Thermal Entanglement of Spins in an Inhomogeneous Magnetic field

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Certificate

Normalize this is to certify that **Mr. Junaid ul Haq** has carried out the work contained in this dissertation under my supervision and is accepted by the Department of Physics, Quaid-i-Azam University, Islamabad as satisfying the dissertation requirement for the degree of Master of Philosophy in Physics.

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To my beloved Parents

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Abstract

We investigate the thermal entanglement for the Heisenberg XXX model in an external inhomogeneous magnetic field by using negativity. We further exploit a measure called quantum mixedness to study the interaction of our system of spins with the heat bath. We study the properties of thermal entanglement by parametrically controlling the inhomogeneous magnetic field on an individual spin. It is noted that the variation in entanglement is symmetric around the applied magnetic field. In the ferromagnetic case, introducing even a small amount of inhomogeneities in the magnetic field can lead to the production of significant thermal entanglement which shows that the thermal entanglement is highly unstable in a given case.

Chapter 1

Introduction

Entanglement is among the most exciting features in quantum mechanics, which plays a significant role in quantum information science. In recent decades, a considerable amount of intensive research has been done on quantifying the entanglement in condensed matter systems, both quantitatively and qualitatively, with the goal of exploiting them in quantum information and communication task. In solid state structures like spin chains, quantum entanglement is an emerging field of research nowadays [1]. In contrast with other quantum systems, spin chains are the most logical candidates for realizing entanglement. The Heisenberg chain has been utilized to build quantum dots and quantum computers [2]. Entanglement is a very fragile and delegated phenomenon that generally doesn't show robustness when the given system is in thermal contact with its environment such as a thermal bath. Therefore, the investigation of thermal properties of entanglements is inevitable to be researched.

Therefore, in order to study the thermal entanglement in a Heisenberg

model, we are considering the ferromagnetic and the antiferromagnetic case in which spins are aligned parallel and antiparallel respectively, below a certain temperature known as Curie and Neel temperature respectively in the presence of the external magnetic field. Along with the exchange interaction of the spins which is responsible for the specific alignment, temperature also plays an important role in the alignment of the spins and hence on the correlation (Entanglement) of the system, in the presence of the external magnetic field.

There has been a lot of intriguing work being done on the entanglement of the Heisenberg spin model [3]. However, only the uniform field case is thoroughly investigated, but the case of the non-uniform magnetic field is rarely considered. In any solid state system, the possibility of inhomogeneous Zeeman coupling exists [4], during the generation of qubits. Therefore, it is crucial to discuss the thermal entanglement in the presence of the inhomogeneous magnetic field. We are discussing the thermal entanglement in ferromagnetic and antiferromagnetic cases in the presence of the inhomogeneous field for different values of the temperature while using negativity as the entanglement quantifier. We also use quantum mixedness to study the effect of interaction with the external system.

1.1 Spin Hamiltonian

1.1.1 Quantum Spin

Before discussing the Heisenberg model, we have to understand the quantum spin. The electron has an intrinsic angular momentum in addition to its orbital angular momentum known as spin, which has nothing to do with the spatial degrees of freedom. The intrinsic degree of freedom or spin is a completely quantum mechanical notion that has no classical realization. A magnetic dipole moment, μ_L of orbit having an area A, in which a charged particle is in motion which constitutes current I is defined as,

$$\mu_L = IA, \tag{1.1}$$

the loop current associated with orbiting electrons having constant speed v is given by

$$I = \frac{e}{T}, \tag{1.2}$$

where T is the time period of the revolution given as $T = \frac{2\pi}{\omega}$, and ω is the related to the velocity of an electron as $\omega = \frac{v}{r}$, and area of the circular loop for electron orbiting around the nucleus is πr^2.

Using these values in equation (1.2), we get,

$$I = \frac{e\omega}{2\pi} = \frac{ev}{2\pi r}, \tag{1.3}$$

so, equation (1.1) can be written as

$$\mu_L = (\frac{ev}{2\pi r})(\pi r^2),$$
$$\mu_L = \frac{evr}{2},$$

$$\mu_L = \frac{e(m_e vr)}{2m_e},$$

where orbital angular momentum L of the electron is defined as $L = m_e vr$. So, the orbital magnetic moment of negatively charged electrons can be written as;

$$\mu_L = \frac{-e\text{L}}{2m_e}. \tag{1.4}$$

Here, the negative sign shows that the direction of the magnetic dipole moment of the electron is opposite to that of the orbital angular momentum. Similarly, magnetic moment due to intrinsic spin, which is twice that of the orbital magnetic moment of electrons due to relativistic effect is given as

$$\mu_s = \frac{-e\overrightarrow{S}}{m_e}, \tag{1.5}$$

where S represents a vector operator of spin angular momentum which gives magnitude as well as direction. $\overrightarrow{S}$ has three components $\hat{S}_x, \hat{S}_y, \hat{S}_z$ which can be expressed in term of the Pauli matrix given as;

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -\iota \\ \iota & 0 \end{pmatrix}, \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.6}$$

where, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -\iota \\ \iota & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ are the Pauli matrices.

When an electron is placed in an inhomogeneous magnetic field, a force is exerted on the electron's spin dipole moment, the direction and strength of the force are determined by the relative alignment of the field and the dipole. This force has a tendency to align μ_s along the magnetic field, causing μ_s to execute the precessional motion. If μ_s is in the direction of the applied field, the electron will proceed in the direction of the increasing field, but if μ_s is in the direction opposite to the applied field, the electron will move in the direction of decreasing magnetic field. As a result, the atomic beam will deflect in accordance with the spin orientation of the electron.

1.1.2 Hamiltonian

The Hamiltonian is generally stated in the form of the sum of operators relating to a system's kinetic and potential energies.

$$H = K + V, \tag{1.7}$$

Let us consider a special case in which uniform magnetic field B is applied to a system having magnetic moment μ related to both orbital motion and intrinsic spin of the electrons, the potential is given as,

$$V = -\mu.B, \tag{1.8}$$

where, $\mu = \mu_L + \mu_s$.

The major source of ferromagnetism in atoms is the spin of electrons, while the orbital angular momentum of the electron around the nucleus also plays a role, but very small so, we can ignore the orbital magnetic moment of the electron for our special case of ferromagnetism. As we are not considering the orbital motion of electrons so, the Hamiltonian of such a system is given as

$$H = \mu_s.B, \tag{1.9}$$

for our special case of ferromagnetism which has spontaneous magnetization in which spins of electrons are oriented in a specific direction because of the interaction between the spins of electrons with each other and with the environment given below.

1.1.3 Magnetic spin exchange interaction

Pauli's exclusion principle essentially causes exchange interaction. This interaction determines the orientation of spins, especially in ferromagnetic materials, i.e., whether spins are parallel (ferromagnetism) or antiparallel (antiferromagnetism). The repulsive force between parallel spins is caused by the exchange interaction. On the other hand, it produces an attractive force between antiparallel spins. In a ferromagnetic material, the overall resultant force can be represented as the vector sum of the Coulomb forces and exchange forces which is quantum mechanical phenomenon with no classical counterpart. The first is caused by the classical distribution of charge, whereas the second is caused by the quantum distribution of spins. Ferro-

magnetic materials balance these two forces to get the minimumenergy (there might be other interactions that could affect the total magnetic moment of electrons are discussed below). Ferromagnetic materials, achieve their lowest energy by generating magnetic domains of different sizes. Each domain has saturation magnetization, which means that all of the spins in that domain point in the same direction. The addition of all the Coulomb and exchange forces using addition results in a minimal force, indicating the material's stability. Anti parallel spins are also present in the domains of an anti-ferromagnetic substance with attractive exchange force and Coulomb force. Again, the vector sum of the forces across all domains gives the material minimal energy.

1.1.4 Types of interaction

The spin Hamiltonian is a useful way of classifying the coupling mechanism of an electron spin with other magnetic moments in quantum mechanics. This Hamiltonian includes all of the magnetic couplings that will affect the energy of the system. Coupling of an electron's spin vector S with any other type of magnetic moments is often of a mathematical form as described in the following subsections:

1.1.5 Spin-orbit coupling

Spin-orbit coupling is due to magnetic interaction between the electron's spin and their orbital motion. This coupling is based on the orbital featuring the unpaired spin overlapping with other orbitals. The spin-orbit coupling is a

type of internal coupling that contributes to the spin Hamiltonian as,

$$H = \beta S_1.L, \tag{1.10}$$

where, β is the spin-orbit field while, L is the orbital moment of electron interacting with the spin of electrons.

1.1.6 Antisymmetric interaction

The Antisymmetric exchange is also known as (DM) interaction is the interaction between two close spins S_i and S_j. The contribution of such interaction to Hamiltonian is given as,

$$H = \beta.(S_i \times S_j). \tag{1.11}$$

Where β is the spin-orbit field dimensionless parameter and tells about how strong the coupling is between the spins. In order to minimize this effect, it can be seen through the above equation if β is pointing in the direction opposite to the $(S_i \times S_j)$. There is some kind of perturbations like spin-orbit coupling which breaks the symmetry and leads to the antisymmetric interaction or DM interactions. DM interactions are responsible for the ferromagnetic character in antiferromagnetism.

1.1.7 Zeeman coupling

A coupling of the electron's spin with the externally applied field is known as the Zeeman effect. Due to the Zeeman effect, splitting of the spectral lines

occurs. Its contribution to spin Hamiltonian is;

$$H = g\mu_e H_o . S_z, \tag{1.12}$$

Where H_0 is the strength of the applied magnetic field, μ_e represent the magnetic moment and S_z is the value of the spin vector directed along the applied magnetic field.

1.1.8 The electron exchange interaction

Exchange interaction is a purely quantum mechanical phenomenon that occurs among identical particles which do not possess any classical analog. This effect is due to the wave function of indistinguishable particles like the electron being subjected to the exchange symmetry. In other words, this kind of interaction occurs when two indistinguishable particles exchange their spatial parts. Consider two atoms with an electron in their outermost shell having the same spin either up or down. When two atoms are at a distance with two different energy states, then, it is possible for electrons can have the same spin, but when two atoms come close to each other, such that their orbits are overlapping and two electrons of interacting atoms are sharing the same quantum state, then the Pauli exclusion principle does not allow electrons to have the same spins rather have opposite spins. The general Hamiltonian of such a system is given as;

$$H = H_o + H_{ex}, \tag{1.13}$$

Where H_o is usually coulomb interaction part of Hamiltonian which has nothing to do with such kind of exchange interaction, only H_{ex} plays the role which is spin dependent given by Heisenberg as,

$$H_{ex} = -JS_1.S_2. \tag{1.14}$$

$$E_{\pm} = C \pm J. \tag{1.15}$$

Where, C represents energy corresponding to Coulomb interaction and J represents energy corresponding to exchange interaction. Value of J decides in which state system will tend to move either E_+ or E_-.

In the case, J is positive ($J > 0$) then, E_- (ground state) is a more favorable energy eigenstate which corresponds to the anti symmetric linear combination of the two electron spatial wave functions and a symmetric linear combination of the spin wave function gives rise to parallel spins result in ferromagnetism. While for the case, J is negative ($J< 0$) then E_+ (ground state) is a more favorable energy eigen state that corresponds to the symmetric linear combination of the two electron spatial wave functions and an anti symmetric linear combination of the spin wave function give rise to anti parallel spins resulting in anti ferromagnetism. (Note, for our convenience, we are using positive Hamiltonian ($\hat{H_{ex}}$), then $(J > 0)$ is for antiferromagnetism, and the case ($J < 0$) is for ferromagnetism).

1.1.9 Complete Hamiltonian

In the light of the above types of interaction, a complete Hamiltonian in the anisotropic medium under the influence of the magnetic field and due to the perturbations like spin-orbit coupling and Zeeman effect is given as [?]

$$H = JS_1.S_2 + \beta.(S_1 \times S_2) + \gamma\beta.\beta S_1.S_2 + \gamma(S_{1z} + S_{2z}). \tag{1.16}$$

Where, γ is the degree of anisotropy, which gives information about the interactions in different directions. Equation (1.12) is the complete form of the spin Hamiltonian in which the first term is due to Heisenberg exchange interaction, the second, and the third term is due to the spin-orbit coupling type perturbations, and the fourth term is due to the Zeeman effect which is of our interest to study the entanglement in the inhomogeneous field.

