

A Comparative Study of Quantum Correlation Measures in an AF Critical Spin System with Next-Nearest-Neighbour Interaction

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Abstract

Recently some Quantum Information Theoretic measures like Entanglement and Quantum Discord have emerged as very important tools for investigating quantum systems. A number of such measures in a critical Heisenberg spin system (which undergoes a transition from a disordered phase to an antiferromagnetically ordered phase) have been studied in this work and some non-trivial features exhibited by the measures near Quantum Critical Points have been obtained. The nature of variation of those measures with a disorder-enhancing next-nearest-neighbor interaction of the model system has also been investigated. The work indicates that the Quantum discord is more robust than the so-called non-local correlations against some disordering interactions present in the system and also more consistent in signaling the changes brought about in the physical state by tuning the relevant parameters of the system across a Quantum Phase Transition. A novel universal scaling behavior exhibited by the measures has also been found.

Keywords: Quantum Correlations, Phase Transition, Disorder, Spin System, Discord

Introduction

Quantum Entanglement, not only is considered as a resource of quantum computation, quantum cryptography and quantum information processing, but also has proved to be efficient in analyzing the behaviour of various condensed matter systems [Horodecki et al., 2009; Amico et al., 2008]. A familiar example of an entangled state is the singlet state of two spin- $\frac{1}{2}$ particles, $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$, which cannot be written as a product of the spin states of individual spins. In the case of a mixed state, entanglement occurs if the density matrix is not a convex sum of product states. However, it has been established that entanglement does not encompass all kind of substantive correlations of quantum nature present in quantum systems. Quantum discord (QD) [Henderson et al., 2001; Ollivier et al., 2002], defined as the discrepancy between quantum versions of two classically equivalent expressions for mutual information, has been demonstrated to be a novel resource for quantum computation [Datta et al., 2008; Knill et al., 1998]. Following the seminal work, people have recently proposed several new measures of quantum correlations

and non-locality that are more general than entanglement [Modi et al., 2012]. It has been experimentally demonstrated using photonic quantum systems that separable states with non-zero quantum discord can outperform entangled states in quantum information protocols like quantum remote state preparation [Dakić et al., 2012].

Quantum phase transitions (QPT) are sharp changes occurring in the ground states of quantum many-body systems when one or more of the physical parameters of the system are continuously tuned at absolute zero temperature [S. Sachdev, 2011]. These radical changes, which strongly affect the macroscopic properties of the system, are manifestations of quantum fluctuations. Despite the fact that reaching absolute zero temperature is practically impossible, QPTs might still be observed at sufficiently low temperatures, where thermal fluctuations are not significant enough to excite the system from its ground state. In recent years, the methods of quantum information theory (QIT) have been widely applied to quantum critical systems. In particular, entanglement and quantum discord have been shown to identify the quantum critical points (QCP) with success in several different critical spin chains, both at zero and finite temperature [Osborne et al., 2002 and references therein].

In this work, we investigate the pair-wise quantum correlations in a one-dimensional spin-1/2 Heisenberg chain with anisotropic nearest neighbour (NN) and next nearest neighbour (NNN) interactions depicted in [Datta et al., 2005]. The Hamiltonian of the anisotropic Heisenberg spin chain is given by

$$H^{spin} = -J_1 \sum_j (\sigma_j^+ \sigma_{j+1}^1 + H.c.) + J_Z \sum_j \sigma_j^z \sigma_{j+1}^z - J_2 \sum_j (\sigma_{j-1}^+ \sigma_{j+1}^1 + H.c.) - k \sum_j \sigma_j^z \quad (1)$$

where J_1 and J_Z are exchange coupling strengths along the transverse and the longitudinal directions respectively, J_2 is the NNN coupling and the coefficient of the last term represents coupling to a longitudinal magnetic field. This Hamiltonian has been obtained by an exact mapping of an effective polaronic interaction Hamiltonian, exact to second order in perturbation, for the spin-less one-dimensional Holstein model to the one written above. The system with $J_2 = 0$, i.e., without NNN interaction, has been shown to undergo a disordered (Luttinger liquid in the original spin-less Polaronic system) to antiferromagnetically ordered phase (Charge Density Wave phase in the Polaronic system) transition at zero magnetization ($\sum_j \sigma_j^z = 0$) at $J_Z = 2J_1$ and at non-zero magnetization is always disordered [F.D.M.

