Concurrence and Quantum Discord in the Eigenstates of Chaotic and Integrable Spin Chains

Atefeh Ashouri, Saeed Mahdavifar, Grégoire Misguich, and Javad Vahedi *

There has been some substantial research about the connections between quantum chaos and quantum correlations in many-body systems. This paper discusses a specific aspect of correlations in chaotic spin models, through concurrence (CC) and quantum discord (QD). Numerical results obtained in the quantum chaos regime and in the integrable regime of spin-1/2 chains are compared. The CC and QD between nearest-neighbor pairs of spins are calculated for all energy eigenstates. The results show that, depending on whether the system is in a chaotic or integrable regime, the distribution of CC and QD are markedly different. On the other hand, in the integrable regime, states with the largest CC and QD are found in the middle of the spectrum, in the chaotic regime, the states with the strongest correlations are found at low and high energies at the edges of spectrum. Finite-size effects are analyzed, and some of the results are discussed in the light of the eigenstate thermalization hypothesis.

1. Introduction

In the recent years, a great deal of attention has been devoted to quantum chaos, one challenge being to identify quantum signatures of chaos, in particular in systems which may lack a clear classical limit. Different signatures have been identified to discriminate chaos from integrability in quantum systems, including level spacing statistics, spectral density of quantum states, the structure of wave functions, and the out-of-time-ordered correlators. We are here interested in quantum chaotic or integrable systems behavior, from the point of view of quantum information. The goal here is to investigate how the chaotic properties of a quantum system affects some quantum information properties of the many-body eigenstates. We wish to describe consequences of chaos on some quantum-information related quantities. More precisely, we will focus on correlations and entanglement, two quantities at the heart of quantum mechanics and many-body physics. We will in particular consider a quantity called as quantum discord (QD), introduced in refs. [9–11]. The QD measures specifically the quantum nature of correlations between two subsystems, and vanishes in classical systems. It is defined as the difference between two classically equivalent expressions for the mutual information associated to two subsystems, but which are in general different in the quantum realm. The second quantity we will analyze is the concurrence (CC), which is a measure of the amount of entanglement between two spins.

Spin-1/2 chains are natural candidates to study the relations between quantum correlations, entanglement and quantum chaos. They are relatively simple many-body systems, but rich enough to exhibit integrable and chaotic regimes. In the present work we numerically study the distribution of CC and QD in the eigenstates of spin-1/2 Ising-Heisenberg chains with the presence of a defect and Dzyaloshinskii–Moriya (DM) interaction. The signature of quantum chaos in this model has been investigated by three of us in ref. [34], and a Poissonian to Wigner–Dyson transition has been found in the energy level
3. Quantum Chaos and Level Spacing Statistics

We begin by characterizing the level spacing statistics as a function of $D$, and then proceed to examining quantum correlations properties (CC and QD) in the following sections.

One of the most commonly used signatures of quantum chaos is the energy level distribution, $P(s)$, where $s(n) = E_{n+1} - E_n$ is the spacing between consecutive unfolded eigenvalues. The unfolded spectrum consists of locally rescaled eigenvalues $E_n$, in which the (local) mean level density is set to unity. Interested readers can find more detailed explanations of the method in ref. [50].

For a quantum integrable system, the distribution is typically Poissonian, $P(s) = \exp(-s)$. While in a chaotic quantum system the energy levels are correlated and “repel” each other (crossings are avoided), The precise form of the level spacing distribution then depends on the symmetry properties of the Hamiltonian matrix. Systems with time-reversal invariance and spin rotation symmetry are described by the Gaussian orthogonal ensemble (GOE), which corresponds to an ensemble of real symmetric matrices, whose elements $H_{ij}$ are independent random numbers chosen from a Gaussian distribution. The corresponding level spacing distribution is the Wigner–Dyson surmise, $P(s) = (\pi s/2) \exp(-\pi s^2/4)$.[4,5]

It is known that the XXZ chain is integrable.[52,53] In this case, the level spacing distribution is Poissonian for all values of the anisotropy parameter[54,55] apart from some special ones that may lead to additional degeneracies. It is shown that chaos may develop by adding at least a single defect in the bulk of the XXZ chain, whereas the model with defect at the boundary is still integrable.