Although theoretically, investigations of entanglement for various forms of anisotropic interactions are interesting, they may or may not have considerable practical application in the physical realization of qubits. We neglect anisotropic perturbations in our thesis due to their small effects and the fact that ways to cancel such anisotropies have been developed [?]. The inhomogeneous Zeeman coupling is always possible in solid state qubit construction so, we are only considering the Hamiltonian of the type including spins exchange interactions and Zeeman effect given as,

$$H = JS_1.S_2 + \gamma(S_{1z} + S_{2z}). \tag{1.17}$$

1.2 The Heisenberg Model

Werner Heisenberg introduced the Heisenberg model in 1926. This model is used to describe the interacting spin systems and also includes the study of magnetic systems. The model contains discrete variables known as spins, which are arranged parallel or antiparallel manners at low temperatures in a lattice. This model is used to find out the Hamiltonian for the spin system including magnetism. The Hamiltonian for the nearest neighbor interaction in the Heisenberg model [5] is given as,

$$H = \sum_{n=1}^{N} (J_x S_n^x S_{n+1}^x + J_y S_n^y S_{n+1}^y + J_z S_n^z S_{n+1}^z). \tag{1.18}$$

The S_n^x, S_n^y, S_n^z are the local spin operators for the n^{th} site, and the J_x, J_y, J_z are coupling constants. When the two spins are aligned parallel to each other then, the product of spins will be +1 and if the spins are antialigned then products will be -1. When the value of the coupling constant is greater than zero, then there is antiferromagnetic interaction, and when its value is less than zero, there will be a ferromagnetic interaction. There are three components of spins (x,y,z), while interactions may have only one (Ising model), two (XX, YY model), or three (XXX, XYZ, XXZ) components.

1.2.1 The Ising Model

The Ising model is the most primitive theoretical explanation of ferromagnetism. Wilhelm Lenz invented this model in 1920 and solved it by his student, Ernst Ising [6]. In the Ising model, the interaction between the

spins is more effective in one direction (i.e. J_z), which is a special case of the Heisenberg model, then the other directions like (J_x, J_y), can be written as $J_z > J_x$ and $J_z > J_y$. Let's consider an external magnetic field having strength B is applied to N identical atoms forming a spin $\frac{1}{2}$ system. From equation (1.14), Hamiltonian of such a system is given by,

$$H = J\sum_{i=1}^{N} s_i s_{i+1} + B\sum_{i=1}^{N} s_i. \tag{1.19}$$

Where s_i is the i^{th} atomic spin with a component in the z-direction and J represents the spin-spin interaction.

There is an energy difference between the two cases, i.e. when two neighboring atoms spins are aligned parallel to each other as in the ferromagnetic case and the antiparallel alignment of spins in the case of the antiferromagnetic. The Pauli exclusion principle is largely responsible for this effect. Due to the Pauli exclusion principle electrons can't share the same quantum state. This implies that two electrons with parallel aligned spins on neighboring atoms can't come close to each other, but for the antiferromagnetic case, where the spins of electrons are aligned in antiparallel order, the Pauli exclusion principle allows them to share the same quantum state and occupy the proximity. Therefore, the exchange energy term J is different for the two cases due to their different spatial separation.

1.2.2 XXX Model

If J_x=J_y=J_z, this implies that the coupling constant has the same value along with all three directions, then the interaction will be kind of XXX model of

Heisenberg. Hamiltonian for this case is given as,

$$H = J\sum_{n=1}^{N}(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + S_n^z S_{n+1}^z). \tag{1.20}$$

$J > 0$ for the antiferromagnetic and $J < 0$ for the ferromagnetic case (as explained above). If $J_x \neq J_y \neq J_z$ then, the Heisenberg model is known as the XYZ model shows that the coupling constant has not the same value along with all three directions.

1.2.3 Heisenberg XY Model

The Hamiltonian for the nearest neighbor interaction is for the 1D anisotropic XY model is [7],

$$H_{XY} = \sum_{n=1}^{N}[(1+\gamma)S_n^x S_{n+1}^x + (1-\gamma)S_n^y S_{n+1}^y]. \tag{1.21}$$

Where, γ is the degree of anisotropy given as, γ=$J_x - J_y$ and $J_x + J_y$=1. The XY model is soluble for each value of γ, as gamma approaches to 1, XY model tends to the Ising model and for γ=0, it tends to XX model [8]

1.2.4 Heisenberg XXZ model

The Hamiltonian for the nearest neighbor interaction of the Heisenberg XXZ model is given as

$$H_{XXZ} = J\sum_{n=1}^{N}(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z), \tag{1.22}$$

where, Δ is the anisotropy parameter along the z-axis. For Δ=1, XXZ model $J_x = J_y = J_z$ turns into a XXX model having the Hamiltonian,

$$H_{XXX} = J \sum_{n=1}^{N} (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + S_n^z S_{n+1}^z), \tag{1.23}$$

and for Δ=0, XXZ model changes to the XX model given as,

$$H_{XX} = J \sum_{n=1}^{N} (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y). \tag{1.24}$$

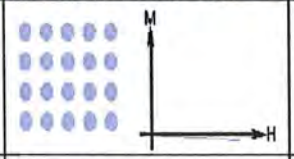
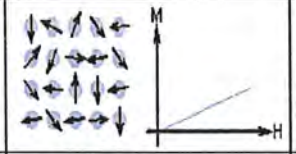
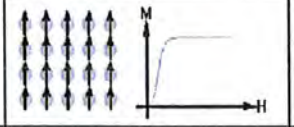
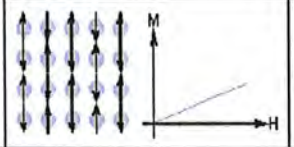
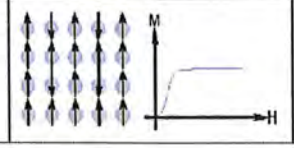
Type of Magnetism	Susceptibility	Atomic	Magnetic Behavior	Example	Susceptibility
Diamagnetism	Small & negative.	Atoms have no magnetic moment		Au Cu	-2.74×10^{-6} -0.77×10^{-6}
Paramagnetism	Small & positive.	Atoms have randomly oriented magnetic moments		β-Sn Pt Mn	0.19×10^{-6} 21.04×10^{-6} 66.10×10^{-6}
Ferromagnetism	Large & positive, function of applied field, microstructure dependent.	Atoms have parallel aligned magnetic moments		Fe	~100,000
Antiferromagnetism	Small & positive.	Atoms have mixed parallel and anti-parallel aligned magnetic moments		Cr	3.6×10^{-6}
Ferrimagnetism	Large & positive, function of applied field, microstructure dependent	Atoms have anti-parallel aligned magnetic moments		Ba ferrite	~3

Figure 1.1: Properties of materials

1.3 Postulates of Quantum Mechanics

1.3.1 Density matrix

We can comprehend the universe of subatomic particles, atoms, and molecules because of quantum mechanics theory. Two types of methods can be used to extract information from the physical quantum mechanical system. The state vector approach comes first, followed by the density matrix approach. State vector algebra is computed by solving the Schrodinger equation and is used for the particles in their pure state, but the density matrix technique is used when dealing with an ensemble of particles. Both procedures are comparable, but solving the Schrodinger equation becomes impossible when dealing with multipartite systems. As a result, the density matrix technique is preferred.

Pure quantum states and mixed quantum states are the two types of quantum states. A pure state is a quantum system in which the quantum state is known, whereas mixed states are quantum mechanical systems in which the complete information is unknown. Because it is impossible to construct a state vector for a mixed state, the density operator is used instead. The density operator is a general concept that can be used to describe both the pure and mixed states of any quantum system.

We suppose a quantum mechanical system exists in quantum state $|\psi_j\rangle$ with associated probabilities p_j, forming a statistical ensemble $[p_j,|\psi_j\rangle]$ of states to construct a density matrix theoretically. The density matrix is the

weighted average of the operators $|\psi_j\rangle\langle\psi_j|$, given as;

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|. \tag{1.25}$$

The quantum mechanical universe exists in an infinite-dimensional Hilbert space, which is a complex linear vector space with the property of commutativity and the density matrix is also known as the density operator since matrix in Hilbert space algebra correlates to operators in quantum mechanics. As a result, the two terms are interchangeable.

When there is only one known state, the equation (1.21) reduces to $\rho = |\psi><\psi|$, which is a pure state. For the determination of the state ρ whether it is pure or mixed, we have the following method, for the pure state,

$$Tr(\rho^2) = 1, \tag{1.26}$$

whereas for mixed state,

$$Tr(\rho^2) < 1. \tag{1.27}$$

So, in general, $P = Tr(\rho^2)$ is known as purity of the state. If purity is one, the state will be pure and will be mixed for the rest of the case.

1.3.2 Properties of density matrix

Properties of density matrix ρ related to an ensemble $[p_j, |\psi_j\rangle]$ are given as,

1. 1) The condition $Tr(\rho^2) = 1$ is basically trace preservation condition.

$$\begin{aligned}
\rho &= \sum_j p_j |\psi_j\rangle\langle\psi_j|, \\
\rho' &= \sum_j p_j Tr(|\psi_j\rangle\langle\psi_j|), \\
\rho' &= \sum_j < \psi_j(|\psi_j\rangle\langle\psi_j|)|\psi_j >, \\
\sum_j p_j &= 1.
\end{aligned} \tag{1.28}$$

where, $(Tr(\rho) = \rho')$.

1. 2) The fact that is a positive operator ρ means that its eigenvalues or probabilities are positive, implying that it fulfills the positivity criterion. To clarify the trace property, Assume that $|\eta >$ is an arbitrary Hilbert space state vector. Then,

$$\begin{aligned}
< \eta|\rho|\eta > &= \sum_j p_j| < \eta|(|\psi_j\rangle\langle\psi_j|)|\eta >, \\
&= \sum_j p_j| < \eta||\psi_j > |^2 \geq 0.
\end{aligned} \tag{1.29}$$

hence, positivity condition is fulfilled.

1. 3) Average value of an observer O is given as

$$\begin{aligned}
\langle O\rangle &= \sum_j p_j < O >_j, \\
&= \sum_j p_j Tr[O\rho_j], \\
&= Tr[O\sum_j p_j\rho_j], \\
Tr[A\sum_j p_j\rho_j] &=< O > .
\end{aligned} \tag{1.30}$$

1.3.3 Density matrix based postulates of quantum mechanics

The standard formulation of quantum mechanics in terms of the state vector is well known. However, taking the density matrix approach to quantum mechanics as opposed to the state vector approach is particularly productive in terms of solving multipartite problems. The next sections show how to reformulate quantum mechanics postulates in terms of density matrices.

