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5 Introduction

5.1 Classical Information Theory

Classical information theory was first studied by Claude Shannon who stated and justified the main mathematical definitions and the two fundamental theorems of information theory. His contribution was considered to be the greatest contribution to the modern science in that time. It is based on the mathematical aspects of information–processing tasks such as storage and transmission of information. This includes the study of classical mechanics and the information theory.

The two core results of the classical information theory established in his landmark 1948 paper explained briefly as

1. Suppose Alice sent a message to Bob to inform something over a noiseless bit channel i.e., If Alice sends a bit '0' to Bob, he receives a bit '0' and If Alice sends a bit '1' to Bob, he receives a bit '1', the message won't be disturbed through a noiseless channel, how the data or the message can be compressed because It is very expensive to the channel for the communication, so it is needed to minimize the number of times they use this noiseless channel.

2. It is not possible to have a error-free communication over a noisy channel to communicate without any disturbance or third party involved in it. The second core result says that at what rate Alice and Bob can communicate over a noisy channel.

Both the results by Claude Shannon talk about the redundancy. One of the key insight by Shannon was the entropy to quantify the redundancy. Entropy is the one which can be used to measure the information sent.

All the physical systems registers some bit of information, where 'information' is a measurable quantity which is the message conveyed through some channel to the other party, also known as the classical information and the entropy measures how much information does a system possesses.

Classical information theory is based on formulations of classical mechanics and probability theory where the information is transmitted in classical bits i.e., $\{0, 1\}$, such that the outcome would be either 0 or 1 at a time.

To understand better, we are considering a random variable X as a message containing list of messages $\{x_1, x_2, x_3, ..., x_n\}$, where each one has the possibility

$\{p(x_1), p(x_2), p(x_3), ..., p(x_n)\}$ to occur is called the probability distribution denoted as p_X. Considering simplest situation we assume that the random message $x = \{0, 1\}$ ALice feeds into a channel and $y = \{0, 1\}$ emerges through a channel shown in the figure below.

Figure 1: Alice transmitting information to Bob through channel.

5.2 Classical Mutual Information

Let us consider simple experiment to understand the logic behind classical mutual information. The concept of classical mutual information is to determine the correlation between two events.

Consider two random variable X and Y, Alice holds the information encoded in a random variable X and the correlation Alice and Bob share, Bob has some "side information" about X in the form of random variable Y, the **conditional entropy** reads as

$$H(X|Y) = H(X, Y) - H(Y) \tag{1}$$

where $H(X, Y)$ is the joint entropy.

We now introduce a measure of information based on the Shannon entropy which is known as the **Mutual Information**. Alice possesses some information X and Bob possesses some information Y, the mutual information quantifies the correlation between the random variable X and Y then this correlation could be measured by the formula given below as

$$I(X : Y) = H(X) - H(X|Y) \tag{2}$$

Classically, it has another equivalent form of mutual information given as

$$I(X : Y) = H(X) + H(Y) - H(X, Y) \tag{3}$$

where conditional entropy $H(X|Y)$ is equivalent to $H(X, Y) - H(Y)$ but in the quantum domain, the criteria changes, this equality does not hold anymore.

5.3 Shannon Entropy and Its Properties

We will understand here how we can measure the classical information. The concept of Shannon entropy was introduced by Claude Shannon who expressed a relation to measure the information in his paper [1]. The classical entropy is denoted as $H(X)$ where X is some random variable.

As we discussed earlier, given the probability distribution p_X for a random variable X with possible outcomes $\{x_1, x_2, x_3, ..., x_n\}$, its Shannon entropy is given as

$$H(X) = -\sum_{i}^{n} p_X(x_i) log_2 p_X(x_i). \tag{4}$$

Similarly, given two random variables X and Y with the possible outcomes x_i and y_j, we may define another term named **Conditional Entropy** as

$$H(X|Y) = -\sum_{i,j} P(x_i, y_j) log_2 (\frac{P(x_i, y_j)}{P(y_j)}) \tag{5}$$

where $P(x_i, y_i)$ is the probability that $X = x_i$ and $Y = y_j$.

There are some important mathematical properties to understand the Shannon entropy $H(X)$ as follows

1. The Shannon Entropy is a non negative quantity for any probability distribution p_X:
$$H(X) \geq 0. \tag{6}$$
2. The Shannon entropy $H(X)$ for a deterministic variable vanishes because the entropy is interpreted as the uncertainty of experiment done randomly.
$$H(X) = 0. \tag{7}$$
3. The maximum value of the Shannon entropy $H(X)$ for a random variable X with d different realizations is
$$H(X) \leq logd \tag{8}$$

5.4 Quantum Information Theory

Quantum information theory is based on the study of quantum mechanics and classical information theory. As we know that quantum information theory runs on the postulates of quantum mechanics, so it is fundamentally different from the classical information theory. The postulates quantum mechanics is based on which only hold for the closed or isolated quantum systems. Whereas, there are no such closed or isolated quantum systems exist in the real world.

Quantum information theory runs on the very important aspects of quantum theory i.e., Superposition and Entanglement, otherwise there are some aspects which exist in the classical theory i.e., Uncertainty, Interference and Indeterminism.

1. Quantum theory is **indeterministic** because the quantum theory is based on the predictions about the probabilities of the event happens. Classical theory is deterministic and is possible to predict with the certainty.

2. **Interference** is an another aspect of quantum theory which is there in the classical wave theory also. Interference is of two types, Constructive interference and destructive interference. When the crest on one wave meets the crest of another wave is known as the constructive interference while the crest of one wave meets the trough of another wave is known as the destructive interference where the wave can occur as a result of many particles.

3. The **uncertainty** is the another feature of quantum theory which is fundamentally different from the classical theory. The uncertainty principle states that It is impossible to know both, the particle's position and the its momentum accurately.

4. The **superposition** principle is purely the quantum phenomena in the quantum theory. The superposition principle states that the quantum state in a quantum system can be written as a linear combination of states. For example , The state $|0\rangle$ and $|1\rangle$ passes through a Hadamard gate which results in a linear combination of $|0\rangle$ and $|1\rangle$ given as

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \;\; |\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle), \tag{9}$$

5. The last and the most important feature of quantum theory is **entanglement**. There is no classical study and theory of entanglement. Entanglement is one of the strong quantum correlation in which two or more parties are involved. It is the strong correlation than any kind of correlation exist in the classical theory. We will study the measure of quantum entanglement in this report later.