In a previous work by three of us, we considered different limits of the XXZ model in the presence of the DM interaction.[34] The main purpose of that work was to answer the following questions: does spin-orbit interactions lead quantum chaos in the XXZ model? The results, plotted in Figure 1, can be summarized as follows: i) the DM interaction induces chaos in the Ising ($J = 0$) and XXZ chain in presence of a defect. ii) The XX chain ($J = 0$) with added DM interaction does not show any chaotic feature, even in presence of a defect. We also stress that determining precisely the value of $D$ where the level spacing is no longer Poissonian is not an easy task, and goes beyond the scope of this work. In particular, we cannot exclude that the strength $D$ needed to clearly observe a Wigner–Dyson statistics might go to zero when increasing the system size, as found in other 1D systems.[57]

It is worth discussing heuristically why the DM interaction could favor a chaotic behavior. To this end, let us perform a unitary transformation of the Hamiltonian of Equation (1), to eliminate the $D$ term. We use local spin rotations about the $z$-axis: $S_x^n \rightarrow S_x^n e^{ian}$, with tan $(a) = D/J$. This maps the Hamiltonian to the XXZ model $H = \sum_n J(S_x^n S_x^{n+1} + S_y^n S_y^{n+1}) + J_z(S_z^n S_z^{n+1})$, with a new $xy$ exchange term $J = \sqrt{J^2 + D^2}$. In the absence of defect, this model is integrable. The defect term however breaks the integrability. We thus need to compare the defect energy $\epsilon$ with the term in $H$ which is responsible for the “delocalized” character of the eigenstates (in the $z$-basis), which is the $J$ term. If $J$ is very small, the eigenstates will be almost localized in in the $z$ basis, and this will induce a Poissonian statistics. On the other hand, increasing $D$ (and thus $J$) will make them more delocalized and...
The concurrence associated to the sites \( i \) and \( j \) can be obtained from the reduced density matrix \( \rho_{ij} \) as

\[
C(\rho_{ij}) = \max \{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\}
\]

where \( \lambda_a \) are the eigenvalues of the matrix \( R = \rho \rho^\dagger \), in decreasing order, and \( \rho_{ij} = (\sigma_i^x \otimes \sigma_j^x)\rho_{ij}^*(\sigma_i^y \otimes \sigma_j^y) \). \( \rho_{ij}^* \) is the conjugate of \( \rho_{ij} \) and \( \sigma^y \) is the \( y \) component of the spin-1/2 Pauli operator. As we have mentioned, there are different measurement tools of quantum correlations. The QD is a measure of the nonclassical correlations between two systems, and it coincides with the entanglement entropy if the two systems form a pure state. For mixed states, the QD and entanglement entropy are however different. The QD has motivated some search for a complete description of all quantum correlations, specially where no entanglement exists.\(^{[61,62]}\)

The QD associated to a pair of quantum systems \( A \) and \( B \) can be calculated by

\[
QD_{A,B} = I_{AB} - C_{A,B}
\]

where \( I_{AB} \) and \( C_{A,B} \) are respectively the quantum mutual information and the classical correlation. The mutual information is defined from the von Neumann entropies \( S(A) \) and \( S(B) \) of each subsystem, and their joint entropy \( S(AB) \):

\[
I_{AB} = S(A) + S(B) - S(AB)
\]

The classical correlation, \( C_{A,B} \), is given by

\[
C_{A,B} = S(A) - \min S(A|\{\pi^A_\alpha\},\{\pi^B_\beta\})
\]

where \( \alpha \) labels the different outcomes of a projective measurement on the system \( B \) and \( \{\pi^B_\beta\} \) represents the associated set of projectors. As for \( S(A|\{\pi^A_\alpha\}) \), it is the quantum conditional entropy of \( A \) given the above measurement on \( B \). In the present work we focus on the case where \( A \) and \( B \) are single sites \( i \) and \( j \), and the quantities above can therefore be obtained from the reduced density matrices \( \rho_i, \rho_j, \) and \( \rho_{ij} \). To calculate numerically the QD in this case we follow Sarandy’s paper formalism.\(^{[63]}\)