1.3.4 Postulate 1

There is an operator ρ called density operator associated with any ensemble $(p_i, |\psi_j)$ that is a positive definite (hermitian) with trace one working on the Hilbert space of any isolated physical system in complex linear vector space (LVS) or Hilbert space where the inner product is specified. The density operator of the system is if the system is in some state j with matching probability p_j is given as,

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|.$$

1.3.5 Postulate 2

The time dynamics in closed systems are unitary and are described by Unitary Transformation. That is the quantum state ρ at time t_1 and $\rho^{'}$ a state a later time t_2 are related by a unitary operator, which only depends on the

limits of time.

$$\rho' = \sum_j U p_j |\psi_j\rangle\langle\psi_j| U^\dagger, \tag{1.31}$$

$$\rho' = U\rho U^\dagger. \tag{1.32}$$

1.3.6 Postulate 3

In quantum physics, measurements are characterized mathematically by a set of measurement operators called M_m, which acts on the density matrix of the quantum system being measured. The measurement result of the experiment is represented by the index m. The completeness connection applies to these measuring operators.

$$\sum_m M_m^\dagger M_m = I, \tag{1.33}$$

If the system is initially in the $|\psi_j\rangle$ state, the possibility of attaining outcome "m" is

$$P(m|j) = \langle\psi_j|M_m^\dagger M_m|\psi\rangle = Tr(M_m^\dagger M_m|\psi_j\rangle\langle\psi_j|), \tag{1.34}$$

the probability of getting results "m" is based on Baye's law of probability.

$$\begin{aligned} p(m) &= \sum_j P(m|j)P_j, \\ &= P_j Tr(M_m^\dagger|\psi_j\rangle\langle\psi_j), \\ P(m) &= Tr(M_m^\dagger M_m), \end{aligned} \tag{1.35}$$

the post measurement state can be defined as,

$$|\psi_j^m\rangle = \frac{M_m|\psi_j\rangle}{\sqrt{\langle\psi_j|M_m^\dagger M_m|\psi\rangle}}, \tag{1.36}$$

we have a post-measurement ensemble of state $|\psi_j^m\rangle$ that produces an outcome "m" with probability $p(i|m)$. The post-measurement density operator ρ_m is now defined as;

$$\begin{aligned} \rho_m &= \sum_j P(j|m) M_m|\psi_j^m\rangle\langle\psi_j^m|), \\ \rho_m &= \sum_j P(j|m) \frac{M_m|\psi_j\rangle\langle\psi_j|M_m^\dagger}{\langle\psi_j|M_m^\dagger M_m|\psi_j\rangle}, \end{aligned} \tag{1.37}$$

from elementary probability theory

$$P(j|m) = \frac{P(m,j)}{P(m)} = \frac{P(m|j)}{P(m)},$$

using relation in above equation

$$\rho_m = \sum_j \frac{P(m|j)}{P(m)} \frac{M_m|\psi_j\rangle\langle\psi_j|M_m^\dagger}{\langle\psi_j|M_m^\dagger M_m|\psi_j\rangle}. \tag{1.38}$$

gives the post measurement quantum state of the system.

1.3.7 Postulate 4

The tensor product of the Hilbert spaces of different parts of the physical system equals the Hilbert space of the composite system. If we have a multipartite system with a number ranging from 1 to n and states n, the system's

composite quantum state is;

$$\rho = \rho_1 \otimes \rho_2 \otimes \rho_3. \tag{1.39}$$

1.4 The reduced density matrix

In quantum physics, we are sometimes more interested in parts of a composite system than the total physical system when dealing with multipartite systems. For example, if we have a two-particle system with density matrix ρ_{AB} and we want to discover its parts ρ_A and ρ_B, we can use the partial trace operation on ρ_{AB}. The partial trace procedure eliminates the information from one portion of the subsystem while keeping the information from the other part of the subsystem untouched in AB. To locate ρ_A from ρ_{AB}, for example, we must conduct a partial trace concerning subsystem B to find then,

$$\rho_A = Tr_B(\rho_{AB}), \tag{1.40}$$

In the same manner, for system ρ_B, partial tracing across subsystem A is used.

$$\rho_B = Tr_A(\rho_{AB}), \tag{1.41}$$

Also, for 2 state vectors ψ_1 and ψ_2 in subsystem A and ϕ_1 and ϕ_2 vectors in subsystem B then, partial trace over B and A becomes

$$\begin{aligned} \rho_A &= Tr_B(|\psi_1\rangle\langle\psi_2| \otimes |\phi_1\rangle\langle\phi_2|), \\ &|\psi_1\rangle\langle\psi_2|Tr_B|\phi_1\rangle\langle\phi_2|, \\ &|\psi_1\rangle\langle\psi_2|Tr_B\langle\phi_1|\phi_2\rangle, \\ \rho_B &= Tr_A(|\psi_1\rangle\langle\psi_2| \otimes |\phi_1\rangle\langle\phi_2|)|, \end{aligned} \tag{1.42}$$

$$\rho_B = |\psi_1\rangle\langle\psi_2|Tr_A\langle\phi_1|\phi_2\rangle. \tag{1.43}$$

We exploited the fact that the trace of any operator O, which is effectively an outer product, turns into an inner product $Tr(|o\rangle\langle p|) = \langle o|p\rangle$ in equations, (1.23) and (1.24).

1.5 The classical information entropy

In information theory, our primary goal is to send a message from the transmitter to the receiver over a channel. To do this, the transmitter delivers a succession of partial messages or a single message to the receiver, which are combined to generate the original message. The content of one of these incomplete messages is used to determine how much uncertainty is removed from the receiver's interpreter. The predicted content of the information provided by a stochastic or random data source is known as the information entropy. Assume, we have a stochastic data source represented by a random variable X, which has a finite number of outcomes, also known as events.

Let's say, we take a measurement of X and get a value. Then entropy is described as the quantity of the knowledge gained after measuring X or as the amount of uncertainty present before measuring X. Both statements are mutually exclusive. Entropy is a measure of the various possible values of event or outcome probabilities of random variable X. Assume that the variable's sample space is

$$X = P_1, P_2, ...P_{n-1}, P_n, \tag{1.44}$$

The Shannon entropy of random variable X is defined as follows:

$$H(X) = H(P_1, P_2, ...P_{n-1}, P_n) = -\sum_j P_j \log_2 P_j, \tag{1.45}$$

With 0(log(0))=0, an event with zero probability and thus no chance of occurring has zero entropy. The negative sign is since $log(p_j < 1)$ produces a negative number, and as entropy cannot be negative, the minus sign of this log, together with the predetermined minus sign in the equation (1.41), produces positive entropy.

Bits are used to define entropy. The information entropy of an occurrence with a low probability will be high, and vice versa.

1.5.1 Binary Entropy

We'll use the example of a random variable X for a stochastic data source with just two outcomes to better understand the property of information entropy. $X = p, 1-p$, where p is the first event's probability and *1-p* is the

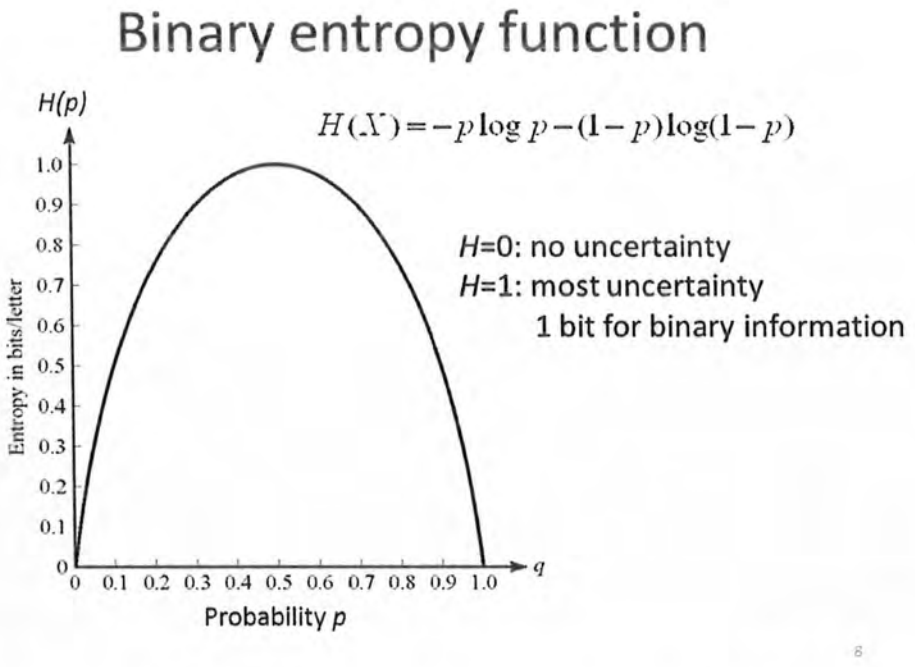


Figure 1.2: Plot of binary entropy H(p) verses probability

second event's binary entropy is the entropy associated with this bipartite system, which becomes,

$$H(X) = -PlogP - (1-P)log(1-P), \tag{1.46}$$

is plotted above. It is clear from the figure of binary entropy that Entropy *H(p)* reaches its highest value at $P = \frac{1}{2}$, which is obvious if we assume we have a fair coin, in which case entropy should be maximum because we cannot expect specific outcomes head or tail because both have half probability, so the entropy should be maximum in this case.

1.5.2 Relative entropy

The relative entropy of two probability distributions *p(x)* and *q(x)* define how close they are to each other. They have a certain amount of entropy, if they coincide, they are the same and their relative entropy is zero and if they are indefinitely apart, their entropy is maximized.

$$H(P(x)||q(x)) \equiv \sum_x P(x) log \frac{p(x)}{q(x)} \equiv -H(x) - \sum_x p(x) log\, q(x), \qquad (1.47)$$

As, it is already defined -0(log(0))=0 and -p(x)log(o)=+ inf, if p(x)>0 The relative entropy is non-negative, with $H(p(x)||q(x)) \geqslant 0$ and equality if *p(x)* = *q(x)*.

1.5.3 Joint entropy

When we want to know the total entropy of a system with a set of random variables, we use the term joint entropy. Assume that a system has two random variables, X and Y. The mathematical definition of joint variable entropy is,

$$H(x, y) = -p(x, y)\, log\, p(x, y), \qquad (1.48)$$

This can be generalized to n number of random variables as,

$$H(x_1, x_2, ...x_n) = -p(x_1, x_2, ..x_n)\, log\, p(x_1, x_2, ...x_n).$$

1.5.4 Conditional entropy

We'll use two random variables, system X and Y, to understand conditional entropy. Now, the definition of conditional entropy answers the question, how much uncertainty is there in the system when the entropy of one of the random variables is identified? The remaining uncertainty of the pair *(X, Y)* is known as conditional entropy if we know the value of Y and hence *H(Y)*. Mathematically,

$$H(X|Y) = H(X,Y) - H(Y), \tag{1.49}$$

So, conditional entropy is the average level of uncertainty we have about the system, taking into account the fact that we know the entropy of one of the random variables.

1.5.5 Mutual Information

The number of mutual information is defined as; it measures how much information is shared random variables X and Y.

$$H(X:Y) = H(X) + H(Y) - H(X,Y), \tag{1.50}$$

using equation (1.45) above eq can be written as,

$$H(X:Y) = H(X) - H(X|Y), \tag{1.51}$$

we are now in a position to discard the Shannon entropy properties.

1. 1) $H(X,Y)=H(Y,X)$, $H(X:Y)=H(Y:X)$,

1. 2) $H(Y|X)\geq 0$ and thus $(X:Y)\leq H(Y)$ where, equality holds when $Y=f(X)$

1. 3) $H(X,Y)\leq H(X)+H(Y)$, where, equality only holds if Y and X don't depend on each other this is known sub-additivity.

1. 4) $H(X)\leq H(X,Y)$ where, equality holds if and only if $Y=f(X)$.

1. 5) $H(Y|X) \leq H(Y)$ and thus $H(X:Y)\geq 0$ where, equality holds if Y and X don't depend on each other.

1.6 The quantum information entropy

In quantum information theory [9], the von Neumann entropy or quantum information entropy is defined similarly to the Shannon entropy, which is calculated on a classical probability distribution in classical information theory. Theorems on Shannon entropies are parallel applied to quantum information theory.

1.6.1 Von Neuman entropy

The Vonn Neuman entropy is a quantum theory counterpart of the Shannon entropy, in which the probability distribution is replaced by a density operator matrix as the source of information. Vonn Neuman entropy is written as,

$$S(\rho) = -Tr\,(\rho\, log\, \rho), \tag{1.52}$$

it is assumed that the logarithm has a base of two. If λ_j are the density matrix eigenvalues, then

$$S(\rho) = -\sum_j \lambda_j log \lambda_j \tag{1.53}$$

with already defined 0(log0)=0.