In quantum information processing systems, the information is stored in the quantum states of a physical system. There are many more interesting aspects from a mathematical or a physical point of view. The bits that are being used in the quantum circuits to transmit the information from one party to another party are being called quantum bits or qubits. For example, the spin of an electron and the polarization of a single photon.

A **Qubit** is the fundamental unit of Quantum Mechanics. In the quantum computation, the information is stored in a qubit which is written as $|0\rangle$ and $|1\rangle$ and the outcome would be in either of the state or the superposition of $|0\rangle$ and $|1\rangle$. A quantum is transmitted through some channel. Our aim is to construct such quantum systems which can transmit the classical information encoded into a quantum state through some noisy channel to another party with the high successful rate.

5.5 Quantum Mutual Information

We follow the mutual information in a quantum domain to understand the quantum mutual information, as this is the standard measure of correlation. As discussed in section 1.3, we study the mutual information to determine the quantum correlation between two parties. Quantum correlation includes several types of measures which we will talk about in this report.

Consider two parties Alice and Bob share some correlation between them. Similar to section 1.3, the conditional entropy $S(\rho_{A|B})$ for a bipartite state ρ_{AB} is the difference of the joint entropy $S(\rho_{A,B})$ and the entropy of the marginal state $S(\rho_B)$, the expression reads as

$$S(\rho_{A|B}) = S(\rho_{A,B}) - S(\rho_B) \tag{10}$$

We now discuss a quantum measure of correlation in a bipartite state i.e., Quantum Mutual Information, holds a relation given as

$$I(\rho_A : \rho_B) = S(\rho_A) - S(\rho_{A|B}) \tag{11}$$

which has an equivalent form of mutual information given as

$$I(\rho_A : \rho_B) = S(\rho_A) + S(\rho_B) - S(\rho_{A,B}) \tag{12}$$

where conditional entropy $S(\rho_{A|B})$ is equivalent to $S(\rho_{A,B}) - S(\rho_B)$ until the state is disturbed. This equality does not hold anymore if any kind of measurement is done on the state.

5.6 Von Neumann Entropy and Its Properties

The study of the measurement of a quantum state in the information theory is the quantum analogue of Shannon entropy, namely the Von Neumann entropy. The Von Neumann entropy is similar to the Shannon entropy, where the classical probability distribution is replaced with the density operator ρ.

Suppose Alice prepares a state ρ_A in a quantum system A. In order to quantify the amount of information or the correlation that a quantum state possesses, It could be measured as

$$S(\rho_A) = -Tr\{\rho_A log \rho_A\} \tag{13}$$

where $S(\rho_A)$ is the Von Neumann entropy.

There are some important mathematical properties to understand Von Neumann entropy $S(\rho_X)$ as follows

1. The Von Neumann entropy $S(\rho_X)$ is a non negative quantity for any deterministic density operator ρ_X given as
$$S(\rho_X) \geq 0. \tag{14}$$
2. For a pure state density operator, the Von Neumann entropy $S(\rho_X)$ for a deterministic density operator vanishes, $S(\rho_X) = 0$.
3. The maximum value of the Von Neumann entropy $S(\rho_X)$ for a d dimensional quantum system is given as
$$S(\rho_X) \leq logd \tag{15}$$
4. (UNITARY INVARIANCE) The Von Neumann entropy is invariant under the action of unitary operations of any density matrix.
5. For a p ure bipartite state ρ_{AB}, the Von Neumann entropy of a subsystem A is equal to the subsystem B.
$$S(\rho_A) = S(\rho_B) \tag{16}$$

6 Tools to Measure Quantum Correlation

6.1 An Introduction to Quantum Correlation

Quantum correlation plays an important role in the many body systems. Quantum entanglement is one of the important measure of correlation in which two or ore parties are involved. Later on, Ollivier and Zurek [1] proposed a new measure of quantum correlation, the Quantum discord, which quantifies the non classical correlation of a given quantum system and is defined as the difference of two classically equivalent forms of mutual information, asnd is given as

$$QD(\rho_{\mathcal{AB}}) = I(\rho_{AB}) - C(\rho_{AB}) \tag{17}$$

where $I(\rho_{AB})$ represents the quantum mutual information and $C(\rho_{AB})$ is the classical correlation where the projective measurements has been performed at the subsystem B.

Let us mention some useful properties of quantum discord [2] and how it performs in different conditions,

1. Quantum discord is a non negative quantity i.e.,nadjw $QD \geq 0$ because measurement disturbs the state which results in $I(\rho) \geq C(\rho)$.
2. Quantum discord is a non symmetric quantity i.e., $QD(\rho_{AB}) \neq QD(\rho_{BA})$ but Quantum mutual information is symmetric i.e., $I(\rho_{AB}) = I(\rho_{BA})$.
3. If the projective measurement done on the subsystem B does not disturb the quantum state, then quantum discord is zero i.e., $QD(\rho_{AB}) = 0$.
4. Quantum Discord reduces to the quantum entanglement for the pure bipartite separable state i.e., $QD(\rho_{AB}) \equiv QE(\rho_A) = QE(\rho_B)$ which is equal to the Von Neumann entropy of the marginal states, in such cases the classical correlation $C(\rho_{AB})$ is zero.

In order to quantify the correlation in the Bell states (pure entangled state), quantum discord and classical correlation, neither of the quantity in such cases is zero. Quantum discord can be measured even if the states are not entangled, and given in a product form $|\psi_{AB}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$, whereas the various measures of quantum entanglement for the pure separable states or bell states (entangled states) give the same result as it is equal to the Von Neumann entropy of the reduced state which is calculated by tracing out one of the subsystem A or B from the composite system, given as

$$QE = tr_B S(\rho_{AB}) = tr_A S(\rho_{AB})$$

For the pure bipartite state, the Von Neumann Entropy of the composite system is zero, $S(\rho_{AB}) = 0$, because of which the entropy of the marginal states are equal.

$$S(\rho_A) = S(\rho_B) \tag{18}$$

6.2 Measures of Quantum Correlation

6.2.1 Quantum Entanglement

Entanglement is the quantum mechanical phenomenon in which at least two parties are involved in such a way that they don't have the individuality of their own. The entanglement of formation is one of an important measure of correlation named **quantum entanglement**.

Entanglement of formation is measured for the pure state as well as for the mixed state, but we study this measure for the pure states only. Considering a pure bipartite state ρ_{AB} where Alice and Bob share some correlation, so the entanglement of formation reduces to the Von Neumann entropy of one of the marginal state.

$$QE = S(\rho_A) = S(\rho_B) \tag{19}$$

We know that the bell states are the four maximally entangled states and the entanglement of formation of such states is one. We will determine it for the bell states with a basic example.