5. Numerical Results

Using numerical exact diagonalizations, we calculate the CC and QD between two spins for different values of the DM interaction strength for chains of size up to \( N = 18 \) spins. In this model, the projection of the total spin along the \( z \)-axis, \( S_z^\text{tot} = \sum_{i=1}^{N} S_z^i \), is conserved and we can therefore diagonalize the Hamiltonian in different \( S_z^\text{tot} \) subspaces. We report numerical results for all the eigenstates in the \( S_z^\text{tot} = 4 \) sector of a chain with \( N = 18 \) sites (Figures 2 and 3), as well as for all the eigenstates in the \( S_z^\text{tot} = 0 \) sector of a chain with \( N = 16 \) sites (Figure 5). In Figures A.1 and A.2 the analysis has been pushed to the \( S_z^\text{tot} = 0 \) and \( N = 18 \).

Importantly, very similar results are obtained in other magnetization subspaces, as well as for other system sizes (see the appendix A). For \( N = 18 \) and \( S_z^\text{tot} = 4 \), the subspace has dimension 8568, which is enough for statistical analysis. We focus on the nearest-neighbor CC, \( C_{i,j+1} \), and the nearest-neighbor QD.
Figure 2. The distribution of the nearest-neighbor concurrence $C_{i,i+1}$ versus the energy. a,b) Ising model; c,d) XX model; e,f) XXZ model in the region $J_z/J < 1.0$; g,h) XXZ model in the region $J_z/J > 1.0$. Numerical results are obtained for a chain of size $N = 18$ in the subspace $S_{tot}^z = 4$. The values of the exchange, DM interaction and magnetic field are chosen same as Figure 1. Insets show the density of states. The blue vertical line is the mean energy $E_{\infty}$ at infinite temperature.

QD$_{i,i+1}$, in the integrable and chaotic regimes of the model. The results do not significantly depend on the position $i$ of this pair, and we also stress that similar results are obtained when considering next nearest-neighbor sites. As for the position of impurity, it can be anywhere in the chain, except for the edges. For the chain with $N = 18$ sites, we put impurity at site $d = 4$.

5.1. Concurrence

In a first step, we calculate the CC for all energy eigenstates of the Ising model, for different values of the DM interaction. The results are presented in Figure 2a,b for two values of the DM interaction, $D = 0.05$ and $D = 0.5$. The first case corresponds to a Poissonian level statistics (Figure 1a), and the second one to a Wigner–Dyson distribution (Figure 1b). As can be seen in Figure 2a, when the model is in the integrable regime, states with large CC can be found in the whole range of energy. On the other hand, when the model is in the chaotic regime, see Figure 2b, the CC is distributed in a completely different way. There, states with large CC are either located at high or at low energies, while the states in the middle of the spectrum (where the density of states is the largest) have very small CC. As already mentioned, the same result is found in other magnetization sectors.
We performed the same calculations for the XX model, with $J = 1.0$ and $J_z = 0.0$, and the results are summarized in Figure 2c,d. The DM interaction is $D = 0.5$ and $D = 1.0$. As mentioned in the preceding section, for the spin-1/2 XX model, we have not found any signature of chaos in the level spacing statistics, even in the presence of a defect. Figure 2c,d again shows the CC distribution for all the eigenstates in the subspace with $S_z^\text{tot} = 4$. In this case, we do not see any qualitative change when increasing $D$, and states with large CC can be found in the whole energy range. Compared with the Ising case, there is no drop of the CC in the middle of the spectrum.

Figure 2e,f shows the results for an XXZ chain in the easy-plane regime, that is, $J_z < J$. The model is integrable but adding a single defect in the middle of chain induces a chaotic-like level statistics (cf. Figure 1e,g). The qualitative shape of the CC distribution does not seem to be sensitive to the DM strength in that case. Contrary to what is observed for the XX model, the eigenstates with large CC are located in two energy bands, one at low energy, and the second one at high energy. In the middle of the spectrum the eigenstates have a vanishingly small CC, and states with large CC can be found in the whole energy range. Compared with the Ising case, there is no drop of the CC in the middle of the spectrum.