1.6.2 Properties of Vonn Neuman entropy

- The entropy of a system is always positive. Only when the entropy is zero. then the quantum state is pure.
- The entropy in n-dimensional Hilbert space is at most equal to log (n). If and only if the quantum state is maximally mixed $\frac{I}{n}$, the entropy is equal to $\log(n)$, where I is the identity matrix of order n.
- When a composite system in a pure state then, *S(A)=S(B).*
- Assume that p_j is the probability and the state j have orthonormal subspace support. Then,

$$S(\sum_j p_j \rho_j) = H(p_j) + \sum_j p_j S(\rho_j), \tag{1.54}$$

- Under unitary translation, the von Neuman entropy is invariant, implying that

$$S(\rho) = S(U \rho U^\dagger).$$

- $S(\rho)$ exists for the independent uncorrelated system addivity. Additivity exists if we have two density matrices ρ_A and ρ_B that correspond to two

parties A and B, respectively.

$$S(\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B). \tag{1.55}$$

- If we have three parties, *A, B, and C*, the entropy *S(ρ)* is subadditive.

$$S(\rho_{ABC}) + S(\rho_B) \leqslant S(\rho_{AB}) + S(_{BC}),$$

it guarantees that the subaddivity exists for *S(ρ)*.

$$S(\rho_{AC}) \leqslant S(\rho_A) + S(\rho_C). \tag{1.56}$$

1.6.3 Quantum relative entropy

Quantum relative entropy is a reasonable statistical measure of quantum state distinguishability. It's a density operator distance measure that's entropic. The measure of distinguishability between two quantum states is quantified by quantum relative entropy if we have two density matrices. The quantum mechanical equivalent of classical relative entropy is defined as

$$S(\rho||\sigma) = Tr(\rho\, log\, \rho) - Tr(\rho\, log\, \sigma), \tag{1.57}$$

below are a few features of quantum relative entropy.

The quantum relative entropy $S(\rho||\sigma) \geqslant 0$ is not negative. When the condition $\rho = \sigma$ is fulfilled, equality is achieved. It is a continuous function if infinities do not exist in the evaluation of quantum relative entropy.

If we have density operators ρ_1, ρ_2, σ_1, σ_2 with probability p_1, p_2, then relative entropy is jointly convex in its argument

$$S(\rho||\sigma) \leqslant p_1 S(\rho_1||\sigma_1) + p_2 S(\rho_2||\sigma_2), \tag{1.58}$$

with $\rho = p_1\rho_1 + p_2\rho_2$ and $\sigma = p_1\sigma_1 + p_2\sigma_2$. The convexity in each argument automatically matches to the convexity in the joint convexity, resulting in

$$S(\rho||\sigma) \leqslant p_1 S(\rho_1||\sigma_) + p_2 S(\rho_2||\sigma). \tag{1.59}$$

Chapter 2

Thermal Entanglement in two qubits Heisenberg XXX model under Inhomogenous magnetic field

2.1 Entanglement

Quantum entanglement is a physical phenomenon that occurs when a set of particles is generated, communicated, or having spatial proximity in such a manner that the quantum state of every particle in the group cannot be characterized independently of the state of all others, even though the particles are isolated. Entanglement, a quantum correlation is not only a fundamental notion in quantum computing, quantum teleportation, and quantum dense coding [10, 11]. To investigate the thermal entanglement in the Heisenberg

spin in order to better comprehend the quantum correlation properties of this model [12, 13].

2.1.1 Thermal Entanglement Quantifier

Let's suppose that a composite system S^{AB} is prepared by Alice or Bob through Local operations on the subsystems S^A and S^B. Alice and Bob can exchange Information through classical communication. During the preparation of the S^{AB} through local operation and classical communication (LOCC), Alice prepares the system S^A in the state ρ_r^A and Bob prepares his system S^B in the state ρ_r^B which is different from that prepared by Alice. The composite state ρ^{AB} is the mixture of the product state as,

$$\rho^{AB} = \sum_{r=1}^{m} p_r \rho_r^A \otimes \rho^B, \tag{2.1}$$

The above equation is valid for the classically correlated state. When the states are non classically correlated, then

$$\rho^{AB} \neq \sum_{r=1}^{m} p_r \rho_r^A \otimes \rho^B, \tag{2.2}$$

To find a correlation between the two subsystems of a composite system, we use the density matrix approach. Density matrix ρ is a mixture of classical and quantum correlations. Von Neuman entanglement entropy or quantum concurrence does give some values, although the states of the density matrix could be classically correlated. So, essentially difficulty with the density matrix is that it is a mixture of classical and quantum correlations, and usually

standard pure state entanglement measures like von Neuman entanglement entropy can not identify these classically prepared states or can not distinguish classical correlations from quantum correlations.

To avoid this problem, let's suppose that one wants to find entanglement between two subsystems, where the entire system is in contact with some thermal bath, then the state of the composite system can be represented by the density matrix $\rho = e^{\frac{H}{KT}}$.

2.1.2 Negativity

Partial transpose could be helpful in integrally characterizing thermal entanglement in such states. By taking the partial transpose of a density matrix, one may get negative eigenvalues which is an indication of the nonseparable entangled states, then one may define a measure of entanglement in terms of the absolute value of those negative eigenvalues are known as negativity. Entanglement negativity measures quantum dimensions of underlying degrees of freedom on the chain spins system. Negativity is entanglement monotone and easy to compute. Negativity is a simple way to compute a measure of quantum entanglement in quantum physics. It's a criterion for separability [14] derived from the PPT criterion.

The positive partial transpose **PPT criterion** or Peres-Horodecki criterion is an essential condition of the joint density matrix of two systems A and B to be separable. For the state $\rho^{'}$ of composite system $H_A \otimes H_B$

$$\rho^{'} = \sum_{ijkl} P_{kl}^{ij} |i\rangle\langle j| \otimes |k\rangle\langle l|, \tag{2.3}$$

its partial trace over B, is given as

$$Tr_B(\rho^{'}) = \sum_{ijkl} P_{kl}^{ij} |i\rangle\langle j| \otimes |l\rangle\langle k| = \sum_{ijkl} P_{lk}^{ij} |i\rangle\langle j| \otimes |k\rangle\langle l|. \tag{2.4}$$

$\rho^{'}$ is separable for positive eigenvalues of the $Tr_B(\rho^{'})$ and for negative eigenvalues, $\rho^{'}$ is entangled. The partial transpose of the density matrix of a separable state (not entangled) is also a valid state. One or more than one negative eigenvalue appears in the partial transpose of a non separable state. The degree to which a state violates the positive partial transposition separability condition is indicated by the negativity of the state. In terms of a density matrix, the negativity of subsystem A can be defined as:

$$N(\rho) = \frac{Tr_A(\rho) - 1}{2} \tag{2.5}$$

2.1.3 Quantum Mixedness

The constant interaction of quantum systems with the environment results in decoherence has an impact on the purity of any quantum state. Noise causes mixedness in the quantum system, resulting in information loss. As a result, characterizing it is an important challenge in quantum information protocols. The mixedness, which is nothing more than the system's disorder, can be expressed using entropic functions. For a given d dimensional state, we define quantum mixedness as,

$$M = \frac{d}{d-1}[1 - Tr(\rho^2)]. \tag{2.6}$$

Where d represents the dimension of given state ρ. For a pure state, having a density matrix ρ, $\mathrm{Tr}(\rho^2)$=1 and for a mixed state, $Tr(\rho^2) < 1$. As a result, mixedness fluctuates between 0 and 1 for each quantum system. No quantum system is completely isolated, due to this interaction information loss due to an increase in entropy of the quantum system. So, it's very important to discuss the decoherence effect. In our present system as we are discussing the thermal effect on the entanglement in which our system is contacting with the heat bath for which we use quantum mixedness to study the interaction between the spins system and heat bath. The states that achieve the maximum entanglement for a given mixedness are called maximally entangled mixed states.

The maximal entanglement that may be produced between a quantum system and an incoherent ancillary through incoherent operations are limited by the system's mixedness. All effective asymptotic entanglement metrics are either the same or fail to yield uniformly consistent density matrix orderings given by Virmani and Plenio. Furthermore, determining the MEMS form requires quantifying the mixedness of a state and for mixedness, there can also be ordering issues. This shows that the MEMS may depend on mixedness measurements as well.

2.2 The Model

Consider two qubit system placed in an independently controllable non-uniform magnetic field *(B-b)* and *(B+b)*, for which the Hamiltonian is defined

as;

$$Hxxx = J(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y + \sigma_1^z\sigma_2^z) + (B-b)\sigma_1^z + (B+b)\sigma_2^z, \tag{2.7}$$

where, J is the exchange coupling constant between spins, $\sigma_n^\alpha(\alpha = x, y, z)$ are the Pauli spin operators. The $J < 0$ corresponds to the ferromagnetic case and $J > 0$ corresponds the antiferromagnetic chain case. The degree of inhomogeneity in uniform magnetic field B is indicated by b which shows an independent magnetic field. We're treating our system in units B, b, *and* J thus, we're in dimensionless units. Since we are using natural units or geometrized units, so we set Planck's and Boltzmann's constants into one h=k=1. The augmented matrix form of Hamiltonian can be written as in the conventional computational base $|00\rangle, |01\rangle, |10\rangle, |11\rangle$ can be written as follows.

$$H = \begin{pmatrix} J-2B & 0 & 0 & 0 \\ 0 & -J+2b & 2J & 0 \\ 0 & 2J & J-2B & 0 \\ 0 & 0 & 0 & J+2B \end{pmatrix} \tag{2.8}$$

The corresponding eigenvalues and eigenvectors of H are given as,

$$\begin{aligned} E_o &= -J + 2B, \\ E_1 &= -J - \sqrt{J^2 + b^2}, \\ E_2 &= -J + \sqrt{J^2 + b^2}, \\ E_3 &= 2B + J, \end{aligned} \tag{2.9}$$

$$
\begin{aligned}
\psi_0 &= |00\rangle, \\
\psi_1 &= N_1(a_1|01\rangle + |10\rangle), \\
\psi_2 &= N_2(a_2|01\rangle + |10\rangle), \\
\psi_3 &= |11\rangle,
\end{aligned}
\tag{2.10}
$$

where, functional form of constants a_1, a_2, N_1, N_2 are given as;

$$
\begin{aligned}
a_1 &= \frac{-b - \sqrt{J^2 + b^2}}{J}, \\
a_2 &= \frac{-b + \sqrt{J^2 + b^2}}{J}, \\
N_1 &= \frac{1}{\sqrt{a_1^2 + 1}}, \\
N_2 &= \frac{1}{\sqrt{a_2^2 + 1}}.
\end{aligned}
\tag{2.11}
$$

2.3 Thermal properties

As a two qubit system is in thermal contact with the heat bath which maintains its constant temperature T. After establishing thermal equilibrium between system and surrounding is established so, we can write thermal state of the system is given below;

$$
\rho(T) = \frac{e^{-\frac{H}{KT}}}{Z}, \tag{2.12}
$$

where, $Z = tr([e^{\frac{H}{KT}}])$ is the system's partition function, and K represent Boltzmann constant. In the current system, the partition function and den-

sity matrix are as follows:

$$Z = exp(\frac{2B-J}{KT}) + exp(\frac{J+\sqrt{J^2+b^2}}{KT}) + exp(\frac{J-\sqrt{J^2+b^2}}{KT}) + exp(\frac{-2B-J}{KT}), \tag{2.13}$$

$$\begin{aligned}\rho(T) = \frac{1}{Z}exp(\frac{2B-J}{KT})|\psi_0\rangle\langle\psi_0| + exp(\frac{J+\sqrt{J^2+b^2}}{KT})|\psi_1\rangle\langle\psi_1| \\ +exp(\frac{J-\sqrt{J^2+b^2}}{KT})|\psi_2\rangle\langle\psi_2 + exp\frac{-2B-J}{KT}|\psi_3\rangle\langle\psi_3|,\end{aligned} \tag{2.14}$$

Putting (2.5) in (2.4) and (2.4) in (2.8), we get

$$\rho(T) = \frac{1}{Z}\begin{pmatrix} u & 0 & 0 & 0 \\ 0 & w & y & 0 \\ 0 & y & x & 0 \\ 0 & 0 & 0 & v \end{pmatrix}, \tag{2.15}$$

where,

$$\begin{aligned} u &= exp(-\frac{E_0}{KT}), \\ v &= exp(-\frac{E_3}{KT}), \\ y &= N_1^2 a_1 exp(-\frac{E_1}{KT}) + N_2^2 a_2 exp(-\frac{E_2}{KT}), \\ w &= N_1^2 a_1 exp(-\frac{E_1}{KT}) + N_2^2 a_2 exp(-\frac{E_2}{KT}), \\ x &= N_1^2 exp(-\frac{E_1}{KT}) + N_2^2 exp(-\frac{E_2}{KT}). \end{aligned} \tag{2.16}$$

Now, we are going to numerically discuss the results of thermal entanglement by using a major called negativity discussed below.