Given a maximally entagled state $|\psi\rangle = \frac{1}{\sqrt{2}}\big(|00\rangle + |11\rangle\big)$ forms a density matrix given as

$$\begin{aligned} \rho_{AB} =& |\psi\rangle\langle\psi| \\ =& \frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|) \end{aligned} \tag{20}$$

The entanglement of formation, a measure of quantum entanglement for a pure bipartite state is given as

$$EOF = S(\rho_A) \tag{21}$$

Now, to determine the Von Neumann entropy of the marginal state, $S(\rho_A)$, we will trace out the subsystem B from the state ρ_{AB} i.e., $S(\rho_A) = tr_B S(\rho_{AB})$, then we get

$$\rho_A = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) \tag{22}$$

where the eigenvalues of state ρ_A are $\lambda = \frac{1}{2}, \frac{1}{2}$, where the Von Neumann entropy is measured as

$$S(\rho_X) = -\sum_i \lambda_i log_2 \lambda_i$$

Then, the entropy for state ρ_A would be

$$S(\rho_A) = -\frac{1}{2}log_2(\frac{1}{2}) - \frac{1}{2}log_2(\frac{1}{2}) = 1$$

Hence, the entanglement of formation is 1 which states that the bell state which we chose as an example is the maximally entangled state. If the entanglement of formation is 0, then the state is separable and there is no entanglement.

6.2.2 Quantum Discord

Considering two random variable X and Y, where Alice holds some information X, and due to the correlation between them Bob holds some incomplete prior information Y. The correlation between the given random variables could be measured by their mutual information

$$I(X:Y) = H(X) + H(Y) - H(X,Y) \tag{23}$$

where $H(X)$ and $H(Y)$ are the Shannon's entropy of X and Y and $H(X,Y)$ is the joint entropy.

To gain the complete information of X, Alice would send some additional information to Bob, so that Bob would have full knowledge of X given his prior information Y, that is given by the conditional entropy as

$$H(X|Y) = H(X,Y) - H(Y) \tag{24}$$

Another expression for the mutual information using Eq. (4), we could rewrite the Eq. (3) as

$$I(X:Y) = H(X) - H(X|Y) \tag{25}$$

In quantum information theory, the Von Neumann entropy is the quantum generalization of Shannon's entropy where in order to write an expression of mutual information in the quantum regime, we would replace the classical probability distribution by the density matrices, then the quantum mutual information is

$$I(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}) \tag{26}$$

where $S(\rho_A) = -\sum_i \lambda_i log_2 \lambda_i$, and λ_i are the eigenvalues of the density matrix ρ_A.

Another expression for quantum mutual information conditioned over the subsystem B is given as

$$J(\rho_{AB}) = S(\rho_A) - S(\rho_{A|B}) \tag{27}$$

where $S(\rho_{A|B})$ is the conditional Von Neumann entropy which is classically equivalent to Eq. (4), but in quantum case, they are not equivalent.

We know that a quantum state can possess the various correlations i.e., quantum entanglement, classical correlation, and etc. We have discussed how much a composite state can possess the quantum correlation which can be measured using the expression of quantum mutual information, similarly, how much the state possess the classical correlation could be obtained by the expression which we are going to discuss now.

In case of the bipartite state ρ_{AB}, we assume to perform a local set of projective measurement $\{B_i\}$ on the subsystem B in the computational basis $\{0, 1\}$, the post-measurement state [3], conditioned on the measurement would be given as

$$\rho_i = \frac{1}{p_i} tr_B \big[(I \otimes B_i) \rho_{AB} (I \otimes B_i) \big] \tag{28}$$

where $p_i = tr_{AB} \big[(I \otimes B_i) \rho_{AB} (I \otimes B_i) \big]$, the identity operator will act on the Alice's system and B_i on the Bob's system, where B_i is given as

$$B_i = U \prod_i U^\dagger$$

where $\prod_i = |i\rangle\langle i|$, $i = 0, 1$ and U is the unitary operator with unit determinant i.e., $U^\dagger U = 1$.

The expression for conditional quantum mutual information, measurement performed on the subsystem B given as

$$J(A : \{B_i\}) = S(\rho_A) - S(\rho_{A|\{B_i\}}) \tag{29}$$

where

$$S(\rho_{A|\{B_i\}}) = \sum_i p_i S(\rho_i) \tag{30}$$

which is the summation of Von Neumann entropy corresponding to the probabilities in given basis $\{0, 1\}$ and here, $J(A : \{B_i\})$ represents the classical correlation which is classically equivalent to Eq. (6), which differs in quantum case because the conditional entropy in Eq. (6) and Eq. (9) differs.

As we discussed earlier, the term quantum discord could be defined easily as we have the expression for quantum mutual information and the classical correlation, which is written as

$$QD(\rho_{AB}) = I(\rho_{AB}) - C(\rho_{AB}) \tag{31}$$

where $C(\rho_{AB})$ is given as following where the maximization is taken over all possible measurement [2] done on the subsystem B,

$$C(\rho_{AB}) = max_{\{B_i\}} J(A : \{B_i\}) \tag{32}$$

7 Quantum Correlation in Quantum Many-Body Systems

7.1 Introduction

The quantum information theory has a major role for simulating the quantum many-body systems in the development of classical fundamental methods. In this report, we mostly focus on the analysis of bipartite entanglement in quantum many-body systems and along with that we discuss another measure of correlation, quantum discord to measure the correlation between the particles at sites in a spin chain.

7.2 A General Hamiltonian for a Spin-1/2 Models

The general expression of the Hamiltonian for the spin-1/2 models is given as

$$H = J\sum_{\langle i,j\rangle}^{N} \frac{1+\gamma}{2}\sigma_x^i\sigma_x^j + \frac{1-\gamma}{2}\sigma_y^i\sigma_y^j + \Delta\sigma_z^i\sigma_z^j + B\sum_{i=1}^{N}\sigma_z^i \tag{33}$$

where $\langle i, j\rangle$ represents the nearest neighbour spins in a spin lattice and N is the number of spins in that lattice. Here, σ_x^i, σ_y^i and σ_z^i are the Pauli matrices at site i, J is the strength of the spin-spin coupling and B is external field along the z-axis. Lastly, γ and Δ are the parameter that fix the anisotropy of the interaction in the XY plane.

Given the Hamiltonian H in which the interacting pair of spin-1/2 systems exhibits the Z_2 symmetry which implies the commutation of H with the parity operator $\otimes_{i=1}^{N}\sigma_z^i$, where N is the total number of spins and σ_z^i is the pauli matrix along the z-axis at site i.

