frac{3J}{T}\right) & 0 \\ 0 & 0 & 0 & -\frac{2}{3}e^{-\frac{B}{T}}\sinh\left(\frac{3J}{T}\right) & 0 & -\frac{2}{3}e^{-\frac{B}{T}}\sinh\left(\frac{3J}{T}\right) & \frac{1}{3}e^{-\frac{B-3J}{T}}(1+2e^{\frac{6J}{T}}) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & e^{-\frac{3(B-J)}{T}} \end{pmatrix} \quad (2.4)$$

With

$$Z = e^{-\frac{3(B+J)}{T}} \left(1 + e^{\frac{2B}{T}}\right) \left(1 + e^{\frac{4B}{T}} + 2e^{\frac{2(B+3J)}{T}}\right) \quad (2.5)$$

It is observable that $\text{Tr}\{\rho\} = 1$, $\rho = \rho^\dagger$ and $\langle \psi_n | \rho | \psi_n \rangle \geq 0$ describing an eight-level system (three interacting qubits). Subsequently, we can derive the reduced 4x4 density matrix by performing a trace over qubit $\{1, 2, 3\}$. Obtaining the same matrix for each pair of reduced qubits.

$$\rho^{12|3} = \rho^{23|1} = \rho^{31|2} =$$

$$= \frac{1}{Z} \begin{pmatrix} \frac{1}{3}e^{-\frac{B-3J}{T}} \left(1 + 3e^{\frac{2B}{T}} + 2e^{\frac{6J}{T}}\right) & 0 & 0 & 0 \\ 0 & \frac{1}{3}e^{-\frac{B+3J}{T}} \left(1 + e^{\frac{2B}{T}}\right) \left(1 + 2e^{\frac{6J}{T}}\right) & -\frac{1}{3}e^{-\frac{B+3J}{T}} \left(1 + e^{\frac{2B}{T}}\right) \left(-1 + e^{\frac{6J}{T}}\right) & 0 \\ 0 & -\frac{1}{3}e^{-\frac{B+3J}{T}} \left(1 + e^{\frac{2B}{T}}\right) \left(-1 + e^{\frac{6J}{T}}\right) & \frac{1}{3}e^{-\frac{B+3J}{T}} \left(1 + e^{\frac{2B}{T}}\right) \left(1 + 2e^{\frac{6J}{T}}\right) & 0 \\ 0 & 0 & 0 & \frac{1}{3}e^{-\frac{3(B+J)}{T}} \left(3 + e^{\frac{2B}{T}} + 2e^{\frac{2(B+3J)}{T}}\right) \end{pmatrix} \quad (2.6)$$

Tracing over any remaining qubit results in the same 2x2 reduced density matrix for an isolated qubit.

$$\begin{aligned}\rho^{1|23} &= \rho^{2|13} = \rho^{3|12} = \\ &= \frac{1}{Z} \begin{pmatrix} \frac{1}{3} e^{-\frac{B+3J}{T}} \left(1 + 2e^{\frac{2B}{T}} + 3e^{\frac{4B}{T}} + 2e^{\frac{6J}{T}} \left(1 + 2e^{\frac{2B}{T}} \right) \right) & 0 \\ 0 & \frac{1}{3} e^{-\frac{3(B+J)}{T}} \left(3 + e^{\frac{2B}{T}} \left(2 + e^{\frac{2B}{T}} \right) \left(1 + 2e^{\frac{6J}{T}} \right) \right) \end{pmatrix}\end{aligned}$$

2.4 ✂ Thermodynamic Functions

2.4.1 ✂ Thermal Machines

Qubits exhibit functionalities that transcend mere information processing. For example, when configured within a specific physical system, they can operate as a Quantum Heat Engine, which possesses numerous astonishing properties. This concept originated from a proposal on how to extract work from a single thermal bath via quantum negentropy [48]. Subsequently, the innovative development of primary quantum protocols, in which a single qubit can be employed to perform work from a single thermal bath [49], seemed to locally infringe upon the second law of thermodynamics. Nevertheless, more advanced protocols have been introduced, demonstrating alignment with the second law and illustrating the ability of single qubits to extract work from sophisticated thermal baths [50–53]. Insightful researchers have unveiled a plethora of findings through the use of Heisenberg models with entangled chains, which encompass both open and closed configurations. These configurations exhibit unique properties due to their topological nature, such as geometric frustration [35, 54, 55]. Notably, two- and three-qubit systems have been demonstrated to function as engines or refrigerators, revealing a diverse range of behaviors and applications. These systems span from Carnot engines to various Otto and Stirling engine designs, achieved by modulating magnetic fields, variation exchange components, and employing both adiabatic and non-adiabatic methods [17, 30, 40, 43, 44, 56–70].

To initiate the construction of a thermal machine mechanism, calculating the thermodynamic quantities of this 3-qubit triangular system is essential. By deriving the density matrix (2.4) and partition function (2.5), we can compute the free energy F , internal energy U , entropy S , magnetization M , and heat capacity C of the system using standard formulas from statistical mechanics within the canonical ensemble formalism.

$$U = \text{Tr}\{\rho \tilde{\mathcal{H}}\} = -3J + \frac{2(B - \exp\{\frac{4B}{T}\})(B - 3J) + 3J}{1 + e^{\frac{4B}{T}} + 2 \exp\{\frac{2(B+3J)}{T}\}} - B \tanh\left(\frac{B}{T}\right) \quad (2.7)$$

$$\begin{aligned}S &= -\text{Tr}(\rho \ln \rho) = \ln(Z) + \frac{U}{T} \\ &= \ln \left[e^{-\frac{3(B+J)}{T}} \left(1 + e^{\frac{2B}{T}} \right) \left(1 + e^{\frac{4B}{T}} + 2e^{\frac{2(B+3J)}{T}} \right) \right] + \frac{1}{T} \left(-3J + \frac{2(B - \exp\{\frac{4B}{T}\})(B - 3J) + 3J}{1 + e^{\frac{4B}{T}} + 2 \exp\{\frac{2(B+3J)}{T}\}} - B \tanh\left(\frac{B}{T}\right) \right) \quad (2.8)\end{aligned}$$

$$\begin{aligned}F &= -T \ln(Z) = -T \ln \left[e^{-\frac{3(B+J)}{T}} \left(1 + e^{\frac{2B}{T}} \right) \left(1 + e^{\frac{4B}{T}} + 2e^{\frac{2(B+3J)}{T}} \right) \right] \\ M &= -\left. \frac{\partial F}{\partial B} \right|_{J,T} = \frac{\left(-1 + e^{\frac{2B}{T}} \right) \left(3 + 4e^{\frac{2B}{T}} + 3e^{\frac{4B}{T}} + 2e^{\frac{2(B+3J)}{T}} \right)}{\left(1 + e^{\frac{2B}{T}} \right) \left(1 + e^{\frac{4B}{T}} + 2e^{\frac{2(B+3J)}{T}} \right)} \quad (2.9)\end{aligned}$$

$$C = \frac{\partial U}{\partial T} = \frac{8e^{\frac{6B}{T}} \left(2B^2 e^{\frac{12J}{T}} + B^2 (5 + 4 \cosh(\frac{2B}{T}) + \cosh(\frac{4B}{T})) + 4e^{\frac{6J}{T}} \left(\cosh(\frac{2B}{T}) (2B^2 + 9J^2 + (B^2 + 9J^2) \cosh(\frac{2B}{T})) - 24BJ \cosh(\frac{B}{T})^3 \sinh(\frac{B}{T}) \right) \right)}{\left(1 + e^{\frac{2B}{T}} \right)^2 \left(1 + e^{\frac{4B}{T}} + 2e^{\frac{2(B+3J)}{T}} \right)^2 T^2}$$

2.4.2 ✂ Contour plots of Thermodynamic Functions

To gain a more intuitive understanding of thermodynamic functions, it is useful to create a contour plot of these quantities as functions of both the magnetic field and temperature for antiferromagnetic and ferromagnetic systems.

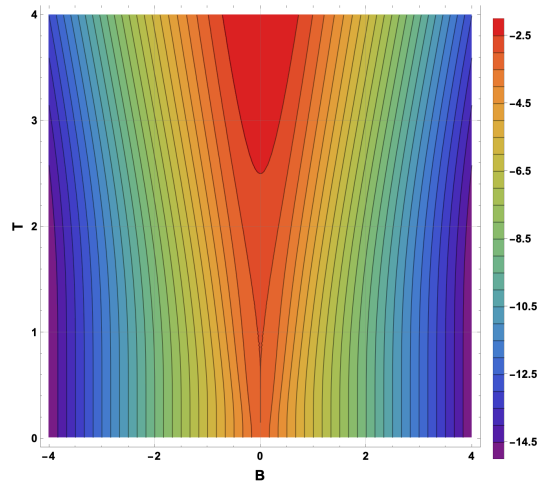


Figure 2.4: Variation of internal energy in units of $|J|$ against magnetic field (B) and Temperature (T) for the ferromagnetic system.

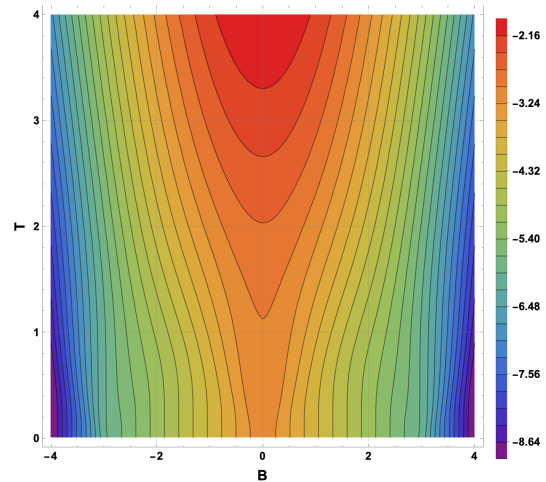


Figure 2.5: Variation of internal energy in units of $|J|$ against magnetic field (B) and Temperature (T) for the antiferromagnetic system.