Haldane, 1980]. The asymptotic behaviour of the static spin-spin correlation function for a chain of length

N is given by $W_N(l) \left(= \frac{4}{N} \sum_{i=1}^N \langle \sigma_j^z \sigma_{j+l}^z \rangle \right) \approx A \frac{(-1)^l}{l^n}$ where A is an unknown constant and n is the spin

correlation exponent. $1 < n \leq 2$ in the disordered (LL) phase, $n = 1$ is the transition point to the ordered (CDW) state and $n = 0$ depicts complete antiferromagnetic order. Interestingly, the NNN exchange interaction term with coupling strength J_2 , being in the transverse direction, does not compete to produce frustration. But on including a non-zero J_2 , the disordering effect increases and the LL to CDW transition takes place at higher values of J_Z . Including J_2 evidently does not change the universality class with the central charge $c = 1$. It is not an integrable model due to the presence of the NNN term and thus cannot be solved by coordinate Bethe Ansatz. Hence we used a modified Lanczos technique to analyze the properties of the effective Hamiltonian numerically [Datta et al., 2005; Gagliano et al., 1987] I have taken $J_1 = 1$ so that the QPT takes place at $J_Z = 2$ for zero J_2 .

As a measure of genuine quantum correlations, we use concurrence [Hill et al., 1997], and a very recently proposed Observable Measure of Quantum Discord (OMQD) [Girolami et al., 2012], which is a simplified version of the geometric measure of quantum discord [Dakić et al., 2010]. A knowledge of the two-site reduced density matrix $\rho(i, j)$, obtained from the full density matrix by tracing out the spins other than the ones at sites i and j , enables one to calculate concurrence, a measure of entanglement between two spins at sites i and j [Hill et al., 1997]. Let $\rho(i, j)$ be defined as a matrix in the standard basis. One can define the spin-reversed density matrix as $\tilde{\rho} = (\sigma_y \times \sigma_y) \rho^* (\sigma_y \times \sigma_y)$, where σ_y is the Pauli matrix. The concurrence is given by $C = \text{Max}\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}$ where λ_i 's are square roots of the eigenvalues of the matrix $\rho\tilde{\rho}$ in descending order. An equivalent way of writing C is $C = \text{Max}\{|\rho(3,2)| - \sqrt{\rho(1,1)\rho(4,4)}, 0\}$. $C = 0$ implies an unentangled state whereas $C = 1$ corresponds to maximum entanglement.

Geometric measure of quantum discord has been introduced to overcome the difficulties in the evaluation of the original quantum discord which involves a tedious optimization job [Dakić et al., 2010]. It measures the nearest distance between a given state and the set of zero-discord states. Mathematically, it is given by:

$$D_G(\rho_{ab}) = 2 \text{Min}_{\chi} \|\rho_{ab} - \chi\|^2 \quad (2)$$

where ρ_{ab} is the composite state of two spins labeled by a and b and the minimum is taken over the set of zero-discord classical-quantum states $\{\chi\}$. If we express the state in the Bloch basis

$$\rho_{ab} = \frac{1}{4} \sum_{i,j=1}^3 R_{ij} (\sigma_i \times \sigma_j) = \frac{1}{4} \left(\mathbb{I}_4 + \sum_{i=1}^3 x_i (\sigma_i \times \mathbb{I}_2) + \sum_{j=1}^3 y_j (\mathbb{I}_2 \times \sigma_j) + \sum_{i,j=1}^3 t_{ij} \sigma_i \times \sigma_j \right) \quad (3)$$

we obtain the three-dimensional Bloch column vectors \vec{x} and \vec{y} associated to a and b and the correlation matrix t . In a recent work, Girolami et. al. has obtained an interesting analytical formula for the geometric discord of an arbitrary two-qubit state $D_G(\rho_{ab}) = 2(\text{Tr}(S) - \text{Max}\{k_i\})$ where $S = \vec{x}\vec{x}^t + t t^t$ and $\{k_i\}$ are the eigenvalues of S , given by $k_i = \frac{\text{Tr} S}{3} + \frac{\sqrt{6\text{Tr} S^2 - 2(\text{Tr} S)^2}}{3} \text{Cos}\left(\frac{\theta + \alpha_i}{3}\right)$ with $\{\alpha_i\} = \{0, 2\pi, 4\pi\}$ and

$\theta = \text{Cos}^{-1}\left\{ \frac{2\text{Tr} S^3 - 9\text{Tr} S \text{Tr} S^2 + 9\text{Tr}(S^3)}{\sqrt{2/(3\text{Tr}(S^2) - \text{Tr} S)^3}} \right\}$. Observing that $\text{Cos}\left(\frac{\theta + \alpha_i}{3}\right)$ reaches its maximum for $\alpha_i = 0$ and choosing θ to be zero, they have obtained a very tight lower bound to the geometric discord, given by:

$$Q(\rho_{ab}) = \frac{2}{3} (2\text{Tr} S) - \sqrt{6\text{Tr}(S^2) - 2\text{Tr} S^2} \quad (4)$$

This quantity (referred as OMQD) can be regarded as a meaningful measure of quantum correlations on its own and it has the desirable feature that it needs no optimization procedure. Besides being easier to manage than the original geometric discord, it can be measured by performing seven local projections on up to four copies of the state. This observable measure has the advantage that it does not require a full tomography of the system, making it experimentally very accessible. I investigate the variation of C and Q (both for NN and NNN spin pairs) in the model system with varying longitudinal coupling strength J_z and the disorder-

enhancing NNN coupling J_2 at zero magnetization with a motivation to obtain non-trivial and physically interesting and important behaviours of usable quantum correlations available naturally in the physical state of the system.