The two-spin density matrix for the Hamiltonian given above at sites $\langle i, j\rangle$ is reduced to the given below as

$$\rho_{\langle i,j\rangle} = \frac{1}{4}\Big[I + \sum_{i=1}^{3}(c_i\sigma_i \otimes \sigma_i) + c_4 I \otimes \sigma_z + c_5\sigma_z \otimes I\Big] \tag{34}$$

Therefore, for a general Hamiltonian, the quantum discord and the entanglement of formation can be determined. The eigenvalues for the density matrix given above are

$$\begin{aligned}
\lambda_0 =& \frac{1}{4}\Big[(1+c_3) + \sqrt{(c_4+c_5)^2 + (c_1-c_2)^2}\Big],\\
\lambda_1 =& \frac{1}{4}\Big[(1+c_3) - \sqrt{(c_4+c_5)^2 + (c_1-c_2)^2}\Big],\\
\lambda_2 =& \frac{1}{4}\Big[(1-c_3) + \sqrt{(c_4-c_5)^2 + (c_1+c_2)^2}\Big],\\
\lambda_3 =& \frac{1}{4}\Big[(1-c_3) - \sqrt{(c_4-c_5)^2 + (c_1+c_2)^2}\Big].
\end{aligned} \tag{35}$$

The expression for mutual information is given as

$$I(\rho) = S(\rho^A) + S(\rho^B) + \sum_{i=0}^{3}\lambda_i log_2\lambda_i \tag{36}$$

where λ_i are eigenvalues for $i = 0, .., 3$.

The marginal density matrices ρ_A and ρ_B of the two-spin reduced density matrix $\rho_{\langle i,j\rangle}$, the reduced density matrices would be

$$\begin{aligned} \rho^A &= tr_B\rho_{AB} = \frac{1}{2}\Big[I + c_5\sigma_z\Big] \\ \rho^B &= tr_A\rho_{AB} = \frac{1}{2}\Big[I + c_4\sigma_z\Big] \end{aligned} \tag{37}$$

we know here, $tr(I) = 2$ and $tr(\sigma_i) = 0$ for i = x,y, and z. So, the reduced density matrix is given as

$$\rho^A = \frac{1}{2}\begin{pmatrix} 1+c_5 & 0 \\ 0 & 1-c_5 \end{pmatrix}, \rho^B = \frac{1}{2}\begin{pmatrix} 1+c_4 & 0 \\ 0 & 1-c_4 \end{pmatrix} \tag{38}$$

The eigenvalues of both the reduced density matrix would be given as

$$\begin{aligned} \lambda_1^A &= 1 + c_5, \lambda_2^A = 1 - c_5. \\ \lambda_1^B &= 1 + c_4, \lambda_2^B = 1 - c_4. \end{aligned} \tag{39}$$

So, the Von Neumann Entropy of the reduced density matrices is

$$\begin{aligned} S(\rho^A) &= -\lambda_1^A log_2\lambda_1^A - \lambda_2^A log_2\lambda_2^A, \\ S(\rho^B) &= -\lambda_1^B log_2\lambda_1^B - \lambda_2^B log_2\lambda_2^B. \end{aligned} \tag{40}$$

Now to determine the classical correlation, considering a set of projectors for local measurement on subsystem B, such that $\{B_k := V\prod_k V^\dagger\}$, where $\prod_k = |k\rangle\langle k|$ for $k = 0, 1$ and V is some unitary matrix such that $V.V^\dagger = 1$, so

$$V = \begin{pmatrix} cos\frac{\theta}{2} & sin\frac{\theta}{2}e^{-i\phi} \\ sin\frac{\theta}{2}e^{i\phi} & -cos\frac{\theta}{2} \end{pmatrix} \tag{41}$$

where $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$.

Now we know that the two-spin reduced density matrix after the local measurement on subsystem B would be

$$p_k\rho_k = (I \otimes B_k)\rho(I \otimes B_k) \tag{42}$$

where $p_k = tr(I \otimes B_k)\rho(I \otimes B_k)$ is the probability which is being cosidered as $\frac{1}{2}$ for bot the cases.

$$\begin{aligned} p_0\rho_0 =&(I \otimes V)(I \otimes \Pi_0)(I \otimes V^\dagger)\rho(I \otimes V)(I \otimes \Pi_0)(I \otimes V^\dagger) \\ =&(I \otimes V)(I \otimes \Pi_0)(I \otimes V^\dagger)\rho(I \otimes V)(I \otimes \Pi_0)(I \otimes V^\dagger) \\ =&\frac{1}{4}(I \otimes V)(I \otimes \Pi_0)\Big(I. + \sum_{i=1}^{3} c_i\sigma_i \otimes V^\dagger\sigma_i V\Big)(I \otimes \Pi_0)(I \otimes V^\dagger) \\ =&\frac{1}{4}(I \otimes V)\Big(I + \sum_{i=1}^{3} c_i\sigma_i \otimes (\Pi_0 V^\dagger\sigma_i V\Pi_0)\Big)(I \otimes V^\dagger) \end{aligned} \tag{43}$$

As the calculation is done and we know now that,

$$
\begin{aligned}
(\Pi_0 V^\dagger \sigma_1 V \Pi_0) &= sin\theta cos\phi \Pi_0, \\
(\Pi_0 V^\dagger \sigma_2 V \Pi_0) &= sin\theta sin\phi \Pi_0, \\
(\Pi_0 V^\dagger \sigma_3 V \Pi_0) &= cos\theta \Pi_0.
\end{aligned}
\tag{44}
$$

So, the Eq. 43 could be written as

$$
\begin{aligned}
p_0\rho_0 = \frac{1}{4}(I \otimes V)\Big(& I \otimes \Pi_0 + c_1 sin\theta cos\phi(\sigma_1 \otimes \Pi_0) + c_2 sin\theta singh\phi(\sigma_2 \otimes \Pi_0) + c_3 cos\theta(\sigma_3 \otimes \Pi_0) \\
&+ c_4 cos\theta(I \otimes \Pi_0) + c_5(\sigma_3 \otimes \Pi_0)\Big)(I \otimes V^\dagger)
\end{aligned}
$$