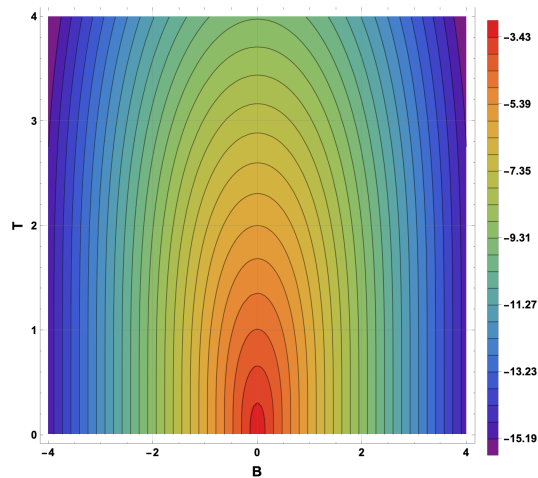


Figure 2.6: Variation of free energy in units of $|J|$ against magnetic field (B) and Temperature (T) for the ferromagnetic system.

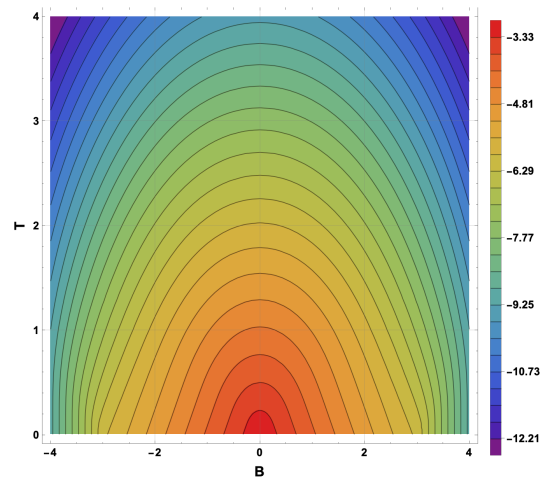


Figure 2.7: Variation of free energy in units of $|J|$ against magnetic field (B) and Temperature (T) for the antiferromagnetic system.

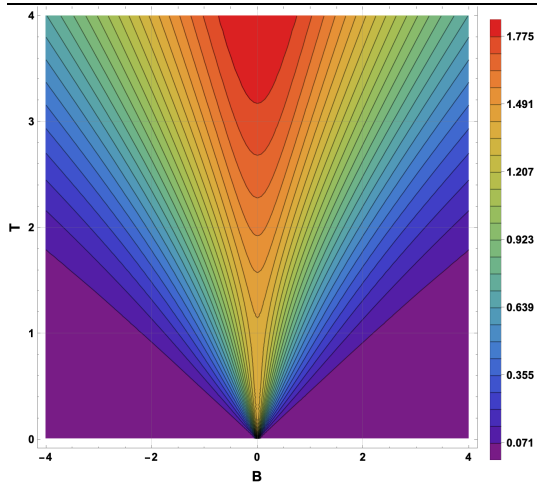


Figure 2.8: Variation of entropy in units of $|J|$ against magnetic field (B) and Temperature (T) for the ferromagnetic system.

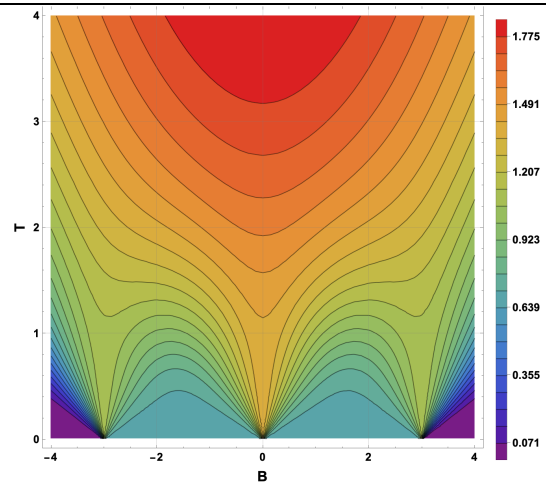


Figure 2.9: Variation of entropy in units of $|J|$ against magnetic field (B) and Temperature (T) for the antiferromagnetic system.

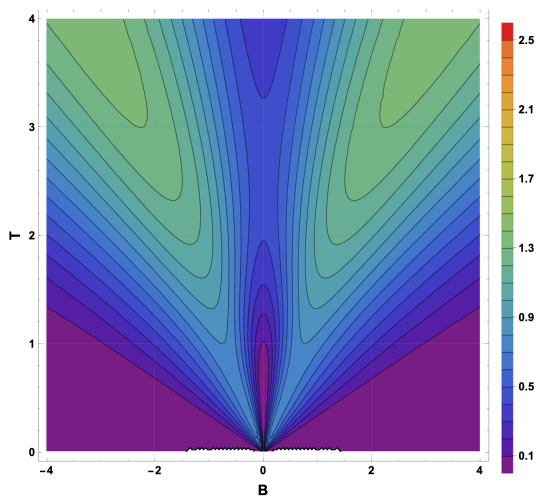


Figure 2.10: Variation of heat capacity in units of $|J|$ against magnetic field (B) and Temperature (T) for the ferromagnetic system.

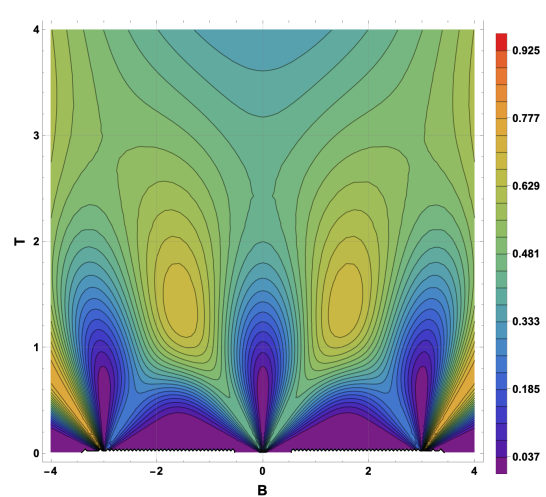


Figure 2.11: Variation of heat capacity in units of $|J|$ against magnetic field (B) and Temperature (T) for the antiferromagnetic system.

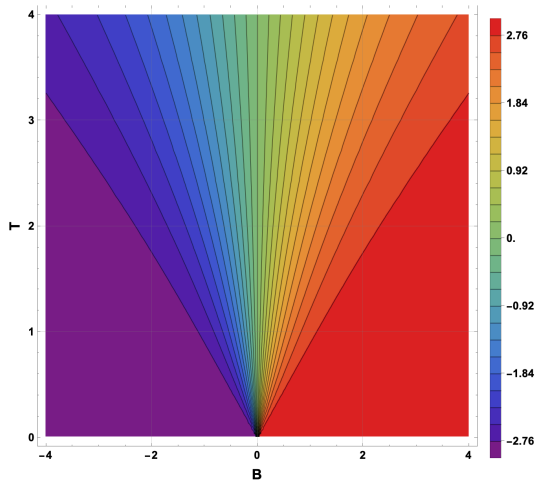


Figure 2.12: Variation of magnetization in units of $|J|$ against magnetic field (B) and Temperature (T) for the ferromagnetic system.

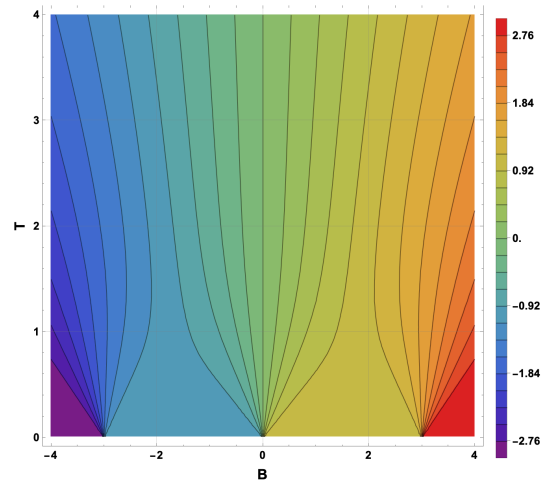


Figure 2.13: Variation of magnetization in units of $|J|$ against magnetic field (B) and Temperature (T) for the antiferromagnetic system.

It is observed that the internal energy of the ferromagnetic system, as illustrated in Fig. 2.4, decreases its energy more rapidly and maintains lower energy levels compared to the antiferromagnetic system shown in Fig. 2.5. Similarly, the free energy exhibits comparable behavior; near the origin, the ferromagnetic system has lower values and diminishes faster than the antiferromagnetic system.

The entropy and heat capacity of the ferromagnetic system, depicted in Figs. 2.8 and 2.10, exhibit only one Quantum Critical Point (QCP) at the origin. In contrast, the antiferromagnetic system, as seen in Figs. 2.9 and 2.11, displays three QCPs, attributable to the parity of the functions against the magnetic field. A parallel trend is evident in the magnetization plots, as demonstrated in Figs. 2.12 and 2.13. However, the signs of the functions correspond to the polarity of the magnetic field, reflecting the distinct magnetic behaviors of the ferromagnetic and antiferromagnetic systems.