Comparative behaviour of Different Correlation Measures

Let's first consider the $J_2 = 0$ case. In the Ising limit $J_Z \rightarrow \infty$, the ground state is exactly the Neel long-range ordered state with vanishing quantum correlations. When J_Z is decreased and made finite, the quantum fluctuations start to play a more and more important role inducing NN disorder in the system, then the Neel state fails to remain an eigenstate of the Hamiltonian. Mathematically, as this fluctuation between two neighbouring sites enhances the value of off-diagonal terms in their reduced density matrix $\rho(i, j)$, the quantum correlations are expected to become larger and larger. At the other extreme limit, i.e., at the "free particle" limit $J_Z \rightarrow 0$, the spin-flip term solely rules the system and all spins flip freely on respective sites. The probabilities of spin up and down at a given site are exactly equal, irrespective of the neighbour spin. Thus, the state $|\uparrow\uparrow\rangle$ share the same probability with $|\uparrow\downarrow\rangle$ or $|\downarrow\uparrow\rangle$. This phenomenon makes $\rho(1, 1)$ or $\rho(4, 4)$ relatively large, making C smaller. But once the J_Z interaction is turned on, the values of $\rho(1, 1)$ or $\rho(4, 4)$ decrease effectively enhancing the concurrence. Hence the competition of disordering quantum fluctuations and ordering interaction must result in a maximum at a certain point. Figure 1 presents the results regarding the quantum correlations quantified by the NN concurrence C and the NN OMQD Q as a function of J_Z for $J_2 = 0$ for a system size $N = 20$. We note that both the measure exhibit maxima at the QCP $J_Z = 2$. The concurrence is greater than the QD for all values of J_Z and exhibits a smooth peak at the QCP. The first derivative, C' of C with respect to J_Z smoothly crosses zero at the QCP (inset of Figure 1). Unlike C , Q shows an arrowhead-like peak and the first derivative Q' , of Q , shows a finite discontinuity at the QCP (inset of Figure 1) which conventionally can be considered as a signature of QPT taking place in the thermodynamic limit (TDL). The results show that, like the pair-wise entanglement, quantum discord also rise with the ordering interaction (J_Z , in our case) in the disordered phase and fall with the same interaction in the antiferromagnetically ordered phase and thus becomes maximum at the transition point. The mathematical reason behind such variation may be similar to the case of C . Discord measure is essentially a function of the elements of the two-site reduced density matrix and the relative changes in the values of the diagonal and the off-diagonal elements due to the change in the interaction strengths of the Hamiltonian results in such variation of Q . The exhibition of a peak by some observable and discontinuity or diverging tendency of its derivatives at some value of the system parameter for a finite sized system can be treated as a precursor of the QPT taking place at the TDL. Repeating the investigation for different sizes of the system, we find similar results (Figure 2 and 3). The value of both the measures depends on the system size and slightly decreases with it at and away from the QCP. One possible explanation is that as the size increases, the correlations get shared among more and more number of parties effectively decreasing the pair-wise part. Figure 4 shows the variation of Q and C respectively with varying N at $J_Z = 2$. But interestingly, the dependence of both the measures on system size becomes flattened as we make the system size larger ($N > 20$). This is totally in conformity with the result shown in [Gu et al., 2003] which shows that for this system, concurrence exhibits a novel size-independent scaling with the correlation length ξ and the measures of quantum correlations calculated for a small system ($N \geq 20$) can well describe the behaviour for very large systems, even the TDL. In the vicinity of the QCP, the concurrence goes like $C = C_0 - C_1(J_Z - J_{ZC})^2$ ($J_{ZC} = 2$ in this case) for high values of N . The values of the constants C_0 and C_1 tend to 0.386292 and 0.188 respectively with increasing system size (matches very well with the values calculated in [Gu et al., 2003] for very large system sizes using Bethe Ansatz. On the other hand, the arrow-head-like variation of the discord measure goes as $Q = Q_0 - Q_1|J_Z - J_{ZC}|$ (this explains the finite jump of the first

derivative of Q at the QCP). The value of the constants Q_0 and Q_1 tends respectively to 0.35 and 0.11 when we increase the system above $N = 20$. The relevant critical exponent of variation is thus 2 (1) for the concurrence (discord) measure.