Chapter 3

Numerical results of thermal Entanglement

We start with ferromagnetic case and antiferromagnetic. Furthermore, there are two magnetic field cases in each of them with a uniform magnetic field ($B\neq0$, $b=0$) and non-uniform magnetic field ($B=0$, $b\neq0$). Where, the unit of temperature is inverse of the unit of Boltzmann constant while magnetic field is dimensionless.

3.1 Negativity

when J<0

For the sake of simplicity, we set $J=-1$ which is a ferromagnetic case.

3.1.1 Uniform magnetic field in ferromagnetic case

The plot of negativity as a function of temperature T, uniform magnetic field B in ferromagnetic case (J=-1).

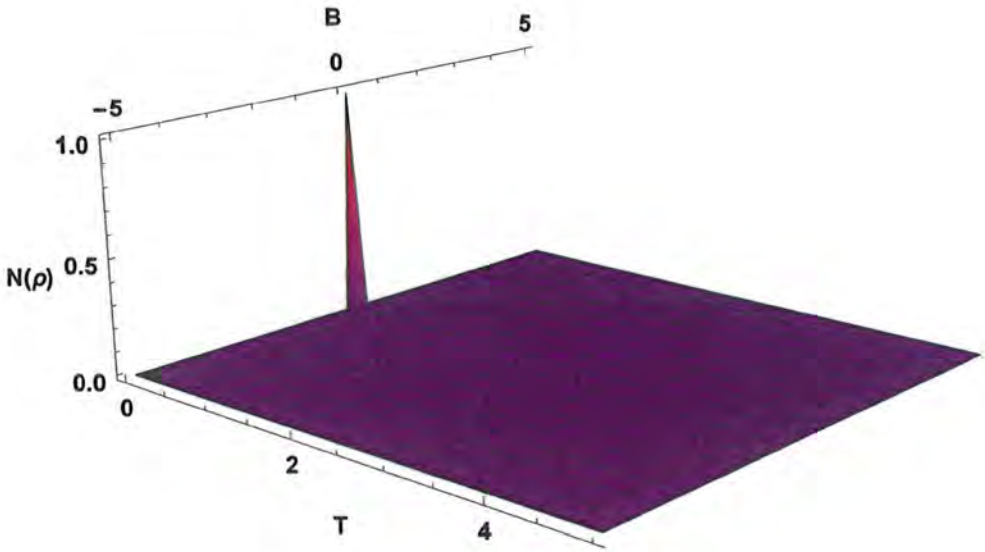


Figure 3.1: N(ρ) plotted against B and T

Figure 3.1 shows that the value of negativity is zero for each value of magnetic field B and temperature except at zero in the case of ferromagnetic in the presence of the uniform magnetic field. This shows that ferromagnetic materials do not exhibit entanglement within the system in the presence of a uniform magnetic field. It can also be observed from the graph that at small values of B approach to zero and at an absolute zero value of temperature negativity shows a peak, which indicates the presence of entanglement that is very sensitive to the magnetic field. As with a small variation in the field B and T from zero, negativity goes to zero. So in general, there is no

entanglement present in the ferromagnetic materials under the influence of uniform magnetic field B at finite temperature.

3.1.2 Ferromagnetic case in non-uniform magnetic field

The plot of negativity as a function of temperature T, non-uniform magnetic field b in ferromagnetic case (J=-1). From figure (3.2), negativity decreases

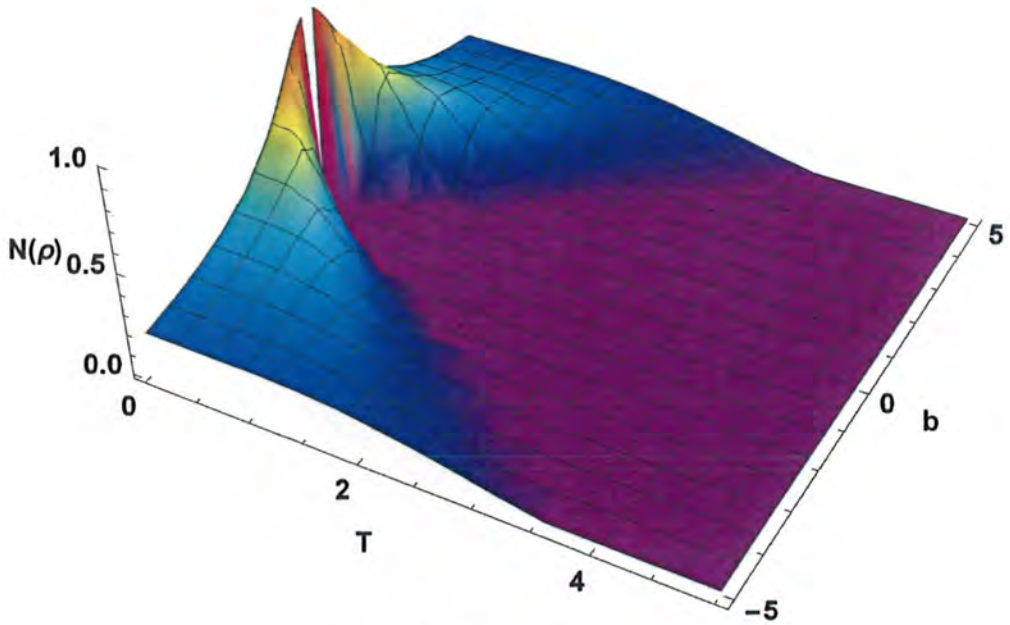


Figure 3.2: N(ρ) plotted against b and T

with increasing both temperature and non-uniform magnetic field as shown in the graph.

Negativity shows a very interesting behavior which is symmetric when plotted against the non-uniform magnetic field b and temperature T. In the

absence of the non-uniform magnetic field and at zero temperature, negativity has the minimum value approaches to zero. For the small values of the non-uniform magnetic field b and at low temperature, negativity is maximum which indicates the presence of the entanglement, but this behavior is only valid for small values of b and with further increase the value of non-uniform magnetic field b and temperature T, negativity also decreases eventually approaches to zero. This shows that in the absence of non-uniform external field and zero temperature, there is no entanglement, but for the smaller values of the non-uniform magnetic field b approaches to zero and at low temperature, there is some entanglement which decreases with increasing non-uniform magnetic field b and temperature T. This means that an infinitesimal magnetic field applied in opposite directions to the two spins at zero temperature maximizes the entanglement between two spins which decreases with increasing magnetic field.

when J>0

For the sake of simplicity, we set J=1, which is a antiferromagnetic case.

3.1.3 Antiferromagnetic case with uniform magnetic field

The plot of negativity as a function of temperature T, uniform magnetic field B in antiferromagnetic case (J=1). Figure (3.3), shows that the negativity is maximum when the external magnetic field is zero or very small and symmetric. It can easily be seen that negativity is maximum in the

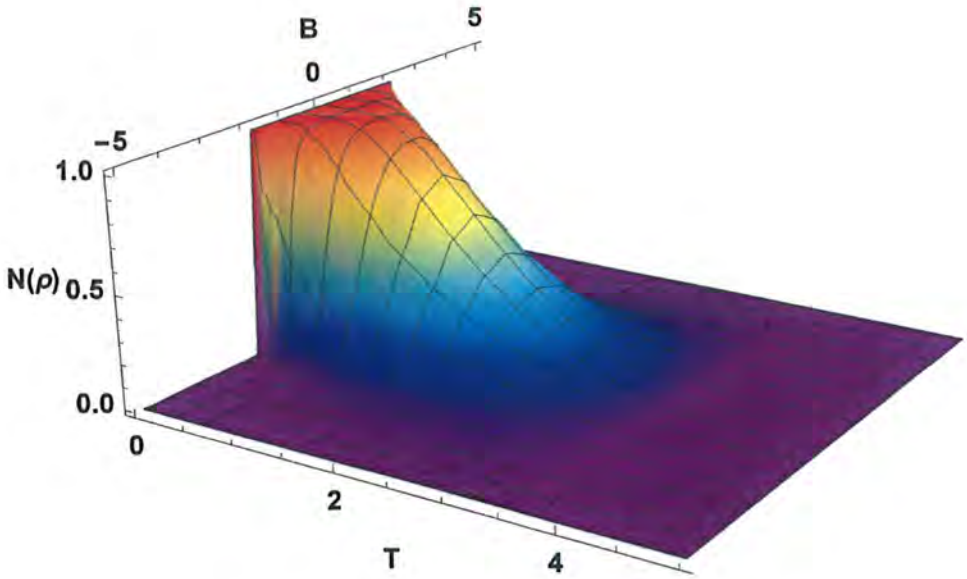


Figure 3.3: N(ρ) plotted against B and T

limit $-2 < B < 2$ and absolute zero value of temperature T. So, entanglement decreases, increasing temperature in the antiferromagnetic case with the uniform magnetic field. Negativity shows an abrupt transition at B=2 to zero i.e. entanglement in the system becomes zero at this specific value of the field also it decreases with increasing the temperature and eventually goes to zero when the temperature is large enough.

3.1.4 Antiferromagnetic case with non-uniform magnetic field

Figure (3.4), negativity in the presence of non-uniform magnetic field for antiferromagnetic case plotted against b and T, shows that negativity decreases with increasing temperature and magnetic field and eventually goes to zero for higher temperatures. For small values of the non-uniform magnetic field

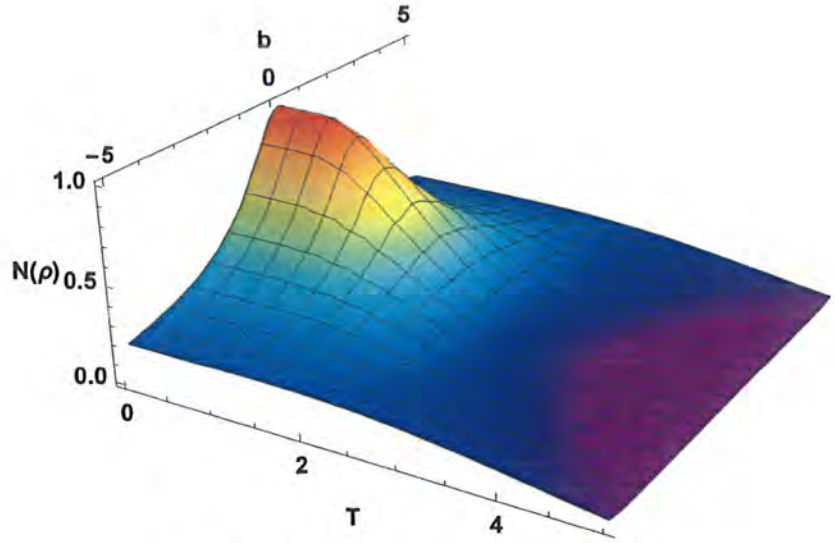


Figure 3.4: N(ρ) plotted against b and T

b and temperature T, negativity is large and hence entanglement is present and is maximum in the absence of inhomogeneous magnetic field and at an absolute zero value of temperature T.

Figure (3.4), also represent that negativity shows the symmetric behavior when plotted against non-uniform magnetic field b and decreases with increasing non-uniform magnetic field and also with temperature and hence entanglement decrease with increasing non-uniform magnetic field and also with temperature.

3.2 Quantum Mixedness

when $J<0$

For the sake of simplicity, we set J=-1 which is the ferromagnetic case.

3.2.1 Ferromagnetic case with uniform magnetic field

The plot of quantum mixedness as a function of temperature T, uniform magnetic field B in ferromagnetic case (J=-1).