Now, cosidering that $w_1 = sin\theta cos\phi$, $w_2 = sin\theta sin\phi$, and $w_3 = cos\theta$, we have

$$
\begin{aligned}
p_0\rho_0 = \frac{1}{4}\Big(&(1 + c_4 w_3) I \otimes V\Pi_0 V^\dagger + c_1 w_1(\sigma_1 \otimes V\Pi_0 V^\dagger) + c_2 w_2(\sigma_2 \otimes V\Pi_0 V^\dagger) \\
&+ (c_3 w_3 + c_5)(\sigma_3 \otimes V\Pi_0 V^\dagger)\Big)
\end{aligned}
$$

$$
p_0\rho_0 = \frac{(1 + c_4 w_3)}{4}\Big[I + \frac{c_1 w_1 \sigma_1}{(1 + c_4 w_3)} + \frac{c_2 w_2 \sigma_2}{(1 + c_4 w_3)} + \frac{(c_3 w_3 + c_5)\sigma_3}{(1 + c_4 w_3)}\Big] \otimes V\Pi_0 V^\dagger \tag{45}
$$

Considering that

$$
q_{01} = \frac{c_1 w_1}{(1 + c_4 w_3)}, q_{02} = \frac{c_2 w_2}{(1 + c_4 w_3)}, q_{03} = \frac{(c_3 w_3 + c_5)}{(1 + c_4 w_3)}
$$

Then, the Eq. 45 would be written as

$$
p_0\rho_0 = \frac{(1 + c_4 w_3)}{4}[I + q_{01}\sigma_1 + q_{02}\sigma_2 + q_{03}\sigma_3] \otimes V\Pi_0 V^\dagger \tag{46}
$$

Now, to determine the probability p_0, we take the trace over Eq. 46, and we know that trace of Pauli Matrices σ_1, σ_2, and σ_3 is zero. So,

$$
p_0 = tr((I \otimes B_0)\rho(I \otimes B_0)) = \frac{1}{2}(1 + c_4 w_3) \tag{47}
$$

Dividing the Eq. 46 by the probability calculated in Eq. 47, we would get the two possible density matrices as mentioned

$$
\rho_0 = \frac{1}{2}[I + q_{01}\sigma_1 + q_{02}\sigma_2 + q_{03}\sigma_3] \otimes V\Pi_0 V^\dagger \tag{48}
$$

Note: If we are given a product of two states in which one is the pure state and other one is not, then the Von Neumann entropy can be understand as

$$\begin{aligned}S(A\otimes B)=&-Tr((A\otimes B)[log_2(A\otimes B)])\\=&-Tr((A\otimes B)[log_2A\otimes I+I\otimes log_2B])\\=&-Tr[Alog_2A\otimes B+A\otimes Blog_2B]\\=&-Tr(Alog_2A)\otimes -Tr(B)-Tr(A)\otimes -Tr(Blog_2B)\\=&[S(A)\otimes -Tr(B)]-[Tr(A)\otimes S(B)]\\=&S(A)\end{aligned} \tag{49}$$

Similarly, we can obtain the post measured density matrix ρ_1 in that basis $\{0,1\}$, we get

$$\rho_1=\frac{1}{2}[I+q_{11}\sigma_1+q_{12}\sigma_2+q_{13}\sigma_3]\otimes V\Pi_1V^\dagger \tag{50}$$

From the Eq. 49, because of which $S(V\Pi_kV^\dagger)=0$ for $k=0,1$, we get the density matrix ρ_0 and ρ_1 given as

$$\rho_0=\frac{1}{2}[I+q_{01}\sigma_1+q_{02}\sigma_2+q_{03}\sigma_3],\;\;\rho_1=\frac{1}{2}[I+q_{11}\sigma_1+q_{12}\sigma_2+q_{13}\sigma_3] \tag{51}$$

Let

$$\theta_k=\sqrt{\sum_{j=1}^{3}q_{kj}^2} \tag{52}$$

which depends on the measurement $\{B_i\}$, then we obtain from Eq. 51,

$$S(\rho_k)=-\frac{(1+\theta_k)}{2}log_2\frac{(1+\theta_k)}{2}-\frac{(1-\theta_k)}{2}log_2\frac{(1-\theta_k)}{2} \tag{53}$$

To determine the classical correlation given in Eq. 29 as

$$C(\rho)=max_{\{Bi\}}J(A:\{B_i\})=max_{\{Bi\}}(S(\rho_A)-S(\rho_{A|\{B_i\}})) \tag{54}$$

where

$$S(\rho_{A|\{B_i\}})=\sum_i p_iS(\rho_i)=\frac{S(\rho_0)+S(\rho_1)}{2}+c_4w_3\frac{S(\rho_0)-S(\rho_1)}{2} \tag{55}$$

Putting the Eq. 55 back in the Eq. 54 to determine the classical correlation for the spin interaction at site i and j, we get

$$C(\rho)=max_{\{Bi\}}\Big(S(\rho_A)-\frac{S(\rho_0)+S(\rho_1)}{2}-c_4w_3\frac{S(\rho_0)-S(\rho_1)}{2}\Big) \tag{56}$$

Finally, the expression for quantum discord as the difference of quantum mutual information in Eq. 36 and classical correlation in Eq. 56, we can easily write as

$$QD(\rho_{AB}) = I(\rho_{AB}) - C(\rho_{AB}) \tag{57}$$

8 Calculation

8.1 Quantum Discord and Quantum Entanglement for a Bell State

We have earlier discussed some useful properties of quantum discord and quantum entanglement, which we will try to understand here with some examples. With the prior knowledge we know that the quantum discord for a Bell state is always 1.

First, we will calculate the quantum discord and quantum entanglement for one of the Bell state which is a pure entangled state given as

$$|\psi\rangle = \tfrac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

which can be written in terms of the density matrix ρ_{AB} as

$$\begin{aligned} \rho_{AB} =& |\psi\rangle\langle\psi| \\ =& \frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|) \end{aligned} \tag{58}$$

The Von Neumann Entropy of the composite system is zero if the state is pure, and to check whether ρ_X describes a pure state or not, there are certain steps,

1. The square of any given state, ρ_X results in same i.e., $\rho_X^2 = \rho_X$, is a pure state and if not i.e., $\rho_X^2 \neq \rho_X$, then mixed state.
2. The trace of the square of the above state is equal to 1 i.e., $Tr(\rho_X) = 1$, is a pure state and if not i.e., $Tr(\rho_X) \neq 1$, then its a mixed state.