Figure 1: NN QD Q (Dark Circles) and NN Concurrence C (Squares) as a Function of J_z for $J_2 = 0$ at $N = 20$

First Derivative of Q (Upper Inset) and C (Lower Inset) as a Function of J_z

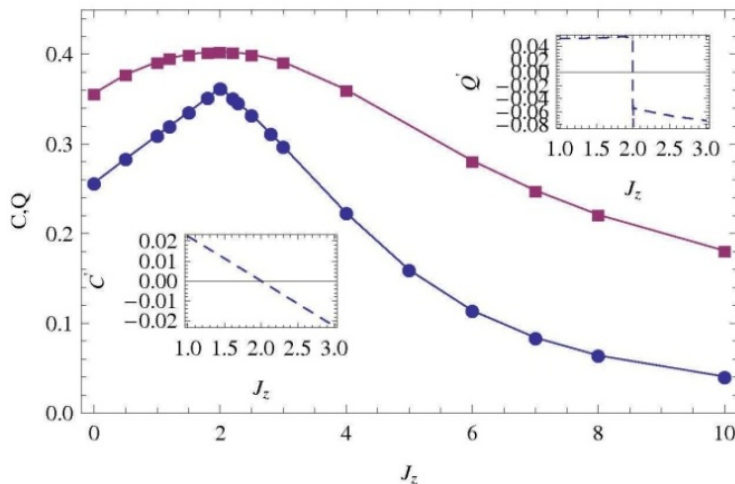
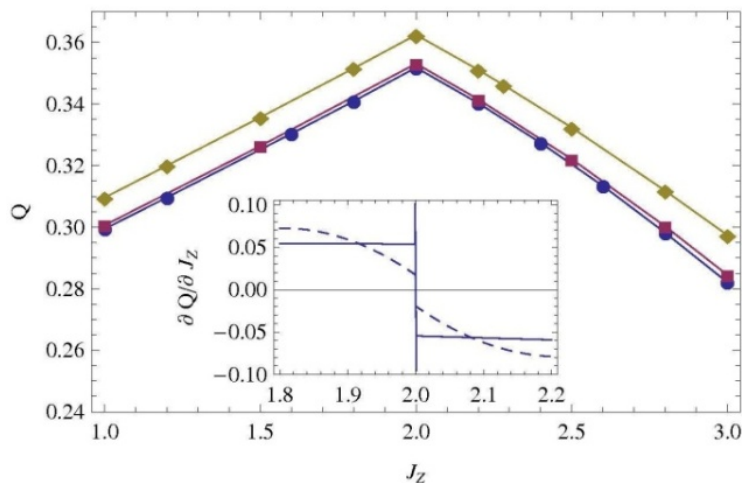


Figure 2: Q as a Function of J_z for $J_2 = 0$ for $N = 20$ (Diamonds), 22 (Squares), and 26 (Circles) Solid Connecting Lines have been Obtained by Fitting $Q = Q_0 - Q_1|J_z - J_{zC}|$ First Derivative of Q (Inset) as a Function of J_z for $N = 18$ (Dashed) and 26 (Solid Line)



**Figure 3: C as a Function of J_z for $J_2 = 0$ for $N = 20$ (Diamonds), 22 (Squares), and 26 (Circles)
Solid Connecting Lines have been Obtained by Fitting $C = C_0 - C_1(J_z - J_{zc})^2$
First Derivative of C (Inset) as a Function of J_z for $N = 18$ (Dashed) and 26 (Solid Line)**