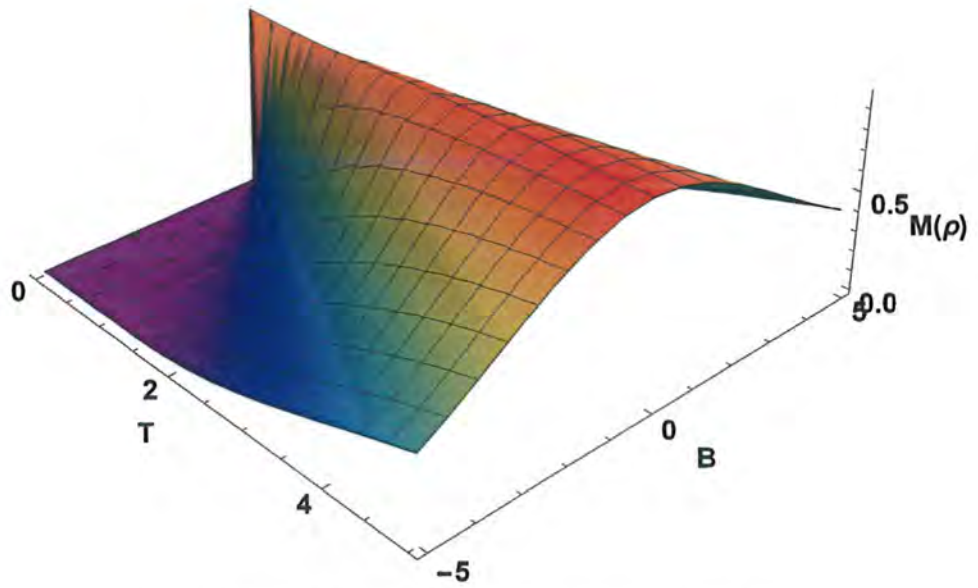


Figure 3.5: QM plotted against B and T

Figure (3.5), it is evident that the QM is symmetric with regard to the uniform magnetic field. Furthermore, it demonstrates that at lower temperatures, the QM decays rapidly as the uniform field increases, whereas at higher temperatures, the QM is maximum but with increasing uniform magnetic field QM decays slowly and has a maximum value in the absence of a uniform magnetic field.

Figure (3.5), also shows that QM for the ferromagnetic case with a uniform magnetic field for different values of B increases with increasing tem-

perature implies that decoherence and the entropy of the system increases which lead to the loss of the entanglement.

3.2.2 Ferromagnetic case in non-uniform magnetic field

The plot of quantum mixedness as a function of temperature T, non-uniform magnetic field b in ferromagnetic case (J=-1).

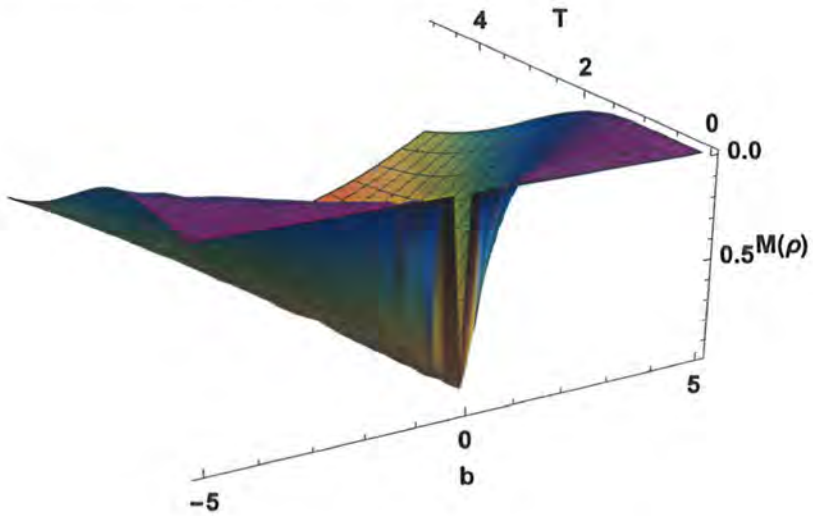


Figure 3.6: QM plotted against b and T

Figure (3.6), for different fixed values of temperatures, it is evident that the QM has symmetric behavior when plotted against the non-uniform magnetic field b. Furthermore, QM has maximum value in the absence of a non-uniform magnetic field b. It demonstrates that at a lower temperature, the QM decays rapidly as the uniform field values increases, whereas at higher temperatures, the QM decays slowly so, for ferromagnetic case in the presence of a non-uniform magnetic field shows a unique behavior than for the rest of the cases which means that non-uniform magnetic field decreases the

entropy of the system.

Figure (3.6), shows that QM for the ferromagnetic case with non-uniform magnetic field for different values of b increases with increasing temperature.

when $J>0$

For the sake of simplicity, we set J=1, which is an antiferromagnetic case.

3.2.3 Antiferromagnetic case in uniform magnetic field

The plot of quantum mixedness as a function of temperature T, uniform magnetic field B in antiferromagnetic case (J=1).

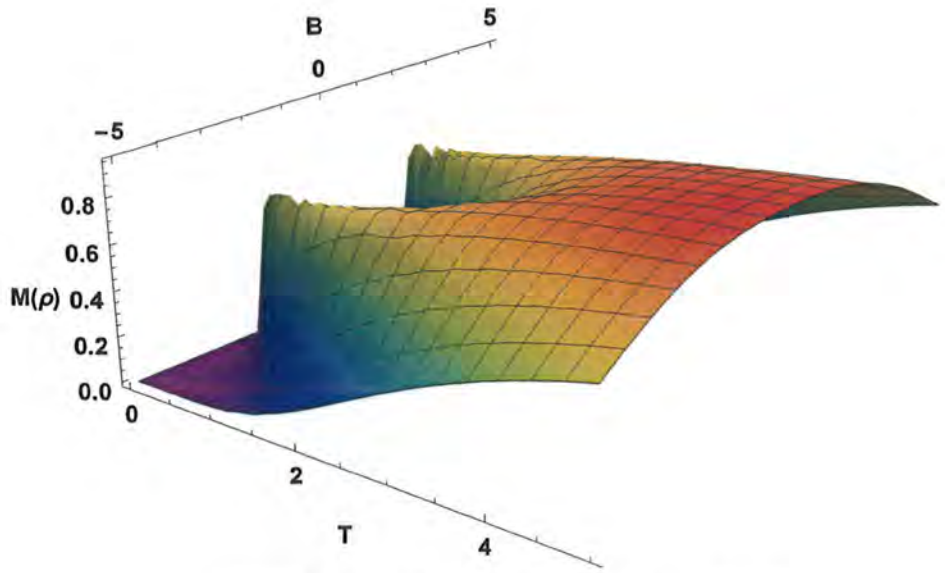


Figure 3.7: QM plotted against B and T

Figure (3.7), shows that QM for the antiferromagnetic case plotted against a uniform magnetic field B and temperature T has the symmetric behavior and has maximum peak value for B=2, on further increasing B beyond 2,

QM starts decreasing eventually to zero. When a uniform magnetic field is zero or in the limit $-2 < B < 2$, QM is zero at low temperature T but for higher temperature T, QM has some value even in the absence of the uniform magnetic field implies that entropy increases.

Figure (3.7), shows that QM has zero value at low temperatures and uniform magnetic field except for higher fixed values of the uniform magnetic field like B=2, mixedness is zero even at zero temperature and start increasing with increasing temperature to the maximum value.

3.2.4 Antiferromagnetic case with non-uniform magnetic field

The plot of quantum mixedness as a function of temperature T, non-uniform magnetic field b in antiferromagnetic case (J=1).

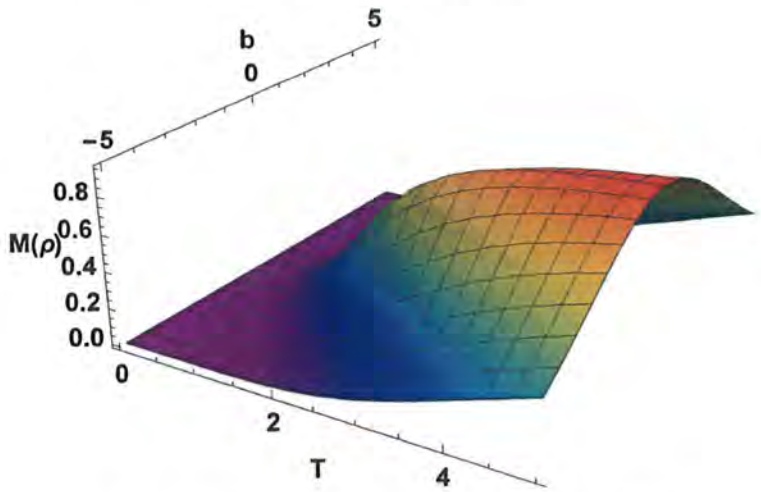


Figure 3.8: QM plotted against b and T

Fig. 3.8, shows that QM for the antiferromagnetic case with non-uniform magnetic field plotted against b has the symmetric behavior and starts decreasing with increasing b and for higher values of temperature T. QM is minimum in the absence of the non-uniform magnetic field b, at low temperature T, but at higher temperature T, QM is maximum even in the absence of inhomogeneous magnetic field and decrease with increasing temperature, which shows that entropy is minimum in the absence or for low values of inhomogeneous magnetic field for the low temperature and start decreasing with increasing temperature.

3.3 Collective study of thermal Entanglement

We have discussed a quantifier to study the thermal entanglement for ferromagnetic and antiferromagnetic cases, for uniform and non-uniform magnetic fields for different values of temperature as negativity and we also use quantum mixedness to study the effect of the heat bath on the spin system, here we are going to compare mentioned two quantifiers. The following graphs for the 2 different quantifiers i.e., negativity(blue solid), quantum mixedness QM (green dotted) is discussed in different cases as mentioned below.

When $J<0$

For the sake of simplicity, we set J=-1 which is a ferromagnetic case.

3.3.1 Ferromagnetic case in uniform magnetic field

The plots of negativity and QM as a function of temperature T, for fixed values of uniform magnetic field B in ferromagnetic case (J=-1).

In figure (3.9), for the ferromagnetic case with a fixed value of the uniform magnetic field B when plotted against temperature T, negativity shows zero response for all values of B and over entire rang of T while for $B=0$, QM has large value even in absence of B and at absolute zero T and increase with increasing temperature T as shown in figure 3.9(a), but in the presence of homogeneous magnetic field B, QM goes to zero for low temperature T approaches to zero and increase rapidly with increasing temperature as shown in figure (3.9)(b, c). It is also observed in absence of homogeneous magnetic field B, negativity is minimum having zero response for all values of the

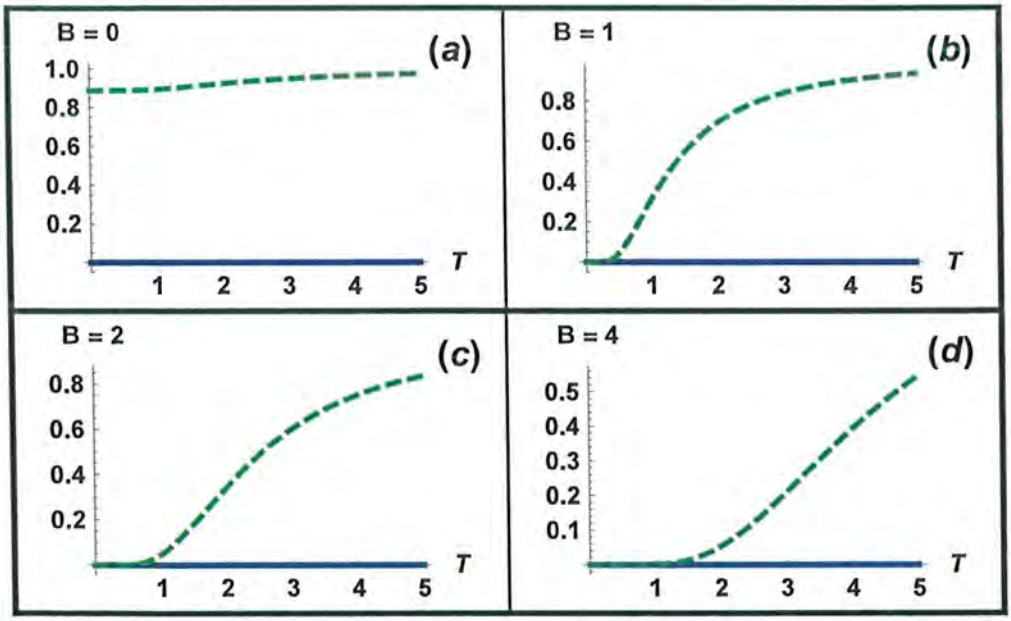


Figure 3.9: N(ρ) and QM plotted against T, for fixed values of B

uniform magnetic field and temperature, but QM shows zero response for small values of uniform magnetic field and temperature approaches to zero are shown in fig 3.9(b, c, d) which is an indication for the presence of the noise in the system which leads the system to the loss of correlation.