2.5 ✂ Magnetic Properties

Given the pronounced behavior of magnetization in both the ferromagnetic and antiferromagnetic systems, it would be relevant to examine their behavior in the limiting case of zero temperature and near-zero magnetic field.

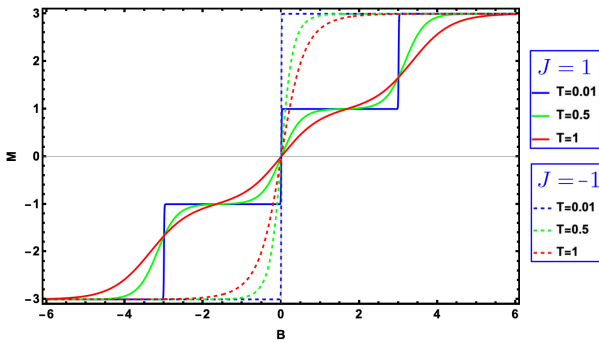


Figure 2.14: Variation in magnetization for the antiferromagnetic system (thick lines) and the ferromagnetic system (dashed lines) as a function of B at zero temperature.

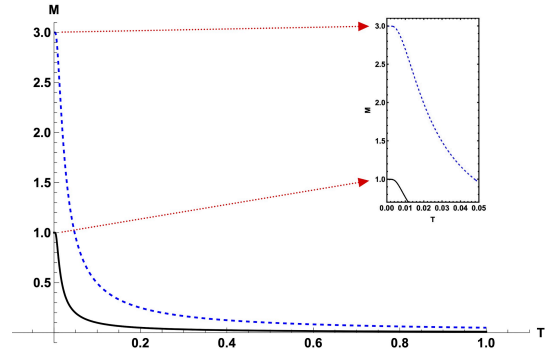


Figure 2.15: Variation in magnetization for the antiferromagnetic system (thick black line) and the ferromagnetic system (dashed blue line) as a function of T in the vicinity of zero magnetic field.

From Fig. 2.14, it is observed that at zero temperature, the ferromagnetic system immediately magnetizes upon the application of a non-zero magnetic field. In contrast, the antiferromagnetic system exhibits a more gradual magnetization, resembling a staircase with the first steps has width $3B$. It eventually reaches the same magnetization level as the ferromagnetic system but requires a larger magnetic field of $\pm 3B$. As the temperature increases, the ferromagnetic system requires a higher magnetic field to reach maximum magnetization. In contrast, the antiferromagnetic system quickly loses its staircase behavior, transitioning to a linear curve as the temperature rises.

Examining the case of zero magnetization in Fig. 2.15, the ferromagnetic system at zero temperature has a magnetization three times greater than the antiferromagnetic system. Furthermore, as the temperature begins to rise, the magnetization of the antiferromagnetic system decreases more rapidly than the ferromagnetic system, indicating that the latter is more resilient to temperature changes. Ultimately, both systems' magnetizations diminish to zero at extremely high temperatures. This behavior of magnetization, as described by (2.9), allows us to compute the magnetic susceptibility (with $\mu_0 = 1$) as:

$$\chi = \frac{\partial M}{\partial B} = \frac{4}{T} \left(-\frac{\left(-1 + e^{\frac{4B}{T}}\right)^2}{\left(1 + e^{\frac{4B}{T}} + 2e^{\frac{2(B+3J)}{T}}\right)^2} + \frac{1}{4} \text{Sech}^2\left(\frac{B}{T}\right) + \frac{1}{1 + e^{\frac{6J}{T}} \text{Sech}\left(\frac{2B}{T}\right)} \right) \quad (2.10)$$

Systems with magnetization at high temperatures exhibit a linear temperature dependence with respect to the inverse of their susceptibility (2.10). Therefore, considering the cases for $J = \{-1, 1, 0\}$ with a small magnetic field $B = 0.01$, we can plot these behaviors alongside a least squares fit from a high temperature range of approximately 30 – 50 (Fig. 2.16). This will highlight the linear behavior at these magnitudes. For the ferromagnetic system at high temperature results can be fitted reasonably well using Curie-Weiss Law ($1/\chi = [T - \Theta]/C$) [45].

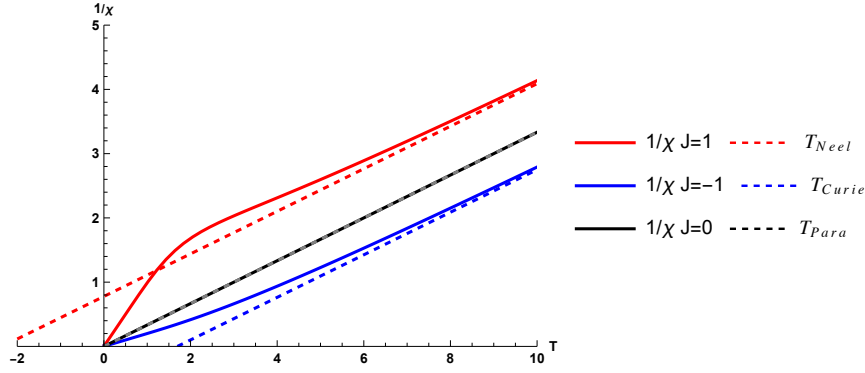


Figure 2.16: The inverse of susceptibility (2.10) as a function of T is shown for $B = 0.01$. The thick red, blue, and black lines represent the inverse of susceptibility for antiferromagnetic, ferromagnetic, and paramagnetic systems, respectively. Meanwhile, the dashed red, blue, and black lines depict the fits according to the Curie-Weiss Law at high temperatures.

$$\left. \begin{array}{lll} T_{Neel} = 0.331082T + 0.777946 & R^2 = 0.999999 & \text{Néel Temperature} \approx -2.34971 \\ T_{Curie} = 0.331255T - 0.561918 & R^2 = 0.999999 & \text{Curie Temperature} \approx 1.69633 \\ T_{Para} = 0.333333T & R^2 = 0.999999 & \text{Para Temperature} \approx 0 \end{array} \right\} \quad (2.11)$$

From (2.11), we observe that the ferromagnetic system has a positive Curie temperature, confirming that the system behaves as a ferromagnetic system in accordance with Curie's Law. Furthermore, the antiferromagnetic system exhibits a negative Néel temperature, aligning with the expected properties for such systems. Lastly, the paramagnetic system lacks a Curie constant, indicating that the susceptibility is inversionally proportional to the temperature.

2.6 ✂ Ground State Effective temperatures

2.6.1 ✂ Reduced Density Matrices of the Ground State

The antiferromagnetic ground state is fourfold degenerate at zero magnetic field. Therefore, it would be intriguing to reduce the system to a single qubit and consider only an effective Hamiltonian where the isolated qubit interacts solely with the magnetic field. All other interactions, such as entangled interactions, are treated as a heat bath. To accomplish this, we need to construct the density matrix of the ground state, assigning zero temperature and zero magnetic field on the reduced density matrices $\rho^{1|23}$, $\rho^{2|31}$ and $\rho^{3|12}$.

$$\rho_0^{23|1} = \rho_0^{13|2} = \rho_0^{12|3} = \begin{pmatrix} \frac{1}{6} & 0 & 0 & 0 \\ 0 & \frac{1}{3} & -\frac{1}{6} & 0 \\ 0 & -\frac{1}{6} & \frac{1}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{6} \end{pmatrix}$$

If we trace over 1, 2, 3 independently, we obtain:

$$\rho_0^{1|23} = \rho_0^{2|13} = \rho_0^{3|12} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \quad (2.12)$$

We can obtain the Von-Neumann entropy ($-\text{Tr}(\rho \ln \rho)$) from the isolated qubits such as:

$$S_{\text{eff}}^{1|2|3} = \ln(2) \quad (2.13)$$

The tripartite antiferromagnetic system distinctively exhibits its spatial symmetry, as evidenced by its triangular configuration (Fig. 2.1). When positioned at any vertex of the triangle, each qubit is surrounded by the same two neighboring qubits, resulting in indistinguishable isolated interactions. Consequently, this symmetry implies that all isolated qubits within the system share the same effective temperature.

2.6.2 $\otimes$ Effective Hamiltonian

Constructing an effective Hamiltonian in which an isolated qubit only experiences the magnetic field in the z-direction, and all other interactions are treated as a heat bath environment, we obtain:

$$\check{\mathcal{H}}_{\text{eff}} = B\hat{\sigma}_z \quad (+\text{Heat Bath})$$

The associated eigenenergies are:

$$E_{\text{eff}}^{\pm} = \pm B$$

The corresponding partition function is given by:

$$Z_{\text{eff}} = 2 \cosh\left(\frac{B}{T}\right) \implies F_{\text{eff}} = -T \ln\left(2 \cosh\frac{B}{T}\right)$$

The associated entropy is:

$$S_{\text{eff}} = \ln\left(2 \cosh\left(\frac{B}{T}\right)\right) - \frac{B}{T} \tanh\left(\frac{B}{T}\right) \quad (2.14)$$

Using expression (2.14), the effective temperature of an isolated qubit within the environment of the other two qubits can be computed. This is achieved by identifying the point where the effective entropy function (2.14) aligns with the effective entropy (2.13), denoted as $S_{\text{eff}} = S_{\text{eff}}^{1|2|3}$. By determining the root we can ascertain the effective temperature corresponding to each isolated system. Employing the dimensionless parameter $x = B/T$, as shown in Fig. 2.17, the roots for the three qubits intersect the x-axis as $T_{\text{eff}} \rightarrow \infty$. This result aligns with the previously analyzed effective entropy. The three qubits possess an infinite effective temperature, indicating that there is no unique effective temperature applicable to all energy levels of the ground state, suggesting that the ground state represents a non-equilibrium steady state [71]. More importantly, it is not feasible to transfer additional entropy to them in the ground state. Consequently, isolated qubits could potentially act as reservoirs of entropy and temperature when considering the ground state.