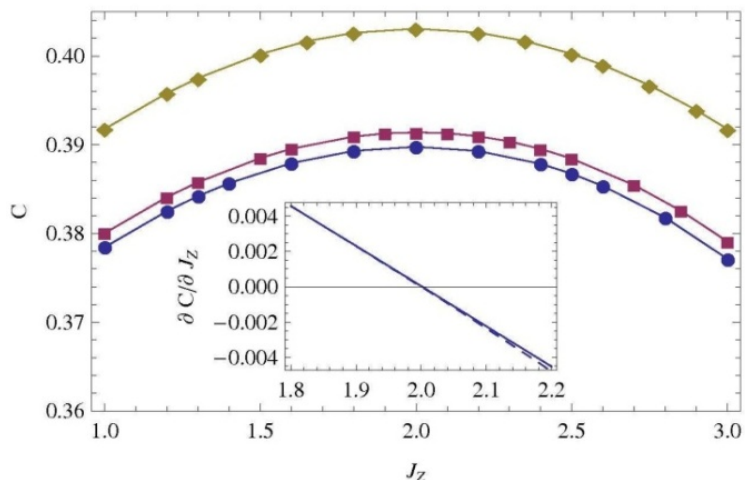


Figure 4: Variation of C and Q with N at the QCP $J_z = 2$

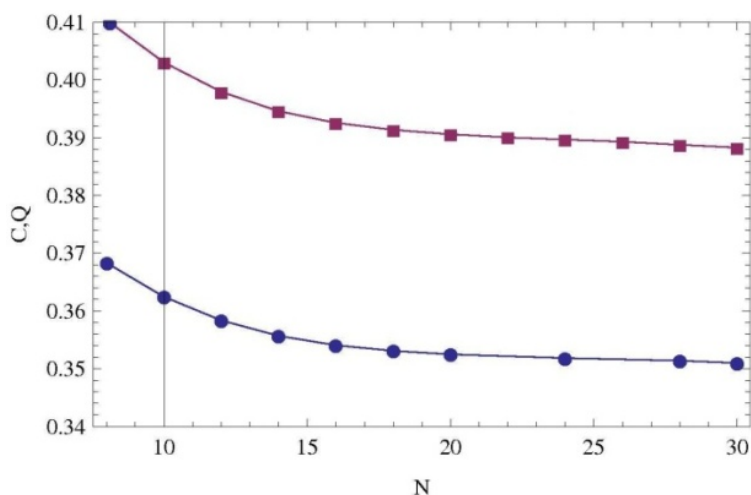


Figure 5: Q (Diamonds), Q_{NNN} (Circles), C (Triangles) and C_{NNN} (Squares) as Functions of J_z for $J_2 = 1$

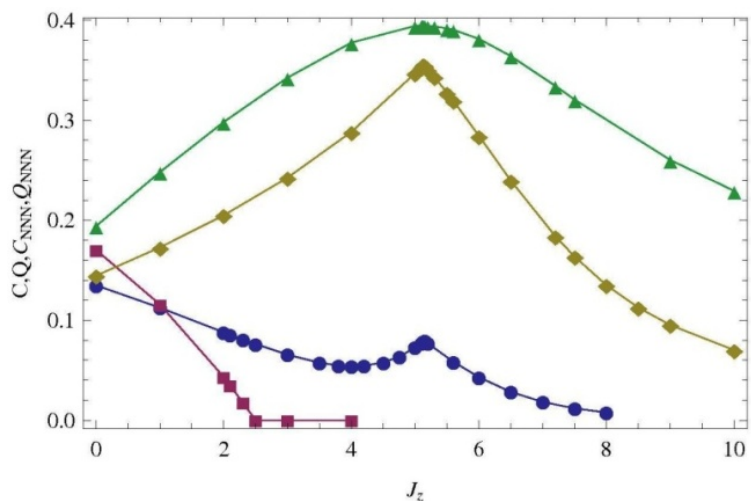


Figure 6: Q (Circles) and C (Squares) as Functions of J_2 for $J_Z = 1$ and 0 (Inset)

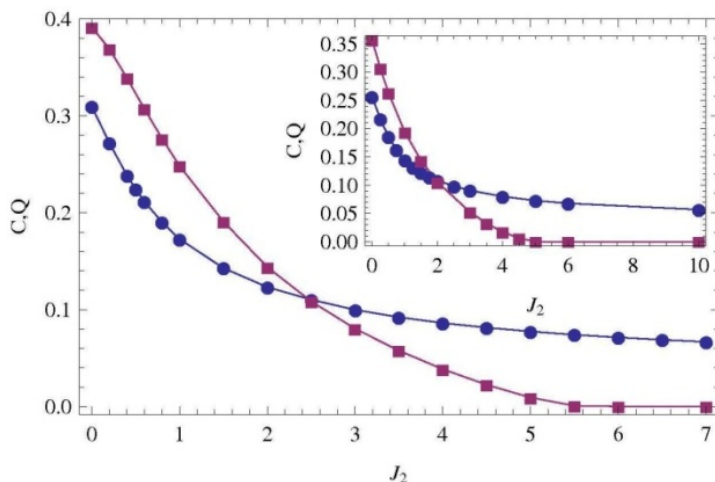


Figure 7: Q and C (Inset) as Functions of J_2 for $J_Z = 0$ (Squares), 1 (Diamonds) 2.5 (Triangles) and 6 (Circles)

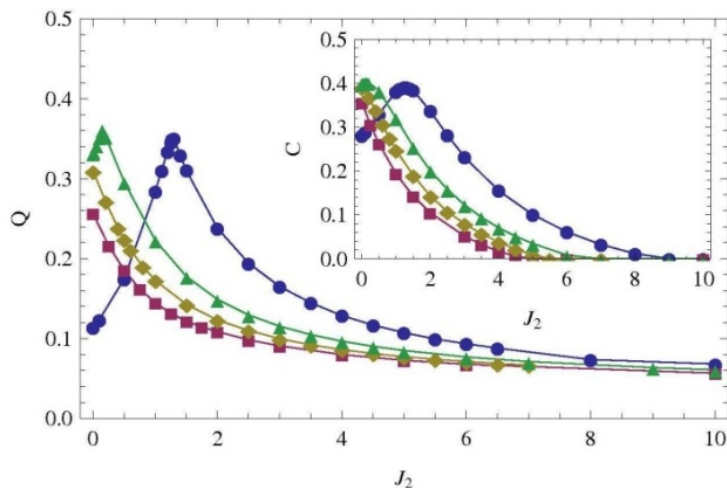


Figure 8: Q (Circles), Q_{NNV} (Diamonds), C (Squares) and C_{NNV} (Triangles) as Functions of J_2 for $J_Z = 0$