In fig. (3.10), in the ferromagnetic case with a fixed value of temperature T, when plotted against uniform magnetic field B, negativity shows zero response for all values of T. For T=0, QM is also zero, mean entanglement does not appear in the system in the absence of the uniform magnetic field, and the absolute value of temperature is shown in fig 3.10 (a). For all the other values of temperature except for T=0, negativity is still zero, but QM is maximum in the absence of homogeneous field and decreases rapidly for small values of temperature T, and slowly for higher values of the temperature with

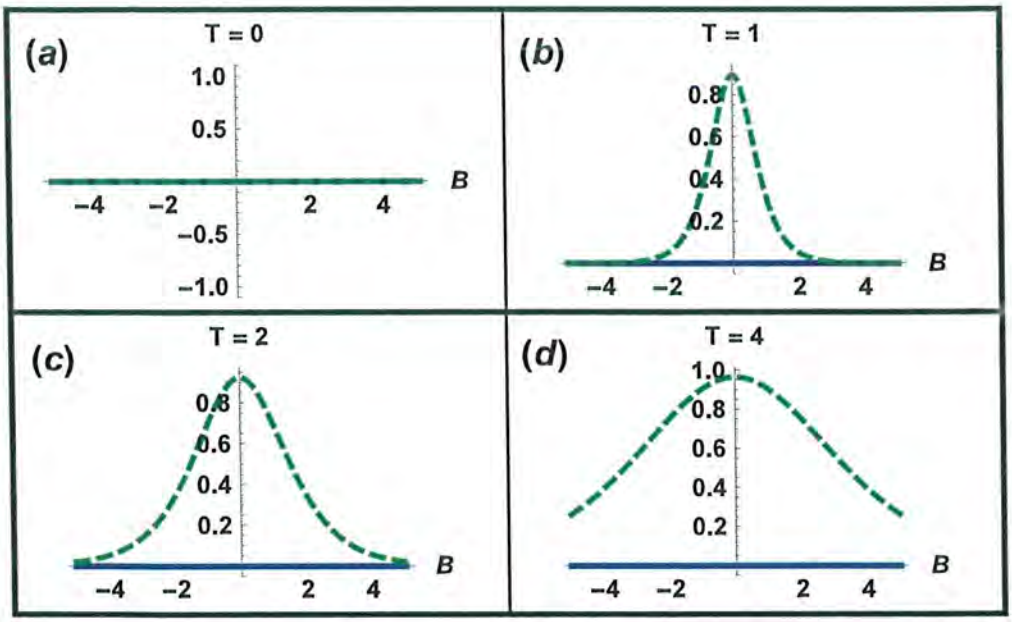


Figure 3.10: N(ρ) and QM plotted against B, for fixed values of T

increasing homogeneous magnetic field B shown in fig. 3.10(b, c, d). These results show that entanglement is present in the system, but very sensitive to temperature and uniform magnetic field.

3.3.2 Ferromagnetic case in non-uniform field

In figure (3.11), for the ferromagnetic case with a fixed value of temperature T when plotted against non-uniform magnetic field b, negativity shows an opposite behavior than the previous one for uniform magnetic field B. At T=0, negativity has some value even at b=0 and decreases with increasing b i.e., in the absence of the b and at T=0, there is maximum entanglement present, which decreases with increasing non-uniform magnetic field b as shown in fig. 3.11 (a) and for T=1, in the absence or small values of the inhomogeneous

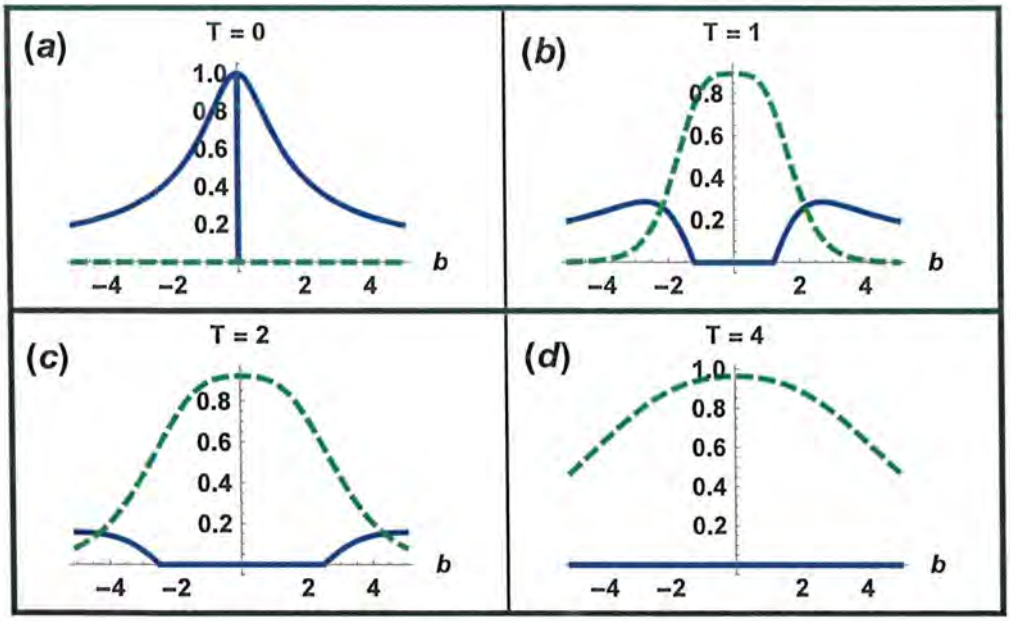


Figure 3.11: N(ρ) and QM plotted against b, for fixed values of T

magnetic field b, QM goes to its maximum value while negativity goes to zero as shown in fig. 3.11 (b) and increase with increasing b along with decreasing QM shows that for small values of temperature and relatively large values of the non-uniform magnetic field, entanglement is present as shown in fig. 3.11 (b, c). While from fig. 3.11 (d), it is clear that with increasing temperature, negativity goes to zero while mixedness increases, which indicates that with increasing temperature T, entanglement also decreases in the presence of the large values of the inhomogeneous magnetic field b.

In figure (3.12), for the ferromagnetic case with a fixed value of non-uniform magnetic field b when plotted against temperature T, in the absence of the b, negativity is zero, but QM is present even for absolute zero T and in the absence of the b and increase with increasing T which shows that no entanglement is present for this case shown in fig 3.12 (a). For higher

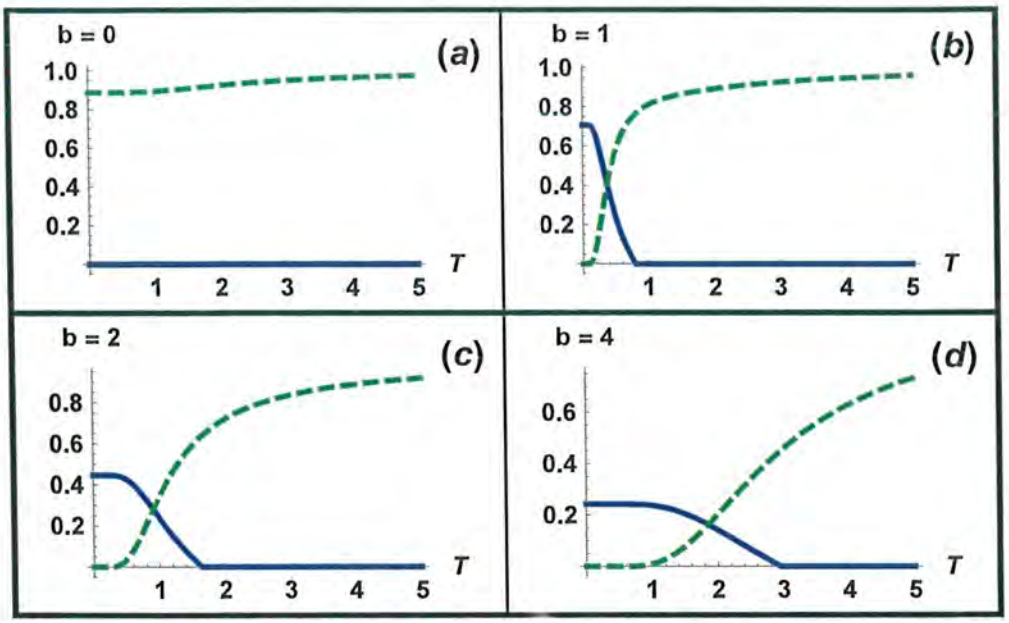


Figure 3.12: N(ρ) and QM plotted against T for fixed values of b

values of b, negativity shows some response even at absolute zero T and decrease quickly with increasing T i.e, entanglement is present for a very short interval of time at very low temperature and comparatively at large values of non-uniform magnetic field b.

when $J>0$

For the sake of simplicity, we set $J=1$ which is antiferromagnetic case.

3.3.3 Antiferromagnetic case in uniform magnetic field

In figure 3.13, for the antiferromagnetic case with a fixed value of temperature T, when plotted against uniform magnetic field B, for T=0, negativity is 1 (maximum) between -2<B<2, on further increasing B, negativity suddenly

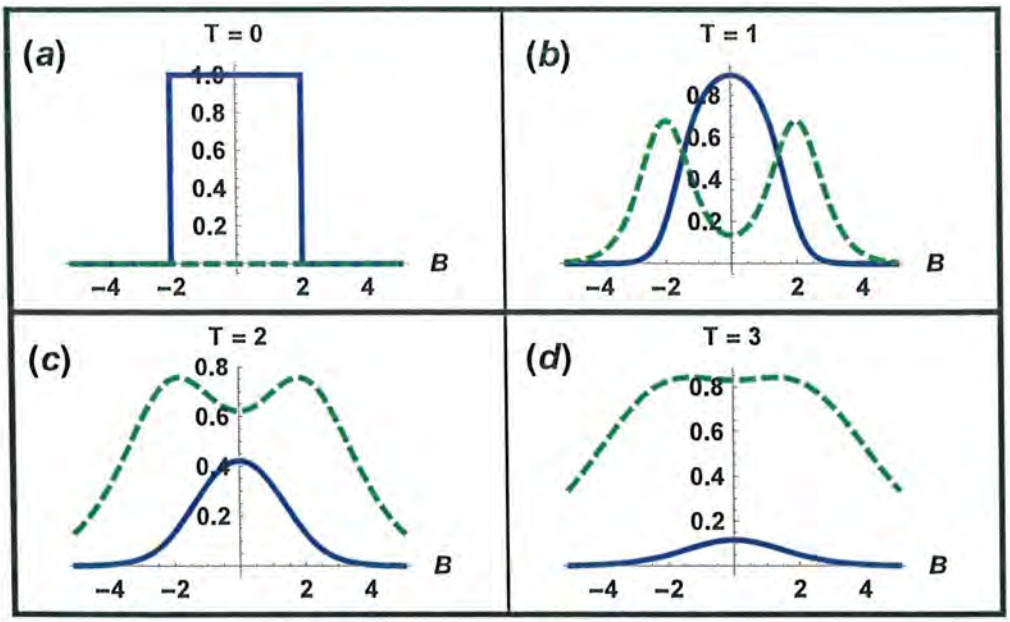


Figure 3.13: N(ρ) and QM plotted against B, for fixed values of T

goes to zero, this shows in antiferromagnetic case entanglement is present for a certain range of the B, QM is zero at T=0 and for all values of B as shown in fig 3.13 (a). Case (b) for T=1, QM plays the role due to which sudden fall down of negativity convert into slowly decreasing pattern. On further increase in temperature as the case (b) and (c), QM starts increasing as resultant negativity goes down, which shows a decrease in the entanglement with a rise in the temperature T.