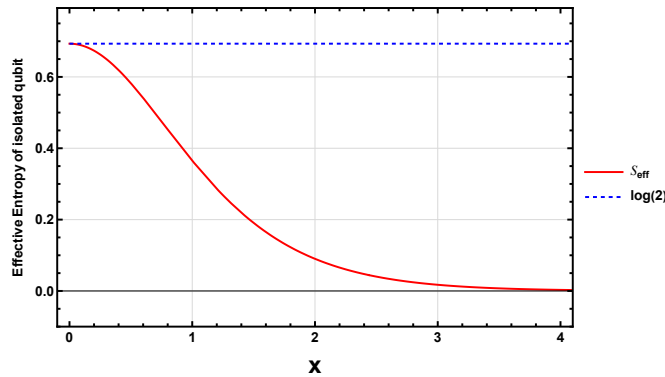


Figure 2.17: Effective entropy function (represented by thick red line) for isolated qubits $\{1, 2, 3\}$ as functions of the dimensionless parameter $x = B/T$, alongside their corresponding effective entropy (depicted by dashed lines).

SPIN CORRELATIONS AND QUANTUM PHASE TRANSITION

3.1 ⌘ Spin correlations and Quantum phase transition

In the specific case of three distinguishable qubits, the correlations (1.5) adhere to the properties $C_{ij}^{\alpha\beta} = C_{ji}^{\alpha\beta}$ and $C_{ij}^{\alpha\beta} = C_{ij}^{\beta\alpha}$. This symmetry reduces the number of necessary calculations for the symmetric tensor $C_{ij}^{\alpha\beta}$ to just the upper diagonal terms, amounting to 9 elements. Additionally, due to the Hamiltonian's symmetry across qubits 1, 2, and 3, we have $C_{ij}^{xx} = C_{ij}^{yy} = C^{xx/yy}$ for the state in thermal equilibrium. For the zz -correlation C^{zz} , it is observed that all three qubits exhibit the same values. Specifically, for $i \neq j$, we find:

$$C^{xx/yy} = -\frac{2e^{\frac{2B}{T}} \left(-1 + e^{\frac{6J}{T}}\right)}{3 \left(1 + e^{\frac{4B}{T}} + 2e^{\frac{2(B+3J)}{T}}\right)} \quad C^{zz} = -\frac{8e^{\frac{4B}{T}} \left(-1 + e^{\frac{6J}{T}}\right) \left(1 + 4e^{\frac{2B}{T}} + e^{\frac{4B}{T}} + 2e^{\frac{6J}{T}} + 2e^{\frac{2(B+3J)}{T}} + 2e^{\frac{4B+6J}{T}}\right)}{9 \left(1 + e^{\frac{2B}{T}}\right)^2 \left(1 + e^{\frac{4B}{T}} + 2e^{\frac{2(B+3J)}{T}}\right)^2} \quad (3.1)$$

Figure 3.1 displays the xx/yy -correlations as defined in Eq. (3.1), while Figure 3.2 presents the zz -correlations, with both sets of correlations plotted as functions of the magnetic field B and temperature T . These plots reveal that as T approaches zero, both $C^{xx/yy}$ and C^{zz} correlations undergo notable transitions around the critical point $B = 3J$. This transition is characterized by a shift from $-1/3$ in $C^{xx/yy}$ and $-4/9$ in C^{zz} to zero in both cases, signaling a first-order Quantum Phase Transition (QPT). Interestingly, at $B = 0$, the C^{zz} correlation exhibits a pronounced peak, transitioning from a mixed state to a Bell state as the magnetic field increases. In contrast, $C^{xx/yy}$ maintains a constant minimum correlation over a wider and more extended range at higher temperatures and near the zero magnetic field regime compared to C^{zz} .

Furthermore, the first-order derivatives of both the xx/yy and zz -correlation functions with respect to the magnetic field display divergences at the critical points, specifically at $B = 3J$, as illustrated in Figs. 3.3 and 3.4. These divergences occur as T approaches zero. With increasing temperature, the peak of the xx/yy -correlations shifts subtly to the right, indicating the system's tendency to favor a disentangled and uncorrelated state. In contrast, the peak of the zz -correlation consistently aligns with the Quantum Critical Point (QCP), influenced by the magnetic field in the z direction.

This phase transition represents a shift from a fermionic magnetic state, where the wave function is antisymmetric upon qubit exchange and associated with spatial symmetry in the triangular qubit topology, to a bosonic magnetic state characterized by a symmetric quantum state upon qubit interchange. This transition signifies a move from an entangled state to a completely disentangled state.

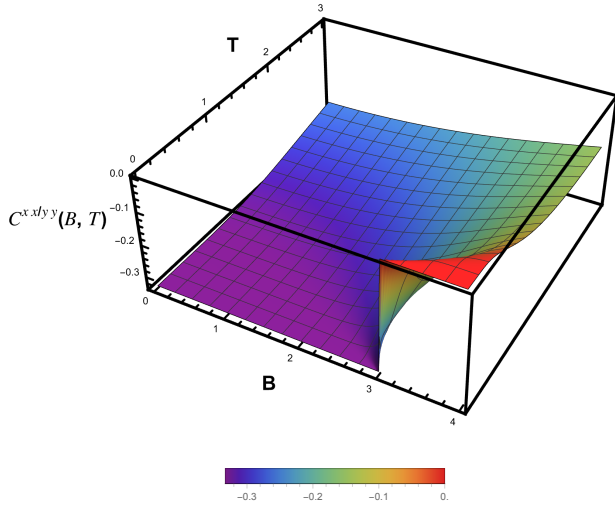


Figure 3.1: Variation of xx/yy correlation of a three-spin system at thermal equilibrium, analyzed as a function of temperature T and magnetic field B , with the exchange parameter set at $J = 1$.

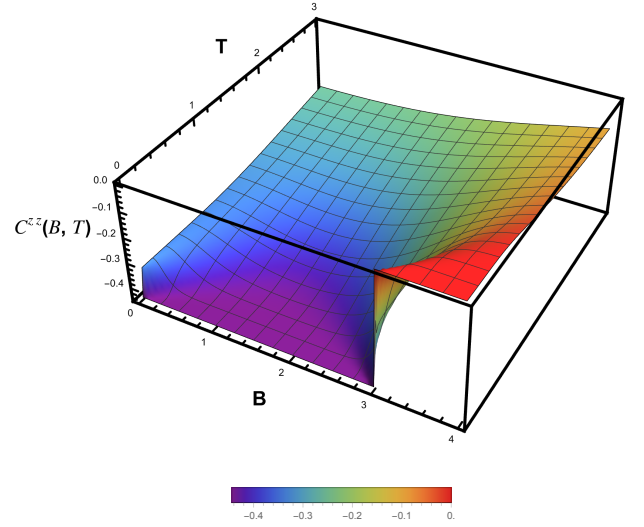


Figure 3.2: Variation of zz correlation of a three-spin system at thermal equilibrium, analyzed as a function of temperature T and magnetic field B , with the exchange parameter set at $J = 1$.

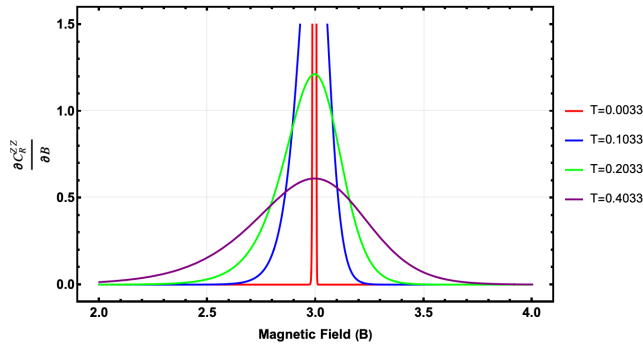


Figure 3.3: Variation of the First-order derivative with respect to the magnetic field of the zz -Correlations at thermal equilibrium across diverse Temperatures with $J = 1$.

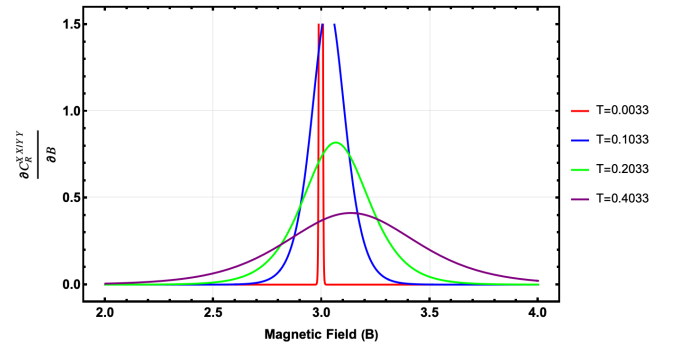


Figure 3.4: Variation of the First-order derivative with respect to the magnetic field of the xx/yy -correlations at thermal equilibrium across diverse temperature with $J = 1$.