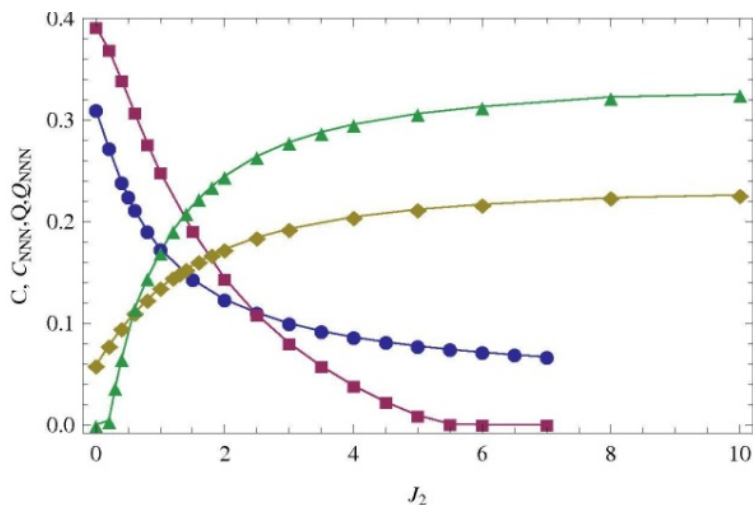
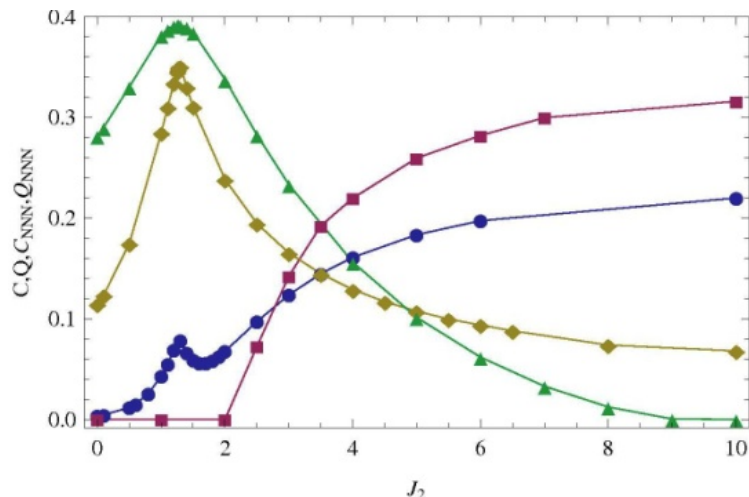
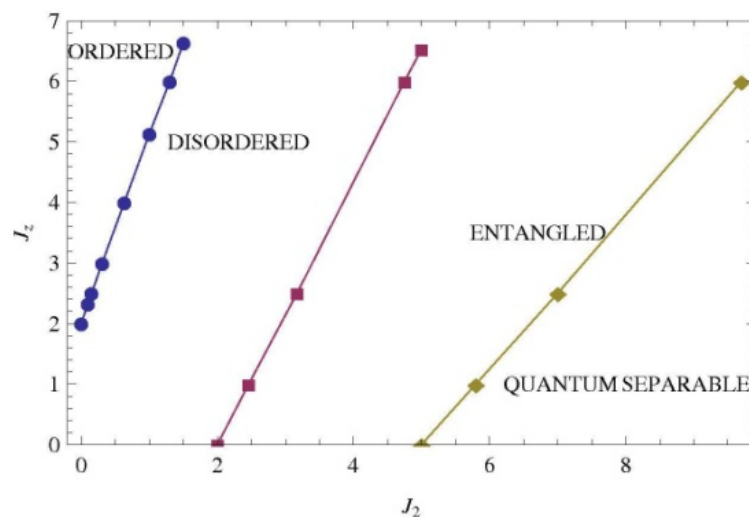


Figure 9: Q (Diamonds), Q_{NNN} (Circles), C (Triangles) and C_{NNN} (Squares) as Functions of J_2 for $J_Z = 6$ **Figure 10: J_{ZC} (Circles), J_{ZCr} (Squares) and J_{ZQS} (Diamonds) as Functions of J_2** 