As the given state in Eq. (29), follows the steps mentioned above and results in a pure state, then the Von Neumann entropy for the state will be zero i.e., $S(\rho_{AB}) = 0$, and followed by Eq. (2) we get $S(\rho_A) = S(\rho_B)$, the quantum mutual information would then be given as

$$I(A:B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}) \tag{59}$$

Since, it is a pure state. Hence, $S(\rho_{AB}) = 0$ and $S(\rho_A) = S(\rho_B)$, then

$$I(A:B) = 2S(\rho_A) \tag{60}$$

Now, to determine the Von Neumann entropy of the marginal state, $S(\rho_A)$, we will trace out the subsystem B from the state ρ_{AB} i.e., $S(\rho_A) = tr_B S(\rho_{AB})$, then we get

$$\rho_A = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) \tag{61}$$

where the eigenvalues of state ρ_A are $\lambda = \frac{1}{2}, \frac{1}{2}$, where the Von Neumann entropy is measured as

$$S(\rho_X) = -\textstyle\sum_i \lambda_i log_2 \lambda_i$$

Then, the entropy for state ρ_A would be

$$S(\rho_A) = -\tfrac{1}{2}log_2(\tfrac{1}{2}) - \tfrac{1}{2}log_2(\tfrac{1}{2}) = 1$$

Hence, the quantum mutual information is, $I(A:B) = 2S(\rho_A) = 2$.

Since, the measurement is done on a subsystem B, obtaining the maximum value of subsystem A i.e., $log_2 d$. According the the definition of quantum discord, the classical correlation $C(\rho_{AB})$, the maximization taken over all possible measurements on subsystem B gives us,

$$C(\rho_{AB}) = max_{\{Bi\}} J(A:\{B_i\}) = log_2 d - min_i S(\rho_{A|\{B_i\}}) \tag{62}$$

where $log_2 d = 1$ for a two dimensional system which results in $J(A:\{B_i\}) = 1 - min_i S(\rho_{A|\{B_i\}})$ and a set of local projective measurement acting on a pure state results in $\sum_i S(U \prod_i U^\dagger) = 0$, which clearly says that the classical correlation is equal to 1.

$$max_{\{Bi\}} J(A : \{B_i\}) = 1 \tag{63}$$

Hence, the numerical value for quantum discord would be difference of the quantum mutual information and classical correlation

$$QD(\rho_{AB}) = I(\rho_{AB}) - C(\rho_{AB}) = 1 \tag{64}$$

8.2 Quantum Discord and Quantum Entanglement for a State with Parameter Delta

Consider an another example for a pure bipartite state given as $|\psi\rangle = |\ 00\rangle + |01\rangle + |10\rangle + \delta|11\rangle$, with the normalizing constant $a = \sqrt{\frac{1}{3+\delta^2}}$, where δ is a constant.

The density matrix, $\rho_{AB} = |\psi\rangle\langle\psi|$ is given as

$$\begin{aligned}
\rho_{AB} =& a^2 \big(|00\rangle\langle 00| + |00\rangle\langle 01| + |00\rangle\langle 10| + \delta|00\rangle\langle 11| \\
& + |01\rangle\langle 00| + |01\rangle\langle 01| + |01\rangle\langle 10| + \delta|01\rangle\langle 11| \\
& + |10\rangle\langle 00| + |10\rangle\langle 01| + |10\rangle\langle 10| + \delta|10\rangle\langle 11| \\
& + \delta|11\rangle\langle 00| + \delta|11\rangle\langle 01| + \delta|11\rangle\langle 10| + \delta^2|11\rangle\langle 11| \big)
\end{aligned} \tag{65}$$

To check whether the above state is pure or not, we would perform the following conditions as

$$\rho_X^2 = \rho_X \text{ and } Tr(\rho_X^2) = Tr(\rho_X) = 1$$

To check whether the state is pure or not, we have

$$\begin{gathered}
\rho_{AB}^2 = a^4 \begin{pmatrix} (3+\delta^2) & (3+\delta^2) & (3+\delta^2) & \delta(3+\delta^2) \\ (3+\delta^2) & (3+\delta^2) & (3+\delta^2) & \delta(3+\delta^2) \\ (3+\delta^2) & (3+\delta^2) & (3+\delta^2) & \delta(3+\delta^2) \\ \delta(3+\delta^2) & \delta(3+\delta^2) & \delta(3+\delta^2) & \delta^2(3+\delta^2) \end{pmatrix} \\
\rho_{AB}^2 = \frac{1}{(3+\delta^2)} \begin{pmatrix} 1 & 1 & 1 & \delta \\ 1 & 1 & 1 & \delta \\ 1 & 1 & 1 & \delta \\ \delta & \delta & \delta & \delta^2 \end{pmatrix} = \rho_{AB}
\end{gathered} \tag{66}$$

Hence, the state is pure. So, $S(\rho_{AB}) = 0$, then the quantum mutual information would be written as

$$I_{AB} = S(\rho_A) + S(\rho_B)$$

where ρ_A and ρ_B are the marginal density matrices given as

$$\begin{aligned}\rho_A =& tr_B(\rho_{AB}) \\ =& a^2\Big(2|0\rangle\langle 0| + (1+\delta)|0\rangle\langle 1| + (1+\delta)|1\rangle\langle 0| + (1+\delta^2)|1\rangle\langle 1|\Big)\end{aligned} \tag{67}$$

where it could be written in a $2 \otimes 2$ matrix

$$\rho_A = \frac{1}{3+\delta^2}\begin{pmatrix} 2 & 1+\delta \\ 1+\delta & 1+\delta^2 \end{pmatrix} \tag{68}$$

As checked from the above matrix, $\rho_A^2 \neq \rho_A$, which confirms the state is not pure i.e., $S(\rho_A) \neq 0$ and the subsystems of the considered state, ρ_{AB} are correlated.

Using the Mathematica software for the calculation, the eigenvalues of the reduced density matrix ρ_A have been determined using $det(A - \lambda I) = 0$, where I is the Identity matrix, given as

$$\lambda_{\pm} = \tfrac{1}{2} \pm \tfrac{(3+3\delta+\delta^2+\delta^3)\sqrt{5-2\delta+\delta^2}}{2(9+6\delta^2+\delta^4)}$$