In fig (3.14), for the ferromagnetic case with a fixed value of uniform magnetic field B when plotted against temperature T, negativity here shows different behavior from all the previous cases and is equal to 1 at B=0 and B=1 case (a,b) and start decreasing with increasing temperature T, this means that entanglement is present in this case which decreases with increasing temperature T, while for B=0 and B=1 case (a,b), initially at B=T=0,

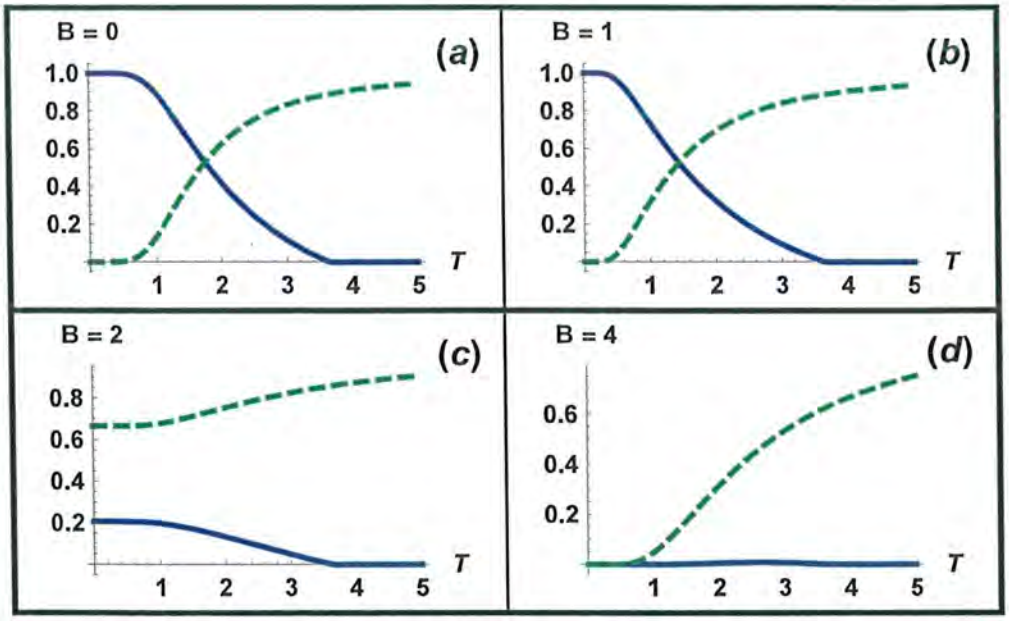


Figure 3.14: N(ρ) and QM plotted against T, for fixed values of B

QM is also zero but with increasing temperature T, QM is also increasing which is a cause of decreasing entanglement. In case (c) B=2, negativity has a small value, but QM is present even at T=0 so, in this case, spins are weakly entangled. In case (d), B=4, negativity shows zero response with an exponential increase in QM which shows no entanglement in the system. So as a conclusion, for the antiferromagnetic case entanglement decrease with an increase in both temperature T and homogeneous magnetic field B.

3.3.4 Antiferromagnetic case in non-uniform magnetic field

In figure 3.15, for the antiferromagnetic case plotted against non-uniform magnetic field b, for fixed values of temperature T, when the negativity is

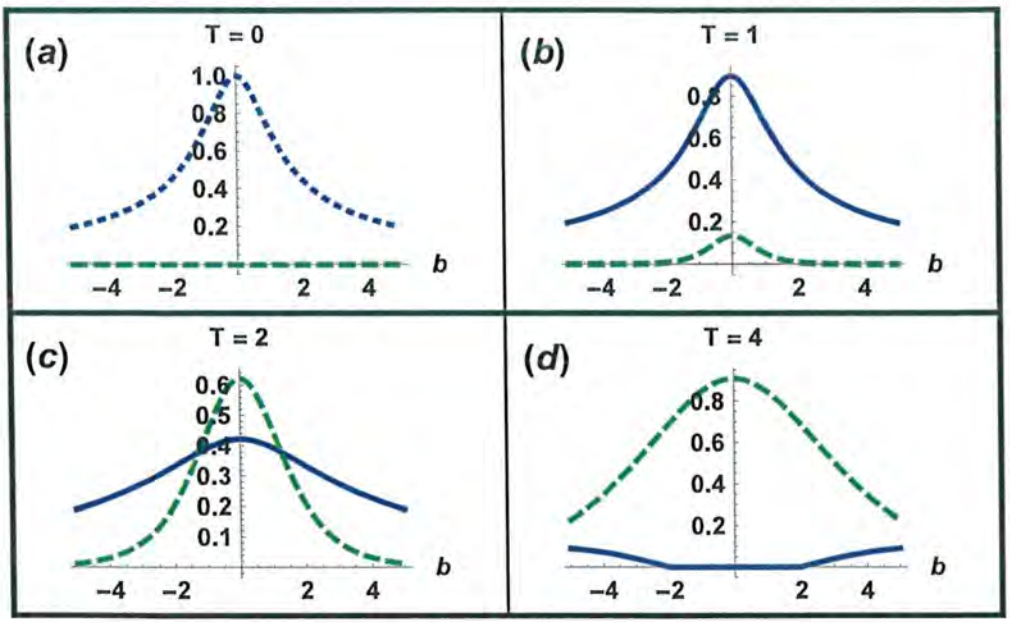


Figure 3.15: N(ρ) and QM plotted against b, for fixed values of T

equal to 1 at B=0 and absolute zero temperature T=0 and start decreasing with increasing T, this means that there is entanglement in the present case (a) which decrease with increasing inhomogeneous magnetic field b and QM is zero for all the values of the b. In case (b), T=1 negativity is almost the same, with a little increment in the QM, with the further increase in the temperature, negativity starts decreasing and QM increases as shown in the case (d) where, for T=4, for small values of b negativity is zero and on further increasing inhomogeneous field, there is a small increment in the negativity along with the decrease in the QM, which is an indication for the entanglement at large values of inhomogeneous magnetic field b. In figure (3.16), for the antiferromagnetic case with a fixed value of non-uniform magnetic field b when plotted against temperature T, negativity is equal to 1 (maximum) at b=0 and start decreasing with increasing temperature T, this means that

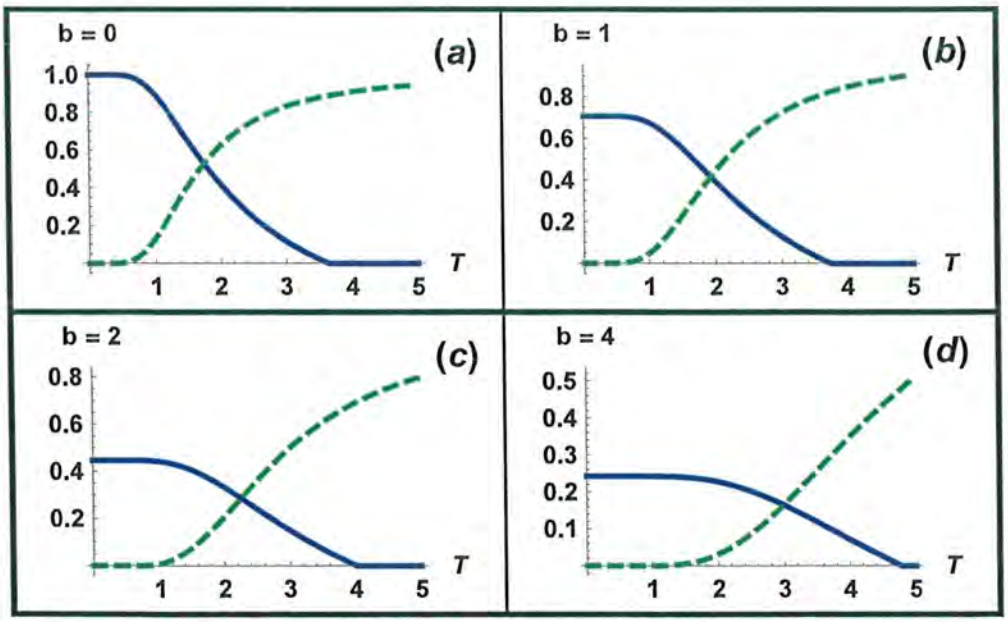


Figure 3.16: N(ρ) and QM plotted against T, for fixed values of b

entanglement is present in this case. Initially, when b=0, for T approaches zero, QM is also zero, which increases with increasing temperature, hence decoherence and entropy increases in the system. With the increasing of the inhomogeneous magnetic field, the maximum value of the negativity at absolute zero temperature T=0 decreases indicate that the maximum value of the entanglement decreases in the system with the increasing inhomogeneous magnetic field.

3.4 Results and Discussion

In this work, the quantification of entanglement measure, negativity is evaluated for two qubit Heisenberg XXX model under the inhomogeneous magnetic field for both ferromagnetic and antiferromagnetic cases. In the antifer-

romagnetic case in the uniform magnetic field B, with an increase in B, there is a critical point at $B{=}B_c{=}2$, negativity becomes a non-analytic function of B which gives the signature of phase transition. Negativity is maximum for $B{<}B_c$ and is minimum for $B{>}B_c$, when $T{=}0$. This means for $B{<}B_c$ at $T{=}0$, the ground state of the system is in an entangled state, whereas for $B{>}B_c$ it is not an entangled state (see **Fig. 3.13**).

Negativity in a non-uniform magnetic field for the antiferromagnetic case, is a single-valued function and so there is no critical point where we can find the non-analytic relation with respect to b and so no quantum phase transition occurs in this case (see **Fig. 3.15**). Moreover, it is seen that QM increases with the increase in T which is trivial as we have calculated the QM for thermal state and in contrast to the uniform antiferromagnetic case, in this case, an increase in the value of b generally slows down the rate of increase in QM with T.

Negativity for the ferromagnetic case in a uniform magnetic field is zero (see **Fig. 3.9**). So, in contrast to the uniform antiferromagnetic case, it is observed that there is no entanglement in this case. It is also observed that QM is zero for all the values of B at $T{=}0$. For small T the behavior of QM is localized at small values of B which becomes delocalize for larger values of T.

In contrast to the uniform ferromagnetic case where is no entanglement at all, in the case of non-uniform ferromagnetic case, entanglement exists which is very sensitive to the values of temperature and non-uniform magnetic field b. At $T{=}0$, negativity is maximum at $b{=}0$ and start decreasing with b (see **Fig. (3.11)**). Whereas for $T > 0$, negativity is zero at $b{=}0$ and starts in-

creasing after a certain value of non-uniform magnetic field b means for finite temperature, negativity start increases and decreases which is unusual. So in this case a very small inhomogeneity is capable of producing large values of thermal entanglement. This shows that the presence of entanglement in the ferromagnetic Heisenberg system is highly unstable against non-uniform magnetic fields.

In general, with the increasing either the magnetic field or temperature, entanglement decreases, finally vanishes. This is due to the fact that the increasing the temperature, the greater the thermal fluctuations, the system is made up of nonentangled and entangled states, and as the temperature rises, the presence of non-entangled states rises resulting in a decrease in entanglement. This shows that at a fixed temperature, a non-uniform magnetic field can minimize the effect on entanglement by thermal fluctuation, hence improving the system's entanglement. We can control the size of entanglement by changing the size of the magnetic field in the inhomogeneous magnetic field, making an entanglement switch.

3.5 Conclusion

The effect of inhomogeneity on ferromagnetic spins is very prominent. An infinitesimal magnetic field applied in opposite directions to the two spins at zero temperature maximizes the entanglement between two spins. It's like as we've twisted the two spins together into an entangled state, which decreases with increasing temperature. When the spins are coupled antiferromagnetically, inhomogeneity can only weaken entanglement.

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