![Figure 3. Same as Figure 2 but for quantum discord (QD).](image)

We now turn to the the distribution of the QD over the eigenstates. For the comparison, we consider the same models and same parameters as for the CC (chain of size $N = 18$ and $S_z^\text{tot} = 4$), and the results are presented in Figure 3. In a way that is quite similar to CC, it can be seen that the QD is distributed in a qualitatively different way, depending if the level statistics is integrable-like (Figure 3a,c,d,g), or chaotic (cf. Figures 3b,e,f,h). As for the CC, we observe that chaotic-like spectra lead to a drop of the QD for eigenstates in the middle of the spectrum.

By comparing the results of CC and QD in the chaotic regimes, it seems that the QD does not vanish completely for eigenstates close to the middle of the spectrum (Figure 3). As we argue below, this is a finite-size effect: both the CC and QD in fact go to zero for eigenstates close to the middle of the spectrum when increasing the system size, but the convergence appears to be slower for the QD than for the CC (see Figures A.1 and A.2 in the appendix).

5.2. Quantum Discord

In this section, we present a simple argument explaining why the CC and the QD associated to pairs of nearby spins vanish in the middle of the spectrum in the chaotic regime. We begin by assuming that the system satisfies the (strong) eigenstate thermalization hypothesis (ETH)\(^\text{[66–68]}\) which is believed to be the case when the spectrum displays some chaotic properties. We then focus on the reduced density matrix $\rho_{ij}$ associated to the eigenstate $|\alpha\rangle$ with energy $E_\alpha$, and to the pair of sites $i,j$. According to the strong ETH, for a large enough system the matrix $\rho_{ij}$ should become a smooth function of the energy $E$, and not of the split bands in the density of state of Figure 2g are due to the relatively large value of $J_z$, for which the spectrum approaches the Ising one, with discrete energies. Increasing the DM strength to $D = 4$, we observe in Figure 2h that the distribution of high CC states again split into two bands, at low and high energy. As for the previous cases with Wigner–Dyson statistics, the eigenstates in the middle of the spectrum appear to have essentially zero two-site entanglement.

5.3. Eigenstate Thermalization Hypothesis

In this section, we present a simple argument explaining why the CC and the QD associated to pairs of nearby spins vanish in the middle of the spectrum in the chaotic regime. We begin by assuming that the system satisfies the (strong) eigenstate thermalization hypothesis (ETH)\(^\text{[66–68]}\) which is believed to be the case when the spectrum displays some chaotic properties. We then focus on the reduced density matrix $\rho_{ij}$ associated to the eigenstate $|\alpha\rangle$ with energy $E_\alpha$, and to the pair of sites $i,j$. According to the strong ETH, for a large enough system the matrix $\rho_{ij}$ should become a smooth function of the energy $E$, and not of...
the choice of one particular eigenstate. In addition, this density matrix should approach its thermal equilibrium value either obtained in the microcanonical ensemble, or canonical ensemble (both giving the same local observable for a large enough system). In the canonical case, the temperature $T(E)$ must be chosen such that $(\hat{H})_{T(E)} = E$. On the other hand, we know that, at high temperature, the canonical ensemble predicts a density matrix $\rho^{\text{therm}}_{ij}$ which will approach a simple diagonal matrix, $\frac{1}{\mathcal{N}}I$, corresponding to uncorrelated spins, and vanishing QD and CC. But in the limit of infinite temperature the (mean) energy goes to a simple limit: $E_{\infty} = \frac{1}{\mathcal{N}} \text{Tr}[\hat{H}]$, corresponding to the “middle” of the energy spectrum. With the present spin chain Hamiltonian, we find $E_{\infty} = (N - 1)Jm^2 + Nh\epsilon m$ with $m = \frac{1}{2}S^z_{\text{tot}}$ (blue vertical lines in Figures 2 and 3). We conclude that, with the hypothesis that the systems is sufficiently large and satisfies the ETH, the reduced density matrix $\rho_{ij}$ will be close to $\frac{1}{\mathcal{N}}I$ for eigenstates with an energy $E_{\infty}$ close to $E_{\infty}$. From the point of view presented above, the fact that the quantum discord and the concurrence become very small in the middle of the spectrum can be viewed as a consequence of the ETH.