3.1.1 ✂ Linking Correlations with Thermodynamics

Establishing a link between thermodynamic quantities—such as internal energy, free energy, and magnetization—and correlations derived from statistical information theory is both intriguing and a new development in the field [17]. For this tripartite system, we can formulate a direct relationship between these thermodynamic functions based on spin correlations using a linear combination of the xx - yy and zz correlation:

$$M = \frac{3K_1(2)K_2(1, -1)}{\sqrt{C^{xx/yy}K_1(4)K_2(1, -1)}}$$

$$U = \frac{-3(BK_1(2)\sqrt{C^{xx/yy}K_1(4)K_2(1, -1)} + J(-C^{xx/yy}(1 + 6C^{xx/yy}K_1(6) - 3C^{zz}) - 3C^{zz}))}{C^{xx/yy}K_1(4)}$$

$$F = 3(B + J) - T \ln \left(\frac{8C^{xx/yy}K_1(4) \left(C^{xx/yy}K_1(4) + \sqrt{C^{xx/yy}K_1(4)K_2(1, -1)} \right) \left(2C^{xx/yy}K_1(2) + 2\sqrt{C^{xx/yy}K_1(4)K_2(1, -1)} - C^{zz} \right)}{K_1(3)(4(C^{xx/yy})^2 + C^{zz})^3} \right)$$

Here $K_1(m)$ and $K_2(m, n)$ are function that depend on the the pair correlations and are given by:

$$K_1(\mathbf{m}) = (1 + \mathbf{m}C^{xx/yy})$$

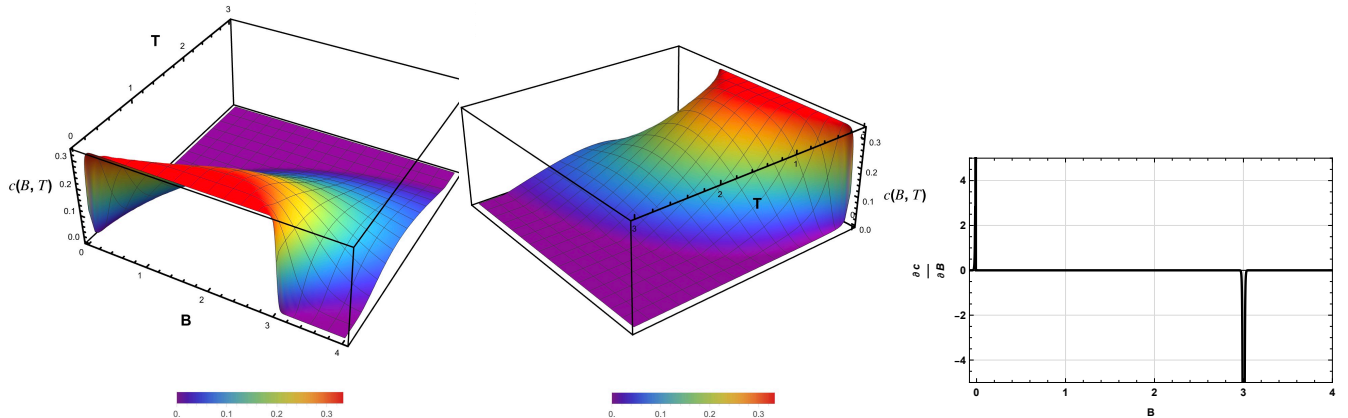
$$K_2(\mathbf{m}, \mathbf{n}) = \mathbf{m}C^{xx/yy} + \mathbf{n}C^{zz}$$

All of these expressions solely rely on the spin correlation functions $C^{xx/yy}$ and C^{zz} . They are applicable across any magnetic field, exchange constant, and temperature, thereby expanding upon previous results obtained at zero temperature.

3.2 ✂ Quantum Entanglement

In the field of information theory, various entanglement measures are recognized as crucial tools for identifying Quantum Phase Transitions (QPTs) [27–29]. In this tripartite system, the reduced 4×4 matrices are identical, a result of translational invariance, which ensures that the concurrence for each pair of nearest neighbors is the same, as detailed in Eq. (1.2). Moreover, the structure of these reduced matrices (2.6) aligns perfectly with the form presented in (1.3), facilitating the application of the concurrence formula (1.4) to this type of system. This compatibility permits an analytical derivation:

$$c(J, B, T) = \frac{2e^{\frac{2B}{T}} \left(-1 - e^{\frac{2B}{T}} + e^{\frac{6J}{T}} \left(1 + e^{\frac{2B}{T}} \right) - \sqrt{\left(1 + 3e^{\frac{2B}{T}} + 2e^{\frac{6J}{T}} \right) \left(3 + e^{\frac{2B}{T}} \left(1 + 2e^{\frac{6J}{T}} \right) \right)} \right)}{3 \left(1 + e^{\frac{2B}{T}} \right) \left(1 + e^{\frac{4B}{T}} + 2e^{\frac{2(B+3J)}{T}} \right)}$$



(a) Variation of concurrence at thermal equilibrium as a function of temperature T and magnetic field B using $J = 1$.

(b) Variation of concurrence observed from a different perspective than that presented in Fig. 3.5a.

(c) Variation of derivative of concurrence of three spins at thermal equilibrium as a function of magnetic field B using $J = 1$ and $T = 0$.

Figure 3.5: Variation of pair concurrences and its derivative at different values for Temperature and Magnetic Field.

The graphs in Figures 3.5a and 3.5b depict the variation of concurrence as a function of the magnetic field B and temperature T , presented from various viewpoints. As T approaches zero, a notable increase in $c(B, T)$ is observed, rapidly rising from near 0 to 0.33 after $B = 0$. This maximum value is 50% less than the maximum possible concurrence achievable in an 3-entangled system [27]. This increase signifies a transition from a disentangled mixed state to a Bell state. Subsequently, there is a significant decrease in concurrence around the critical point $B = 3J$. These changes are characterized by a distinct transition, indicating a shift from a Bell state to a separable state, a hallmark of a first-order Quantum Critical Point (QCP). This shift correlates with the ground state's evolution from a mixed state $\sum_i |\psi_i\rangle$ (where $i = \{1, 2, 3, 4\}$) near the origin, to a state of $|\psi_1\rangle + |\psi_2\rangle$ for $0 < B < 3J$, and eventually to the disentangled state $|000\rangle$ beyond $B = 3J$. Importantly, the first-order derivative of concurrence with respect to B exhibits non-analytical behavior at these critical points when T nears zero, as depicted in Fig. 3.5c. This behavior highlights the transition to an entangled state beyond $B = 0$ and a subsequent shift to a completely unentangled state after $B = 3J$. At higher temperatures, concurrence rapidly diminishes at low magnetic fields, but in the high magnetic field regime, it takes slightly longer to dissipate.

QUANTUM STIRLING AND QUANTUM-QUASISTATIC OTTO CYCLES

4.1 ⌘ Otto and Stirling Engine

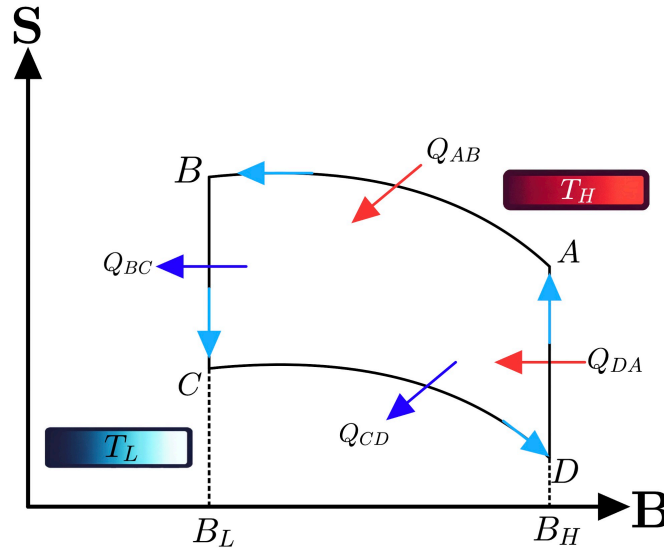


Figure 4.1: Diagram of the Stirling cycle regarding entropy and the external perpendicular magnetic field value along z-axis. Curve AB is an isotherm at $T = T_H$ and curve CD at $T = T_L$

4.1.1 ⌘ Stirling Engine

Mirroring its classical counterpart, the quantum Stirling cycle comprises four distinct phases: two isothermal and two isomagnetic processes. These isomagnetic stages in the quantum cycle are analogous to the isochoric stages in the classical Stirling cycle. Throughout the isothermal phases, the system maintains thermal equilibrium with one of two thermal reservoirs, characterized by temperatures $T = T_H$ and $T = T_L$, where $T_H > T_L$. Concurrently, the external magnetic field oscillates between B_H and B_L , adhering to the criterion $B_L < B_H$. Regarding the isomagnetic phases, the interaction with the thermal baths ceases, prompting the system to undergo a transition at a consistent magnetic field intensity (either at B_L or B_H). This cycle is illustrated in Fig. 4.1, with the external magnetic field B_z serving as the control parameter. Analyzing the cycle stage-by-stage, as presented in the figure, note that the exchange constant J remains fixed at 1.