Then, the Von Neumann entropy of ρ_A is given as

$$S(\rho_A) = -\lambda_+ log_2\lambda_+ - \lambda_- log_2\lambda_-$$

An important measure of quantum entanglement is the entanglement of formation as discussed before, which for the pure state reduces to the Von Neumann entropy of the marginal state,

$$EOF = S(\rho_A) = S(\rho_B) \tag{69}$$

The Von Neumann entropy for the pure state is, $S(\rho_A) = S(\rho_B)$. Then, the quantum mutual information is

$$I_{AB} = 2S(\rho_A) \tag{70}$$

In order to quantify the classical correlation $C(\rho_{AB})$, let us consider the projection operator $\{B_i\}$ in the computational basis {0,1}, performed on the subsystem B, is given as

$$\begin{aligned} C(\rho_{AB}) =& max_{\{B_i\}} J(A|\{B_i\}) \\ =& max_{\{B_i\}}(S(\rho_A) - \sum_i S(\rho_{A|\{B_i\}})) \\ =& S(\rho_A) - min_{\{B_i\}} \sum_i S(\rho_{A|\{B_i\}})) \end{aligned} \tag{71}$$

where the maximization taken over all possible measurements $\{B_i\}$, won't affect the Alice's system as it is taken over the Bob's system. Now, to determine the classical correlation, first we start with the what projector operators would be in the basis $\{0, 1\}$ as

$$B_0 = U \prod\nolimits_0 U^\dagger = (a_0. + a_3)^2|0\rangle\langle 0| + (a_1 - ia_2)^2|1\rangle\langle 1| + (a_0 + a_3)(a_1 + ia_2)[|0\rangle\langle 1| + |1\rangle\langle 0|]$$

where $\prod_i = \sum_i |i\rangle\langle i|$ for $i = 0, 1$ and unitary is $U = a_0 I + \sum_{i=1}^{3} a_i \cdot \sigma_i$ with unit determinant, i.e., $a_0^2 + a_1^2 + a_2^2 + a_3^2 = 1$.

Let us consider here, $A = (a_0 + a_3)^2, B = (a_1 - ia_2)^2$ and $C = (a_0 + a_3)(a_1 + ia_2)$, then

$$\begin{aligned} I \otimes B_0 =& [|0\rangle\langle 0| + |1\rangle\langle 1|] \otimes [A|0\rangle\langle 0| + B|1\rangle\langle 1| + C(|0\rangle\langle 1| + |1\rangle\langle 0|)] \\ =& A[|00\rangle\langle 00| + |10\rangle\langle 10|] + B[|01\rangle\langle 01| + |11\rangle\langle 11|] \\ &+ C[|00\rangle\langle 01| + |10\rangle\langle 11|] + C[|01\rangle\langle 00| + |11\rangle\langle 10|] \end{aligned} \tag{72}$$

Therefore,

$$(I \otimes B_0)\rho_{AB}(I \otimes B_0) = a^2 \begin{pmatrix} A & C & 0 & 0 \\ C & B & 0 & 0 \\ 0 & 0 & A & C \\ 0 & 0 & C & B \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & \delta \\ 1 & 1 & 1 & \delta \\ 1 & 1 & 1 & \delta \\ \delta & \delta & \delta & \delta^2 \end{pmatrix} \begin{pmatrix} A & C & 0 & 0 \\ C & B & 0 & 0 \\ 0 & 0 & A & C \\ 0 & 0 & C & B \end{pmatrix}$$

$$= a^2 \begin{pmatrix} (A+C)^2 & (A+C)(C+B) & (A+C)(A+\delta C) & (A+C)(C+\delta B) \\ (A+C)(C+B) & (C+B)^2 & (C+B)(A+\delta C) & (C+B)(C+\delta B) \\ (A+C)(A+\delta C) & (C+B)(A+\delta C) & (A+\delta C)^2 & (A+\delta C)(C+\delta B) \\ (A+C)(C+\delta B) & (C+B)(C+\delta B) & (A+\delta C)(A+\delta C) & (C+\delta B)^2 \end{pmatrix} \tag{73}$$

Now, to determine the probability distribution $p_0 = tr(I \otimes B_0)\rho_{AB}(I \otimes B_0)$ for the final state which is given as

$$\rho_k = \frac{1}{p_k} tr(I \otimes B_k)\rho_{AB}(I \otimes B_k) \tag{74}$$

where $k = \{0, 1\}$. So,

$$p_0 = a^2\big[(A + C)^2 + (C + B)^2 + (A + \delta C)^2 + (C + \delta B)^2\big] \tag{75}$$

The state post measurement followed by Eq. (8) could be written as

$$\rho_0 = \frac{1}{p_0}\big[tr_B(I \otimes B_0)\rho_{AB}(I \otimes B_0)\big] \tag{76}$$

Similarly, we could write this expression for ρ_1 as

We would simplify the calculation here. To calculate the eigenvalues for a state ρ_0, there would be one real value possible for $a_0 = a_3 = \frac{1}{\sqrt{2}}$ and $a_1 = a_2 = 0$ and for others, eigenvalues will be imaginary. By implementing these values, we get

$$\rho_0 = \frac{1}{p_0}(tr(I \otimes B_0)\rho_{AB}(I \otimes B_0)) = \frac{1}{8}\begin{pmatrix} 4 & 4 \\ 4 & 4 \end{pmatrix} \tag{77}$$

where the eigenvalues for such matrix is $\lambda = 0, 1$ which results in zero Von Neumann entropy i.e., $S(\rho_0) = 0$.

Similarly, the Von Neumann entropy for state ρ_1 would be zero i.e., $S(\rho_1) = 0$,

Hence,

$$min_{\{B_i\}} S(\rho_{A|\{B_i\}}) = \sum_i p_i S(\rho_i) = 0 \tag{78}$$

Then, the expression for classical correlation reduces to the Von Neumann entropy of the marginal state given as

$$C(\rho_{AB}) = S(\rho_A) \tag{79}$$

Hence, the Quantum Discord would be given as

$$\begin{aligned} QD(\rho_{AB}) =& I(\rho_{AB}) - C(\rho_{AB}) \\ =& 2(S(\rho_A)) - S(\rho_A) = S(\rho_A) \end{aligned} \tag{80}$$