Finally, we show in Figure 5 how the QD data get modified for a pair (2,4) of next-nearest neighbor spins. Comparing $QD_{2,4}$ to $QD_{1,3}$ in the Ising model, we observe that the two distributions as a function of energy are qualitatively similar in the chaotic regime, with very small QD in the center of the spectrum and high values toward the edges. The pair of sites (2,4) is relatively short-ranged and the associated reduced density matrix is therefore that of a local subsystem. From the ETH, this density matrix should then again be close to an infinite-temperature density matrix for all the eigenstates close to the center of the spectrum, hence the vanishing QD (bottom panel of Figure 5). On the other hand, we do not expect any direct connection between $QD_{1,3}$ and $QD_{2,4}$ in the integrable regime. In that case, the data associated to QD at distance 1 and 2 (upper panel of Figure 5) have the same overall shape, but with a shift of about $\approx 15\%$ shift in the energy of the maximum.

6. Summary and Conclusion

We have studied quantum correlations and entanglement in the chaotic and integrable regimes of Ising-Heisenberg spin chains. We considered anisotropic spin chains with a defect (localized magnetic field) and DM interactions, to break the integrability of the model. The concurrence and the quantum discord associated to pairs of sites have been used as measures of entanglement and quantum correlations, and these two quantities have been evaluated in all the eigenstates of the Hamiltonian in a given magnetization sector.

The numerical results revealed a strong qualitative difference in the way the quantum correlation and the entanglement are distributed over the energy spectrum, depending whether the energy level spacing statistics exhibits some integrable or chaotic properties. In the integrable regime, that is when the level statistics appears to be Poissonian, the concurrence and quantum discord appear to be weakly correlated with the energy of the eigenstates. In particular, eigenstates with large concurrence or discord can be found at all energies. On the other hand, in the chaotic regime, with a Wigner–Dyson level spacing distribution, states with large concurrence are either found at low or high energy, but are absent from the middle of the spectrum. Moreover,
eigenstates close to the middle of the spectrum have vanishingly small quantum correlations. A very similar phenomenon is observed for the quantum discord, although it does not completely vanish for states in middle of chaotic spectra. We explained how the findings in the chaotic cases may be related to the eigenstate thermalization hypothesis. Finally, the vanishingly small quantum discord in the middle of the chaotic spectra was shown to be also verified for next-nearest neighbor sites, which is also expected from the ETH.

We hope that our results will motivate some further investigations on the difference between chaotic and integrable quantum many-body systems from the point of view of quantum correlations and entanglement measures, and from a quantum information perspective in general.

**Conflict of Interest**

The authors declare no conflict of interest.

**Appendix A: Finite Size Effects**

To verify the robustness of results, different chain sizes are considered. We consider systems with \( N = 14, 16, 18 \) sites. Figures A.1 and A.2 show results of \( C_{i,i+1} \) and \( QD_{i,i+1} \) for different DM interaction strength, respectively. It can be seen that, starting with a distribution of nearest-neighbor concurrence centered in the middle of spectrum in the integrable regime, the distribution gradually splits in two sets of high-concurrence eigenstates. In the chaotic regime, the states in the vicinity of the middle of the spectrum have a vanishing concurrence. Importantly, these results are very similar for the different system sizes we considered.

**Keywords**

quantum chaos, quantum correlation, quantum entanglement, spin chains

Received: November 8, 2019  
Revised: May 8, 2020  
Published online: June 25, 2020

[1] M. C. Gutzwiller, *Chaos in Classical and Quantum Systems*, Springer-Verlag, Berlin 1990.
[2] R. Aurich, J. Bolte, F. Steiner, *Phys. Rev. Lett.* 1994, 73, 1356.
[3] Y. Ashkenazy, L. P. Horwitz, J. Levitan, M. Lewkowicz, Y. Rothschild, *Phys. Rev. Lett.* 1995, 75, 1070.
[4] T. Guhr, A. Müller-Groeling, H. A. Weidenmüller, *Phys. Rep.* 1998, 299, 189.
[5] M. L. Mehta, *Random Matrices*, Academic Press, San Diego, CA 1991.
[6] J. Maldacena, S. H. Shenker, D. Stanford, *J. High Energ. Phys.* 2016, 2016, 106.
[7] M. A. Nielsen, I. L. Chuang, *Quantum Computation and Quantum Information: 10th Anniversary Edition*, Cambridge University Press, Cambridge 2010.
[8] G. Benenti, G. Casati, G. Strini, *Principles of Quantum Computation and Information*, World Scientific, Singapore 2007.
[9] W. H. Zurek, *Ann. Phys.* 2000, 9, 855.
[10] H. Ollivier, W. H. Zurek, *Phys. Rev. Lett.* 2001, 88, 017901.
[11] L. Henderson, V. Vedral, *J. Phys. A: Math. Gen.* 2001, 34, 6899.
[12] W. K. Wootters, *Phys. Rev. Lett.* 1998, 80, 2245.
Figure A.2. Same as Figure A.1 but for quantum discord (QD). Pair sites are the same as Figure 3.