Having discussed the behaviours of the quantum correlations near the QCP for $J_2 = 0$, let us now explore the effect of the non-frustrating NNN interaction J_2 on the QIT measures and the QCP. Introduction of a non-zero J_2 increases the disordering effects (as NNN pairs start to flip now) and shifts the QCP to a higher value. We studied the variations of the correlation measures C and Q with J_2 and J_Z for different system sizes. Figure 5 demonstrates the variation of C and Q with J_Z for $J_2 = 0$ and 1 for $N = 20$. The peaks of C and Q shift to $J_Z \approx 5.13$ for $J_2 = 1$. The measures successfully signal the QPT taking place at a higher value of J_Z . The value of the maxima depends on the system size (decreases with increasing N first significantly up to $N = 20$ and then it gets flattened out) and is lowered as we increase J_2 . Figure 6 depicts the nature of variation of the measures with increasing J_2 for $J_Z = 1$ and 0 (inset) for $N = 20$. Both C and Q decreases monotonically with the NNN interaction strength J_2 for all $J_Z < 2$. Interestingly, C dominates over Q up to a certain value of J_2 and then goes below it and vanishes as J_2 is increased further but Q always remains non-vanishing and tends to a finite value. We may say that in the disordered phase, the NNN interaction keeps enhancing the disorder, taking the system more and more away from the QCP, and diminishing the quantum correlations in that phase, eventually killing the non-local part. But it cant kill all meaningful quantum correlations as the discord measure remains non-zero in the quantum separable state at even very high values of J_2 . Crossing of the entanglement and discord measure at a given J_2 signals the onset of a novel state where the non-local part of quantum correlations is dominated by some other type of

correlations of purely quantum nature measured by the OMQD. If we put $J_Z > 2$, the monotonic nature of variation of C and Q with J_2 changes (Figure 7). Both the measures first increase with J_2 up to a value and then decrease monotonically. The position of the maxima increases with increasing J_Z (inset of Figure 6). For $J_Z > 2$, the system is in a phase with quasi-long range order (depicted by the power law variation of the spin correlations) when $J_2 = 0$. If we increase J_2 in this regime, the correlations first get enhanced due to increasing J_2 as it rapidly takes the system to the order-to-disorder transition point where the correlations become maximum and then in the disordered phase, it starts to decrease again like the $J_Z < 2$ case. This result is important due to entanglement and discord being a resource in quantum computation as it demonstrates the fact that disorder may be beneficial at times in certain regions of the tunable parameter space. The crossing of C and Q happens for $J_Z > 2$ as well and the crossing point shifts to higher J_2 values with increasing J_Z .

We now investigate the variation of NNN concurrence C_{NNN} and NNN OMQD Q_{NNN} with increasing interaction strengths. For $J_2 = 0$, C_{NNN} has been found to be vanishing for all values of J_Z and thus insensitive to the QPT. With no NNN spin flipping interaction, the non-zero NN spin flipping term J_1 and ordering term J_Z make the diagonal elements dominating over the off diagonal elements of the NNN two-site reduced density matrix making the entanglement between two NNN spins vanishing. However, the “quantum separable” state of two NNN pair still contains genuine quantum correlations measured by the QD measure Q_{NNN} . Q_{NNN} is found to be exactly equal to the NN discord Q in this case. For a non-zero J_2 , we get a non-zero C_{NNN} , but it dies a sudden death for a small value of increasing J_Z (Figure 5). But Q_{NNN} , though much smaller in magnitude compared to Q , continues to remain non-zero and signal the QCP exhibiting an arrowhead-type peak (and a discontinuous first order derivative). Figure 8 shows the simultaneous variations of NN and NNN concurrences and OMQDs with increasing J_2 for $N = 20$ and for $J_Z = 0$. Q_{NNN} is zero for $J_2 = 0$ and increases with increasing J_2 and tends to a constant value at higher J_2 values. Q_{NNN} , on the other hand, increases with increasing J_2 , crosses and goes below C_{NNN} at a given J_2 and tends to a constant when J_2 is increased further. The variations of the same measures with same system size for $J_Z = 6$ for have been furnished in Figure 9. Surprisingly, in this case, both Q and Q_{NNN} increases initially with increasing J_2 , shows peaks at the same value of J_2 . But unlike Q , Q_{NNN} in this case goes down unto a certain value of the NNN interaction, shows a dip and then again goes up and tends to a constant value. Near the QCP, unlike entanglement measures, both NN and NNN discord has been found to grow and exhibit local maximum. This is an interesting result. This is a hint of the fact that for some physical systems, we obtain enhancement of usable quantum correlations between NN as well as distant pairs of parties near the QCPs. C_{NNN} is vanishing up to a value of J_2 , suddenly kicks in at that value, increases, goes above Q_{NNN} and finally saturates. The $Q - Q_{NNN}$ crossing points are identically same with the $C - C_{NNN}$ crossing points. The scaling behaviours exhibited by the measures in the vicinity of the QCP for $J_2 > 0$ are similar to the behaviours obtained in the $J_2 = 0$ case with exactly same exponents.