- I. Isothermal Phases: These stages are represented by the trajectories $A \rightarrow B$ and $C \rightarrow D$ in Figure 4.1. During the initial phase $A \rightarrow B$ (and subsequently $C \rightarrow D$), the system's temperature is maintained at a constant T_H (T_L), with entropy alterations ensuing from fluctuations in the external magnetic

field. As a result, the heat exchanged by the system throughout these phases can be ascertained from the entropy's variation during the processes conducted at a uniform temperature, expressed as:

$$\begin{aligned} Q_{AB} &= T_H (S_B - S_A) \\ Q_{CD} &= T_L (S_D - S_C) \end{aligned}$$

II. Isomagnetic Phases: These stages correspond to the trajectories $B \rightarrow C$ (with $B_L = \text{constant}$) and $D \rightarrow A$ (with $B_H = \text{constant}$) depicted in Fig. 4.1 Throughout these phases, no work is performed; hence, the heat exchange is derived from the alteration in internal energy as the system transitions between thermal baths from a temperature of T_H to T_L in the $B \rightarrow C$ phase, and reversely from T_L to T_H in the $D \rightarrow A$ phase. The formulas for the heat exchanges during these phases are as follows:

$$\begin{aligned} Q_{BC} &= U_C - U_B, \\ Q_{DA} &= U_A - U_D \end{aligned}$$

From the first law of thermodynamics and knowing that the variation of the internal energy in a closed cycle is zero the total work is:

$$W = Q_H + Q_L = Q_{AB} + Q_{DA} + Q_{BC} + Q_{CD}$$

In our analysis, we adhere to the following sign convention: a positive (negative) value of Q denotes the system's absorption (release) of heat, while a positive (negative) value of W signifies work performed by (on) the system. Consequently, in the context of a heat engine, the conditions $Q_H > 0$, $Q_L < 0$, and $W > 0$ prevail, meaning the system draws a certain quantity of heat Q_H from the hot reservoir, releases a portion Q_L to the cold reservoir, and utilizes the remainder to execute an amount of work W . The efficiency η is then defined as the ratio of the total work output to the heat absorbed by the system, expressed as:

$$\eta = \frac{W}{Q_H} = \frac{Q_{AB} + Q_{BC} + Q_{CD} + Q_{DA}}{Q_{AB} + Q_{DA}}$$

4.1.2 ✕ Quasistatic Otto Engine

The cycle is thermodynamically defined by two heat reservoirs (hot and cold) and two distinct values of the external field, B_h and B_l . Typically, the stage with lower temperature (T_l) is associated with a lower external field value (B_l), while the stage with higher temperature (T_h) corresponds to the higher external field value (B_h).

Stage A-B. In the cycle depicted in Fig. 4.2, the sequence $A \rightarrow B$ commences with the system at an external magnetic field of B_l , reaching thermal equilibrium at temperature T_l . Subsequently, the magnetic field shifts from B_l to B_h , elevating the internal temperature to T_b along an isoentropic path, thereby performing work.

$$S(T_l, B_l) = S(T_b, B_h) \implies W_{1 \rightarrow 2} = U(T_b, B_h) - U(T_l, B_l)$$

Stage B-C. The system then engages with the hot reservoir, increasing its internal temperature through heat absorption:

$$Q_{in} = U(T_h, B_h) - U(T_b, B_h)$$

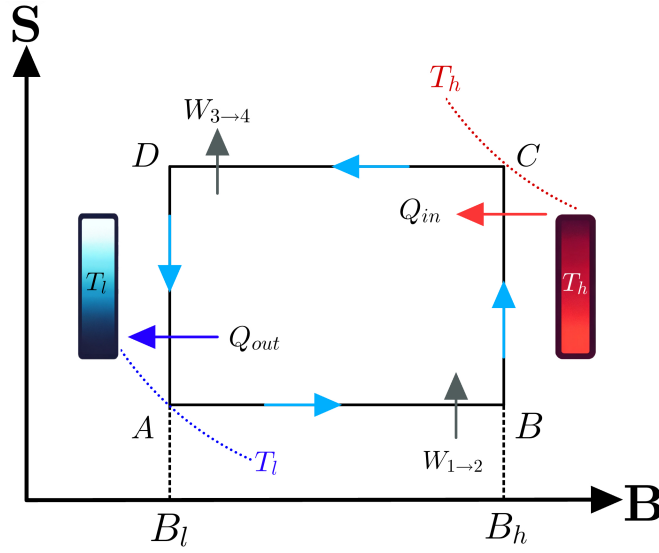


Figure 4.2: Diagram of the Otto cycle regarding entropy and the external perpendicular magnetic field value along z-axis.

Stage C-D. The system disengages from the hot reservoir and altering back the magnetic field from B_h to B_l and traversing an additional isoentropic path, thus executing further work.

$$S(T_d, B_l) = S(T_h, B_h) \implies W_{3 \rightarrow 4} = U(T_d, B_l) - U(T_h, B_h)$$

Stage D-A. Finally, the system interfaces with a cold reservoir at temperature T_l , expelling heat during the transition:

$$Q_{out} = U(T_l, B_l) - U(T_d, B_l)$$

The output power output is quantified as the work conducted over each cycle iteration:

$$W = Q_{in} - Q_{out}$$

Subsequently, the efficiency is articulated as the proportion of total work relative to Q_{in} :

$$\eta = \frac{Q_{in} - Q_{out}}{Q_{in}} = 1 - \left| \frac{Q_{out}}{Q_{in}} \right|$$

4.1.3 ⌘ Quantum Otto Engine

The quantum Otto cycle consists of four stages, each drawing parallels to the quasi-static process. However, there are notable differences that set them apart. The stages are described as follows:

Stage A-B. The system is in thermal equilibrium at temperature T_l under the influence of an external magnetic field B_l . Let the initial occupation probabilities be denoted as p_{il} for its eight eigenstates, where $i \in \{1, 2, \dots, 8\}$ and $j \in \{l, h\}$. Subsequently, the system undergoes a quantum adiabatic process as the magnetic field transitions from B_l to B_h . During this process, the probability of each eigenstate remains conserved, i.e., $p_{il} = p_{ib}$. As a result, work is performed on the system without any heat transfer.

Stage B-C. The system comes into contact with a heat bath at temperature T_h . Consequently, the occupation probability of each eigenstate shifts to p_{ih} . This results in the system absorbing thermal energy from the bath achieving thermal equilibrium. Heat transfer occurs during this stage due to the change in occupation probability, while no work is executed.

Stage C-D. As the system detaches from the heat bath, the magnetic field transitions back from B_h to B_l , setting off another quantum adiabatic process. During this phase, the probability of each eigenstate remains conserved, such that $p_{ih} = p_{id}$, and work is performed on the system.

Stage D-A. When the system engages with a cold bath. During this interaction, heat is transferred as the system releases energy to the thermal reservoir when transitioning from a higher to a lower state. The occupation probability transitions from p_{id} back to p_{il} , thereby restoring thermal equilibrium.

Throughout the cycle, the system interacts with different thermal baths during Stages B-C and D-A, achieving thermal equilibrium only in these stages. In contrast, the quasi-static Otto engine achieves thermal equilibrium at every stage. The occupation probabilities, p_{il} and p_{ih} , depend solely on the temperature of each bath and the energy levels of the system:

$$p_{ij} = \frac{\exp(-E_{ij}/kT_j)}{\sum_i \exp(-E_{ij}/kT_j)}, \quad \text{with } j = \{l, h\}$$

Here, E_{il} and E_{ih} represent the eigenvalues of the system's Hamiltonian, denoted by (2.3), corresponding to the magnetic fields $B = B_l$ and $B = B_h$, respectively.

The heat Q_{in} absorbed during stage B-C and Q_{out} released during stage D-A are given by:

$$Q_{in} = \sum_i E_{ih}(p_{ih} - p_{il}),$$

$$Q_{out} = \sum_i E_{il}(p_{ih} - p_{il}),$$

Energy conservation dictates that the net work done by the system during the quantum adiabatic processes is:

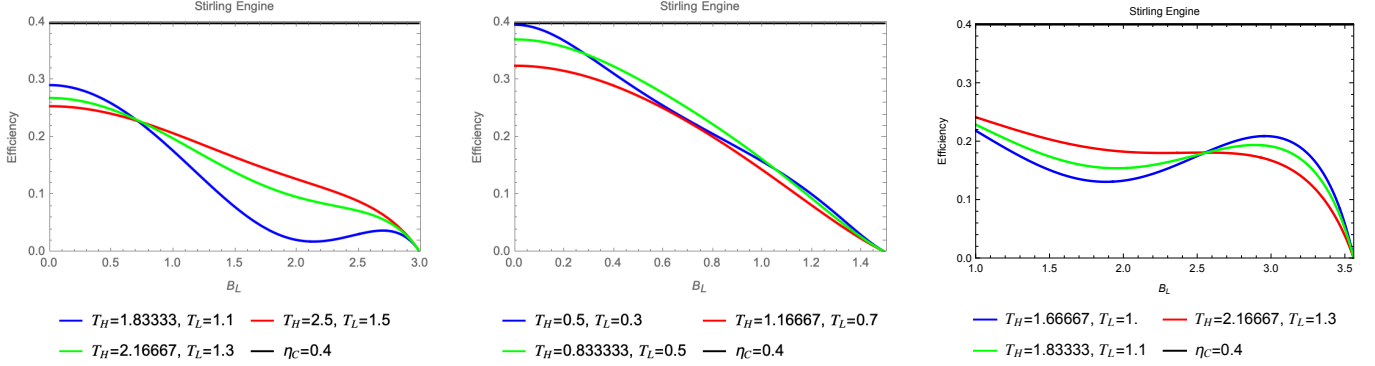
$$W = Q_{in} + Q_{out} = \sum_i (E_{ih} - E_{il})(p_{ih} - p_{il}) > 0 \quad (4.1)$$

The efficiency, η , is defined analogously to that of the quasi-static process:

$$\eta = 1 - \left| \frac{Q_{out}}{Q_{in}} \right| \quad (4.2)$$

PERFORMANCE ANALYSIS OF EACH CYCLE

5.1 ⌘ Stirling Engine



(a) Stirling Engine: Variation of efficiency with respect to B_L at elevated $B_H = 3.0$ values for various hot and cold bath temperatures, given $J = 1$. It is noteworthy that the difference between the lowest $B_L = 0$ and B_H is substantial. The Carnot efficiency for all scenarios remains at $\eta_C = 0.4$.