[13] J. Karthik, A. Sharma, A. Lakshminarayan, Phys. Rev. A 2007, 75, 022304.
[14] W. G. Brown, L. F. Santos, D. J. Starling, L. Viola, Phys. Rev. E 2008, 77, 021106.
[15] X. Wang, S. Ghose, B. C. Sanders, B. Hu, Phys. Rev. E 2004, 70, 016217.
[16] R. Lopez-Sandoval, M. Garcia, Phys. Rev. A 2007, 75, 022304.
[17] W. G. Brown, L. F. Santos, D. J. Starling, L. Viola, Phys. Rev. E 2008, 77, 021106.
[18] J. C. Getelina, F. C. Alcaraz, J. A. Hoyos, Phys. Rev. B 2016, 93, 045136.
[19] R. Lopez-Sandoval, M. Garcia, Phys. Rev. A 2007, 75, 022304.
[20] W. G. Brown, L. F. Santos, D. J. Starling, L. Viola, Phys. Rev. E 2008, 77, 021106.
[21] X. Wang, S. Ghose, B. C. Sanders, B. Hu, Phys. Rev. E 2004, 70, 016217.
[22] J. C. Getelina, F. C. Alcaraz, J. A. Hoyos, Phys. Rev. B 2016, 93, 045136.
[23] R. Lopez-Sandoval, M. Garcia, Phys. Rev. A 2007, 75, 022304.
a large number of symmetry sectors. For this reason, nearby levels typically belongs to different symmetry sectors and do not repel each other.

[52] H. Bethe, Z. Phys. 1931, 71, 205.
[53] R. Orbach, Phys. Rev. 1958, 112, 309.
[54] D. Poilblanc, T. Ziman, J. Bellissard, F. Mila, G. Montambaux, EPL 1993, 22, 537.
[55] T. C. Hsu, J. C. Angle’s d’Auriac, Phys. Rev. B 1993, 47, 14291.
[56] L. F. Santos, J. Phys. A: Math. Gen. 2004, 37, 4723.
[57] L. F. Santos, M. Rigol, Phys. Rev. E 2010, 81, 036206.
[58] R. Modak, S. Mukerjee, New J. Phys. 2014, 16, 093016.
[59] C. H. Bennett, D. P. DiVincenzo, J. A. Smolin, W. K. Wootters, Phys. Rev. A 1996, 54, 3824.

[60] C. H. Bennett, H. J. Bernstein, S. Popescu, B. Schumacher, Phys. Rev. A 1996, 53, 2046.
[61] B. P. Lanyon, M. Barbieri, M. P. Almeida, A. G. White, Phys. Rev. Lett. 2008, 101, 200501.
[62] G. Passante, O. Moussa, D. A. Trottier, R. Laflamme, Phys. Rev. A 2011, 84, 044302.
[63] M. S. Sarandy, Phys. Rev. A 2009, 80, 022108.
[64] S. Luo, Phys. Rev. A 2008, 77, 042303.
[65] T. Werlang, S. Souza, F. F. Fanchini, C. J. Villas Boas, Phys. Rev. A 2009, 80, 024103.
[66] J. M. Deutsch, Phys. Rev. A 1991, 43, 2046.
[67] M. Srednicki, Phys. Rev. E 1994, 50, 888.
[68] M. Rigol, V. Dunjko, M. Olshanii, Nature 2008, 452, 854.