We have observed that the critical value J_{ZC} of the longitudinal interaction strength J_Z , at which the “disordered-to-ordered” transition occurs, increases with the increasing transverse NNN interaction J_2 due to disordering effects of the later. We plotted J_{ZC} with J_2 in Figure 10 (Circles). It is a straight line and when fitted, it goes like $J_{ZC} \approx 2.000 + 3.129J_2$. These values are in fair agreement with the values obtained from the spin correlation exponent calculations [Dutta et al., 2005]. Thus, as depicted in Figure 10, the straight line can be considered as the critical boundary separating the disordered phase from the antiferromagnetically ordered phase in the $J_Z - J_2$ parameter space. We have determined the values of J_{ZQS} at which the NN concurrence vanishes for given J_2 values and plotted it in the same figure. It has also been

found to be a straight line. This line can be considered to be the boundary line separating the region of non-local correlations from the region of pure discordant quantum separable states of a NN pair. Also, the value J_{Zcr} at which the NN entanglement crosses the NN Quantum discord and goes below it has been observed to vary linearly with the value of J_2 (Figure 11). Going from left to right of Figure 10, i.e., with increasing J_2 , we first cross the “ordered-to-disordered” J_{ZC} critical line, then in the disordered phase we cross “ J_{Zcr} line” where each NN pair of system becomes “more discordant than entangled” and finally we cross the J_{ZQS} line where the NN pairs becomes “Quantum separable” with non-vanishing discord.

Conclusion

This paper reports the study of the quantum correlations quantified by both entanglement and discord measures in a one-dimensional anisotropic Heisenberg model which undergoes a continuous QPT from a disordered (LL) to an antiferromagnetically ordered (CDW) phase at a value of the longitudinal coupling strength J_Z . The system contains a NNN exchange interaction J_2 also which is not frustrative but it enhances disordering quantum fluctuations in the system effectively delaying the transition and shifting it to higher values of the longitudinal ordering interaction J_Z . The Heisenberg spin model with such competing interactions has been shown to be realized using atoms in photon coupled cavities [Chen et al., 2010]. I have quantified the entanglement with the well known measure Concurrence C and the quantum discord using a recently proposed observable measure of geometric discord Q in the ground state of the system using a modified Lanczos technique of exact Diagonalization and studied the system for increasing finite sizes. Only the even values of N have been considered to avoid the frustration effects for odd N under periodic boundary conditions. Both the measures Q and C studied here have operational meanings so that the correlations studied can be made useful and Q have been found to show maxima at the QCP in different fashions and their first derivatives behave very differently near the QCP. These results demonstrate that OMQD can be more relevant than some conventional pairwise entanglement measures for identifying QCPs in concrete physical problems. Both the measures have been shown to exhibit a universal size-independent scaling behaviour around the critical point for large system sizes. This result conforms well to the work by Gu et. al. (using Bethe Ansatz technique), where the concurrence has been shown to behave almost system-independent manner for large system sizes ($N > 20$). However, the variation of the QD measure around the QCP demands more complete physical understanding.

The transition point has expectedly been found to shift to higher J_Z values (signalled by the OMQD measure) as we keep on enhancing disordering quantum fluctuations by increasing the transverse NNN coupling J_2 . Interestingly, the non-local measure C , starting with values higher than that of Q , decays sharply with increasing J_2 , goes below Q at a given J_2 , and then vanishes at a higher value of the NNN coupling. On the other hand, Q remains non-vanishing and tends to a minimum value with increasing J_2 . While NNN entanglement C_{NNN} has been found to die sudden death and be fully insensitive to the transition point, NNN discord Q_{NNN} has been found to signal the QCP by exhibiting an arrowhead-type peak, though feebler than its NN counterpart and a discontinuous first order derivative. While studying the correlations, we have found regions of the J_2 parameter space, where the concurrence value is vanishing for NN and NNN pairs, i.e., the system is in quantum separable state but the discord measures are non-vanishing. There are regions also with discord higher than the non-local correlations. The states in those regions are the potential candidates to implement QIT protocols which use geometric quantum discord as a resource. Such crossing of measures of entanglement and discord need further explanations and understanding though. It would also be interesting to study these measures in the thermodynamic limit where the QPT takes place in actuality and also at finite temperatures. The work once again shows that genuine quantum correlations can

be present in a physical state without the so-called non-local correlations and we need more general measures of quantum correlations like QD to quantify it and use it a resource. Those correlations are also more robust compared to the entanglement against the disordering quantum fluctuations present in the system. It also shows that quantum discord measures can signal Quantum phase transitions more successfully and consistently than the entanglement measures and thus can shed light on the areas of condensed matter physics which are not understood well in terms of conventional observable tools. This work can be extended to those systems which are yet unexplored.

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