(b) Stirling Engine: Variation of efficiency with respect to B_L at reduced $B_H = 1.5$ values for various hot and cold bath temperatures, given $J = 1$. The disparity between the lowest $B_L = 0$ and B_H is slight. The Carnot efficiency for all scenarios remains constant at $\eta_C = 0.4$.

(c) Stirling Engine: Variation of efficiency with respect to B_L at elevated $B_H = 3.5$ values for various hot and cold bath temperatures, given $J = 1$. The disparity between the lowest $B_L = 1.0$ and B_H is notably slight. The Carnot efficiency for all scenarios remains constant at $\eta_C = 0.4$.

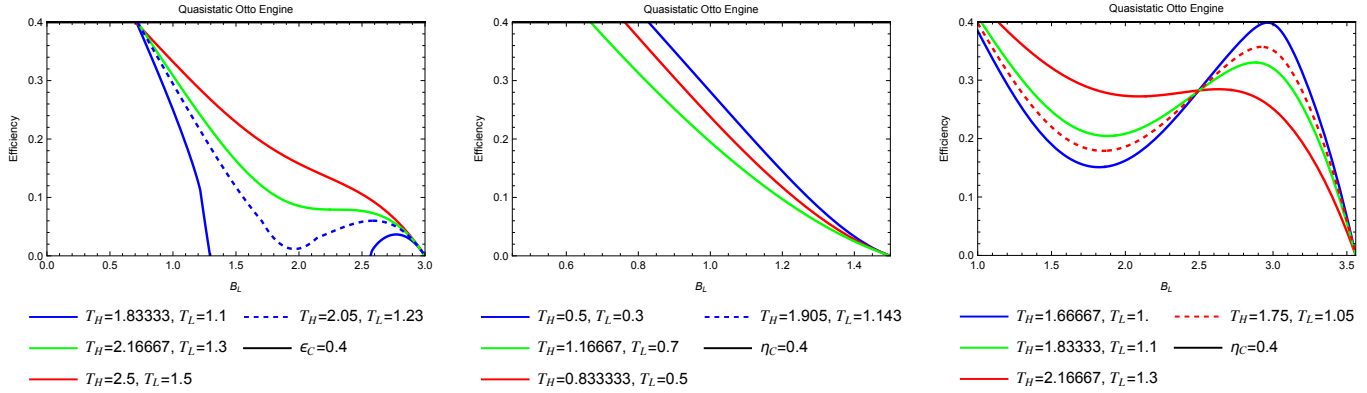
Figure 5.1: Variation of Stirling Engine's efficiency at different values of Temperature and Magnetic Field.

In the high-temperature regime ($T > 1$), the Stirling engine's performance, as shown in Fig. 5.1a, varies significantly with the magnetic field. At low T_L and minimal B_L variations, efficiency is enhanced but declines as B_L nears $B_H = 3.0$. In contrast, engines starting at higher T_L show less efficiency at low B_L but improve as B_L increases, highlighting the influence of initial temperature on efficiency across the magnetic field range.

In the low-temperature regime ($T < 1$), as illustrated in Fig. 5.1b, the engine functions within a magnetic field range from $B_L = 0$ to $B_H = 1.5$. At this regime, the engine starting at lower temperatures initially achieve Carnot efficiency, but this efficiency rapidly diminishes as B_L increases. Conversely, the engine with the highest initial temperatures exhibit the lowest efficiency throughout the entire interval. Interestingly, cycle with moderate initial temperatures begin operation near Carnot efficiency and, at mid-range magnetic fields, alternate in achieving maximum efficiency with the lower initial temperatures.

In scenarios with high T and a broad magnetic field range (Fig. 5.1c), initial higher temperatures yield better efficiency, which decreases with increasing B_H . As B_L grows, lower initial temperatures enhance efficiency, with the lowest temperature case eventually matching its initial efficiency before a rapid overall decline. This pattern indicates that the Stirling engine is more efficient at lower temperatures, with performance sharply deteriorating as the magnetic field extends.

5.2 ✂ Quasistatic Otto Engine



(a) Quasistatic Otto Engine: Variation of efficiency with respect to B_L at elevated $B_H = 3.0$ values for various hot and cold bath temperatures, given $J = 1$. It is noteworthy that the difference between the lowest $B_L = 0$ and B_H is substantial. The Carnot efficiency for all scenarios is maintained at $\eta_C = 0.4$.

(b) Quasistatic Otto Engine: Variation of efficiency with respect to B_L at reduced B_H values for various hot and cold bath temperatures, given $J = 1$. It should be highlighted that the Carnot efficiency for all scenarios remains $\eta_C = 0.4$.

(c) Quasistatic Otto Engine: Variation of efficiency with respect to B_L at elevated $B_H = 3.5$ values for various hot and cold bath temperatures, given $J = 1$. The Carnot efficiency for all scenarios remains constant at $\eta_C = 0.4$.

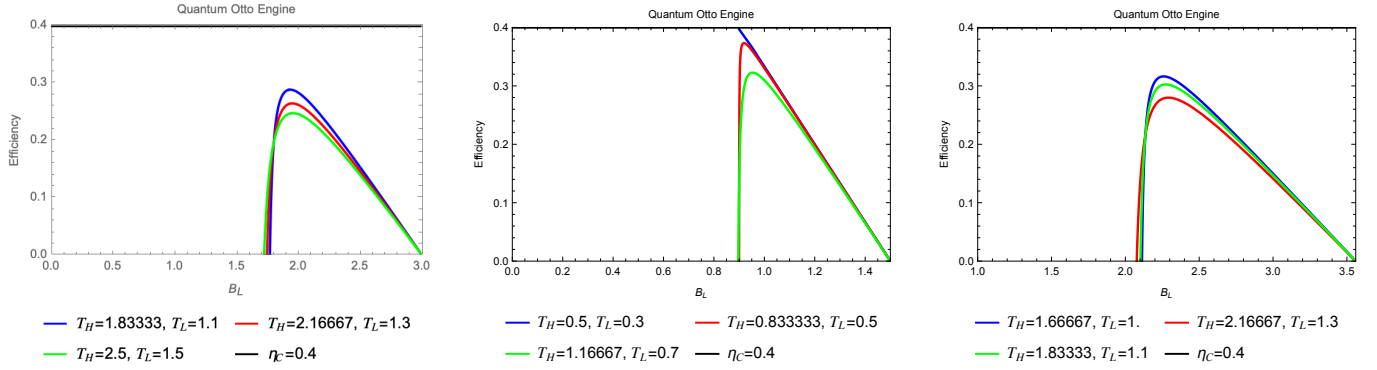
Figure 5.2: Variation of Quasistatic Otto Engine's efficiency at different values of Temperature and Magnetic Field.

In the high-temperature domain ($T > 1$), the quasi-static Otto engine's efficacy, as shown in Fig. 5.2a, is notably absent at low B_L due to the erratic isentropic trajectories at diminished temperatures and magnetic fields, potentially causing engine failure. Upon increasing B_L slightly, all curves initiate at Carnot efficiency, only to rapidly decline with further magnetic field enhancement. The lowest temperature cycle fails almost instantaneously, a consequence of the same erratic behavior. Yet, a slight elevation in initial temperature, indicated by the blue dashed line, allows for successful engine operation. The cycle with the highest initial temperature outperforms the others, followed by the intermediate and then the lowest temperature cycles.

In the cooler regime, characterized by $T < 1$ as depicted in Fig. 5.2b, the engine operates over a range from $B_L = 0$ to $B_H = 1.5$. In this regime, the operational challenges necessitate a higher B_L to ensure stable initiation due to the form of isentropic lines on the entropy (Fig. 2.9). Furthermore, it is observed that all cycles commence with Carnot efficiency. However, engines with a middle starting temperature initiate earlier but exhibit lower efficiency compared to those starting later. Conversely, engines operating at lower temperatures demonstrate higher efficiency when functioning concurrently.

At high temperatures and across a broad magnetic field spectrum, Fig. 5.2c reveals that the cycle with the highest initial temperatures exhibit inefficiencies at low B_L values, consistent with earlier observations. A slight decrease in the initial temperature is crucial to initiate operation at $B_L = 0$ with Carnot efficiency indicated by the red dashed line. The cycle with the lowest initial temperature, initially less efficient, experiences a significant surge in efficiency at $B_L \approx 2.0$, achieving Carnot efficiency at $B_L = 3.0$. This efficiency peak coincides with a quantum critical point at zero temperature. In contrast, the cycle with the highest initial temperature, while more efficient in the mid-range of B_L , becomes the least efficient beyond $B_L \approx 2.5$. Meanwhile, the cycle with an intermediate initial temperature maintains a steady efficiency across the entire range of magnetic field values.