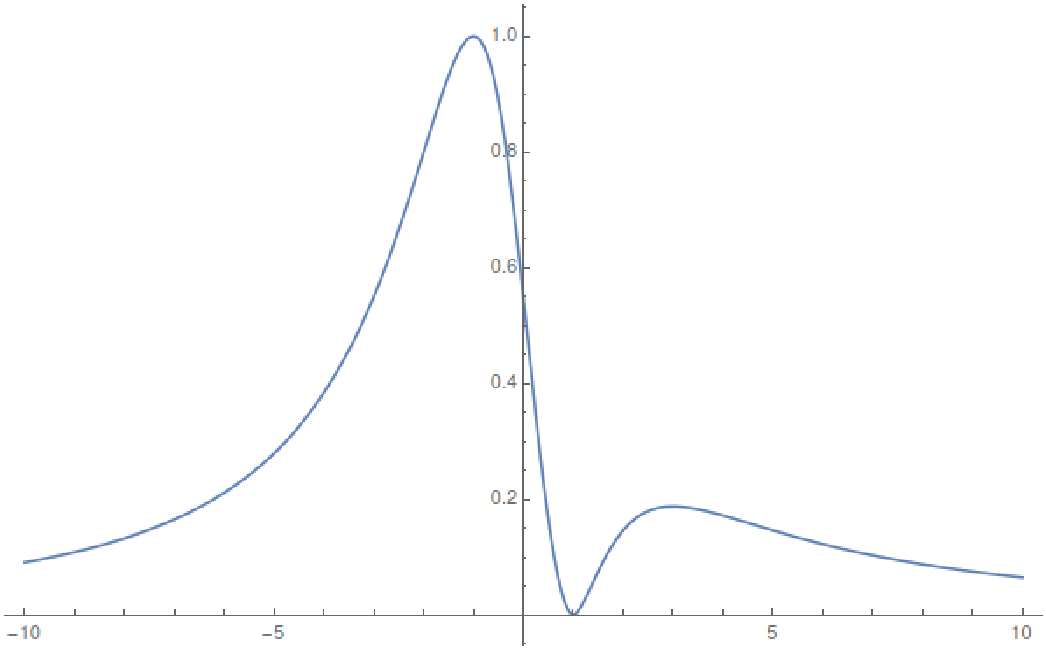

Figure 2: Quantum Discord Vs the parameter δ.

9 Conclusion and Discussion

9.1 For a Bell state

As calculated earlier in section 8.1, the entanglement of formation is 1 and the quantum discord is also 1 but both having the different explanation.

The numerical value of entanglement of formation for a pure state says about how correlated two states are. It says about the nature of a state. If the result says that the entanglement of formation, a quantum entanglement measure of the state is 0, then the states are separable and can written in a product form which shares no entanglement between them but that does not mean that there is no correlation. The correlation can be found in the non-product states as well.

$$EOF = 0, \text{ State is separable. Hence, } \rho_{AB} = \rho_A \times \rho_B$$

If the entanglement of formation of the state is 1, then the states are not separable which shares the correlation. These states are the maximally entangled states.

$$EOF = 1, \text{ State is maximally entangled. Hence, } \rho_{AB} \neq \rho_A \times \rho_B$$

We are clear about the results of Bell states, but if the entanglement of formation is neither 0 nor 1 but lies between them shares the correlation and the states are entangled too but they are not maximally entangled.

9.2 For a State with Parameter Delta

As following section 8.2, the calculation of the entanglement of formation and the quantum discord for a state with some parameter δ says that both quantity varies upon changing the value of the parameter δ as we see in the Figure 2.

In this section 8.2, the result shows that the entanglement of formation and the quantum discord are equal to the marginal state of the composite state $S(\rho_{AB})$.

$$EOF = QD(\rho_{AB}) = S(\rho_A) \tag{81}$$

By looking at the graph, the minimum value of quantum discord which has achieved is 0 at $\delta = 1$ and the maximum value which has achieved is 1 at $\delta = -1$.

At $\delta = 1$, the entanglement of formation is 0 which means the state is separable and can be written in a product form and the quantum discord is also 0 which says that the state shares no correlation but as we change the value of $\delta = -1$, the quantum discord reaches to its maximum value which shares the maximum correlation and the entanglement of formation reaches to its maximum too which says the state is maximally entangled state.

10 Summary

The classical information theory which is based on the formulations of classical mechanics and probability theory. It was first studied by Claude Shannon which states and justifies the the mathematical aspects and two fundamental theorems of information theory. Currently, all the classical system run on some bit of information which gets transmitted through some channel.

In the landmark 1948, Claude Shannon introduced a measure of information, Shannon Entropy. The concept of Shannon Entropy is based on the probability distribution. There exist a measure of information based on the Shannon Entropy which is known as the Mutual Information. The classical and quantum mutual information quantifies the correlation.

The quantum information theory is based on the postulates of quantum mechanics and is fundamentally different from the classical information theory. The quantum physical systems register the bit of information and is stored in a quantum state. In the quantum regime, the Von Neumann Entropy is similar to the formulation of Shannon Entropy. To measure the quantum correlation that a quantum state possess, the concept of quantum mutual information plays a major role in the quantum information theory.

Quantum correlation plays an important role in the quantum many body systems. There exist two ways to measure the correlation, (i) The entanglement of formation, a measure of Quantum entanglement, is one of the important measure of correlation in which two or ore parties are involved and states that either the state is partially entangled or maximally entangled or the state can be written in a product form (the state is separable). (ii) Later on, Ollivier and Zurek [1] proposed a new measure of quantum correlation, the Quantum discord, which quantifies the non classical correlation of a given quantum system and is defined as the difference of two classically equivalent forms of mutual information.

We later reviewed in this report that the quantum discord can also be used to measure the correlation between the particles ate the neighbour sites in a spin chain. Given a general Hamiltonian for any spin-1/2 models, It is possible to analytically determine the correlation between them. We have currently studied for the two qubit X-state and obtained the results for the same.

We briefly reviewed the properties and expressed the relation between the important measures of correlation like quantum discord and quantum entanglement, and compared them with the obtained numerical values. For the state with parameter delta we considered, we have evaluated that the quantum entanglement measure and quantum discord is same but have the different explanation to each which has explained better in section 9 and can be better understood by plot [Fig. 2].

11 Future Plans

We discussed all the important aspects of classical as well as the quantum information theory. We have discussed the measure of correlation for only two qubit states. We aim to study the measure of correlation for three or four qubit states or may be qudits also if possible.

It is easy to quantify the quantum discord for n-qubit states with no arbitrary parameter. When it comes to do the measurement on the subsystem B in a composite system AB and it becomes more tougher when the arbitrary parameter present in a quantum state.

Quantum information theory has helped in understanding the quantum correlation in quantum many body systems. Especially, the bipartite entanglement has become more crucial to characterise and simulate the quantum many body systems. The methods and notions studied in the many body systems does not end with the entanglement in which two parties are involved. The measures, quantum discord and quantum entanglement can be further explored for the multipartite states. There can be other forms of correlation exist in either the ground state, excited state or the thermal states which needs to be further explored in the many body systems.

Finally, apart from the the measures we have studied, I would wish to focus on other measures of correlation like multipartite entanglement, quantum discord for multipartite states and mutual information. There exist some other non-classical correlation like quantum coherence which still needs to be explored in the quantum many body systems.

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