5.3 ✂ Quantum Otto Engine



(a) Quantum Otto Engine: Variation of efficiency with respect to B_L at elevated $B_H = 3.0$ values for various hot and cold bath temperatures, given $J = 1$. It is noteworthy that the difference between the lowest $B_L = 0$ and B_H is substantial. The Carnot efficiency for all scenarios is maintained at $\eta_C = 0.4$.

(b) Quantum Otto Engine: Variation of efficiency with respect to B_L at reduced B_H values for various hot and cold bath temperatures, given $J = 1$. It should be highlighted that the Carnot efficiency for all scenarios remains $\eta_C = 0.4$.

(c) Quantum Otto Engine: Variation of efficiency with respect to B_L at elevated $B_H = 3.5$ values for various hot and cold bath temperatures, given $J = 1$. The disparity between the lowest $B_L = 1.0$ and B_H is notably slight. The Carnot efficiency for all scenarios remains constant at $\eta_C = 0.4$.

Figure 5.3: Variation of Quantum Otto Engine's efficiency at different values of Temperature and Magnetic Field.

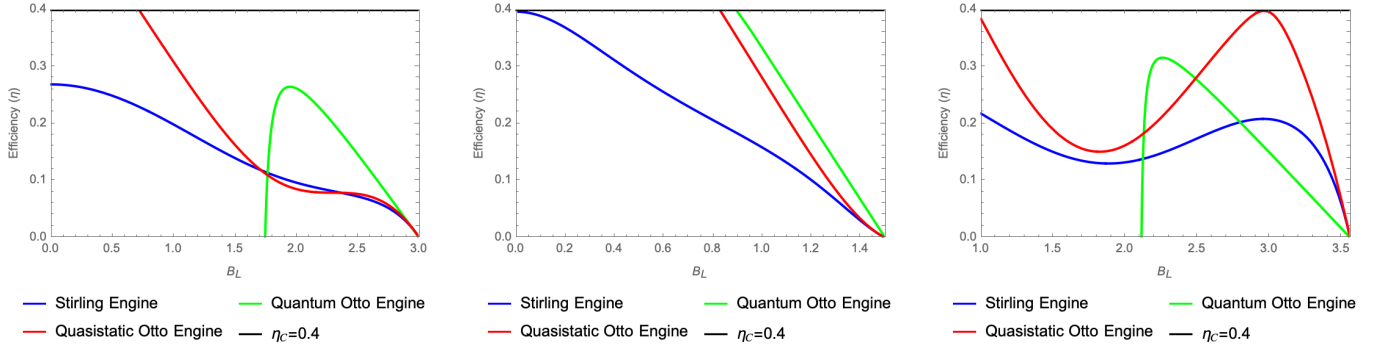
In both high and low temperature regimes, the efficiency of the quantum Otto engine is notably absent at moderately low B_L values. This effect is primarily attributed to the non-conservation of probabilities in these conditions, posing operational challenges for the engine. Interestingly, this situation leads to a transition towards a refrigeration mode, a phenomenon not explored in this chapter.

In the higher temperature regime, as B_L surpasses 1.7 (Fig. 5.3a), the initial temperature critically influences engine performance. Notably, at $B_L \approx 1.8$, cycles with lower initial temperatures outperform others, demonstrating a temperature-dependent inversion in efficiency.

In the regime of low temperatures and magnetic fields, as depicted in Fig. 5.3b, the engine's performance is distinctly influenced by the initial temperature setting. Specifically, the cycle with the lowest initial temperature initially fails to operate but then starts at Carnot efficiency, only to rapidly decline to zero efficiency. In contrast, engines with moderate and high initial temperatures exhibit different efficiency profiles. The engine with the highest initial temperature achieves the lowest maximum efficiency. Meanwhile, the engine with a middle-range initial temperature approaches almost to Carnot efficiency but then experiences a rapid efficiency drop, similar to the other cycles.

In conditions of higher magnetic fields and temperatures, as depicted in Fig. 5.3c, an inverse behavior pattern is observed. The cycle commencing with the highest initial temperature initiates operation first but exhibits the lowest maximum efficiency. This trend continues with the cycle starting at a middle initial temperature, which shows a slightly better efficiency, and finally, the cycle with the lowest initial temperature demonstrates the best performance in terms of maximum efficiency.

5.4 ✂ Comparison between cycles



(a) Comparison of different engines: Variation of efficiency with respect to B_L at elevated $B_H = 3.0$ values for various engine cycles using $T_L = 1.3$ and $T_H = 2.166$. The Carnot efficiency for all scenarios is maintained at $\eta_C = 0.4$.

(b) Comparison of different engines: Variation of efficiency with respect to B_L at lower $B_H = 1.5$ values for various engine cycles using $T_L = 0.3$ and $T_H = 0.66$. The Carnot efficiency for all scenarios is maintained at $\eta_C = 0.4$.

(c) Comparison of different engines: Variation of efficiency with respect to B_L at elevated $B_H = 3.5$ values for various engine cycles using $T_L = 1$ and $T_H = 1.66$. The Carnot efficiency for all scenarios is maintained at $\eta_C = 0.4$.

Figure 5.4: Variation of Three Engine Cycles's efficiency at different values of Temperature and Magnetic Field.

In the high temperature and high magnetic field regime, as shown in Fig. 5.4a, it is observed that the Stirling engine operates across the entire interval. This contrasts with both the quantum and quasi-static engines, which do not start at lower magnetic field regimes. Interestingly, the quasi-static engine initiates operation before the quantum engine and initially reaches the maximum global efficiency at Carnot's efficiency. However, it is quickly surpassed by the quantum engine. This indicates that the Stirling engine is more efficient at lower magnetic fields, the quasi-static engine dominates in the mid-range regime, and the quantum engine excels in the higher regime.

In the regime of lower temperature and lower magnetic field, as depicted in Fig. 5.4b, the Stirling engine commences operation at zero magnetic field with Carnot efficiency, but its efficiency gradually decays to zero across the magnetic field spectrum. In contrast, both the quasi-static and quantum Otto engines do not operate over more than half of the interval. However, when they do start, almost at the same magnetic field, they initially achieve Carnot efficiency but then rapidly decline to zero. A notable difference is observed towards the end of the magnetic field range: the quasi-static Otto engine's efficiency decreases almost exponentially, whereas the quantum engine's efficiency declines linearly. During the period when the Otto engines are inactive, the Stirling engine exhibits superior efficiency. However, as soon as the quasi-static engine becomes operational, it overtakes the Stirling engine, and subsequently, when the quantum engine starts, it surpasses all others in the final stretch.

In the middle temperature and highest magnetic field regime, as illustrated in Fig. 5.4c, both the Quasi-static Otto and Stirling engines initiate operation at the same initial magnetic field. However, the Quasi-static Otto engine starts near Carnot efficiency, in contrast to the Stirling engine, which begins significantly lower and remains below the Quasi-static engine throughout the entire magnetic field range. Both engines exhibit an inflection point around $B \approx 1.9$, where their efficiency increases. Near $B \approx 2.1$, the Quantum Otto engine begins operation and momentarily surpasses the efficiencies of both the Quasi-static and Stirling engines. At $B \approx 2.5$, another intersection point occurs where the Quasi-static Otto engine overtakes the Quantum engine. Remarkably, it reaches Carnot efficiency at $B = 3.0$, a point that corresponds to a Quantum Critical Point (QCP) at zero temperature. Towards the end of the range, the efficiencies of all three engines decline, with the Quasi-static Otto maintaining the highest efficiency, followed by the Stirling engine, and the Quantum Otto exhibiting the lowest efficiency.

CONCLUSIONS

In this study, the thermodynamic behavior of three $\frac{1}{2}$ spin particles, modeled using a Heisenberg XXX-type arrangement in a ring topology, was investigated. The tripartite antiferromagnetic system distinctly exhibits its spatial geometry through the identical results in the reduced thermodynamic components. Additionally, the magnetic susceptibility exhibits the anticipated behavior for the antiferromagnetic system ($J > 0$), ferromagnetic system ($J < 0$), and paramagnetic system ($J = 0$). In these systems, one can readily distinguish their respective Néel temperature, Curie temperature, and the paramagnetic regime, which occurs in the absence of exchange interaction.

The entanglement in this system was analyzed and quantified using spin correlation, concurrence, and thermodynamic entropy. Furthermore, a profound interconnection between information theory and thermodynamics in this tripartite system was explored. It was demonstrated that thermodynamic functions can be expressed in terms of spin correlations, highlighting the intricate link between quantum information and thermodynamic performance.

The primary emphasis in the antiferromagnetic system study was on its performance as a quantum Stirling, quasi static Otto, and Quantum Otto engine, especially in proximity to two Quantum Critical Points (QCPs). The external magnetic field, perpendicular to the system, served as the control parameter for the proposed cycles.

The quantum phase transitions in the antiferromagnetic system at $B = 0$ and $B = 3J$ were analyzed in terms of entanglement and spin correlations. It was found that these QCPs significantly influence the efficiency of the three engine cycles. By carefully selecting cycle parameters T_L, T_H, B_L , and B_H in the antiferromagnetic system ($J = 1$), Carnot's efficiency can be achieved. The findings suggest that at low temperatures, the Stirling engine outperforms the Otto engines, reaching Carnot efficiency at the lower QCP. Conversely, the Otto engines are more efficient at higher temperatures, with the quasistatic engine capable of achieving Carnot's efficiency at the higher QCP.

This thesis lays the groundwork for future research on systems with a greater number of qubits arranged in a ring topology. Such studies could encompass fundamental molecules in biological systems, considering environmental interactions, magnetic anisotropy, or more complex engine and refrigerator cycles.

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