Entanglement and quantum correlations in many-body systems: a unified approach via local unitary operations

M. Cianciaruso, 1 S. M. Giampaolo, 2, 3 W. Roga, 3 G. Zonzo, 1 M. Blasone, 1, 4 and F. Illuminati 3, 4, 5

1 Dipartimento di Fisica “E. R. Caianiello”, Università degli Studi di Salerno, Via Giovanni Paolo II 132, I-84084 Fisciano (SA), Italy
2 University of Vienna, Faculty of Physics, Boltzmanngasse 5, 1090 Vienna, Austria
3 Dipartimento di Ingegneria Industriale, Università degli Studi di Salerno, Via Giovanni Paolo II 132, I-84084 Fisciano (SA), Italy
4 INFN Sezione di Napoli, Gruppo collegato di Salerno, Italy
5 CNISM Unità di Salerno, I-84084 Fisciano (SA), Italy

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Local unitary operations allow for a unifying approach to the quantification of quantum correlations among the constituents of a bipartite quantum systems. The distance between a given state and its image under least-perturbing local unitary operations is a bona fide measure of quantum entanglement, the so-called entanglement of response, for pure states, while for mixed states it is a bona fide measure of quantum correlations, the so-called discord of response. Exploiting this unifying approach, we perform a detailed comparison between two-body entanglement and two-body quantum correlations in infinite XY quantum spin chains both in symmetry-preserving and symmetry-breaking ground states as well as in thermal states at finite temperature.

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I. INTRODUCTION

Quantum correlations arise from the combination of the superposition principle and the tensor product structure of the Hilbert space associated with a composite quantum system. For pure states, they are entirely captured by entanglement. Instead, in the case of mixed states, the situation becomes more subtle since there exist mixed non-entangled states that display non classical features, the so-called classical-quantum states [1–3]. Such states led to the idea that the total amount of quantum correlations cannot be, in general, quantified by the entanglement but rather by a more general feature named quantum discord (or quantumness). Both these two quantities showed to be not only a fundamental resource for quantum information, computation and communication [4–6] but also a key tool for the characterization of quantum many-body systems [7–9]. For example, there are particular quantum phases of matter, as the so called topological ordered phase, which are not characterized by the Landau-Ginzburg paradigm based on symmetry breaking, but rather by the entanglement properties of the ground state of the system [10–12]. This fact led to the awareness that quantum correlations of ground states allow for the most fundamental characterization of complex quantum systems. Such awareness is also strengthened by the fact that, even in systems that do not show any exotic phase, the analysis of some quantities related to entanglement and quantumness of correlations may provide a deeper characterization of the different phases [13–22].

In spite of this big effort to characterize the entanglement and the quantumness of the ground state of complex quantum systems, till now there exists no well posed comparison of the different behaviors of this two quantities on the same system.

This fact is due that, till now, even if there exist many different measures of quantumness and entanglement, they are connected to different aspects of quantum states and hence a strict comparison between two of them, such as the one carried out in Ref. [23], is not well posed. In this paper we want to carry out such direct comparison between entanglement and quantumness, basing our work to the recently introduced unified approach to the quantification of quantum correlations based on local unitaries [24–27]. According to this approach, the distance between a given state and its image after the least disturbing local unitary transformation of the fixed spectrum of the complex roots of unity is a measure of the quantumness of correlations, the so-called discord of response, while the convex roof extension of this measure as well as its reduction to pure states are bona fide measures of entanglement that have been generically dubbed entanglement of response. We apply such results on spin pairs in the one-dimensional XY model in a transverse magnetic field with periodic boundary conditions. We show how the pairwise discord of response dominates with respect to the pairwise entanglement of response in symmetry preserving ground state, particularly at the factorization point and at long distances, and how it decays in symmetry breaking ground states, whereas the pairwise entanglement of response increases slightly for values of the external field below the factorization point. In addition, we show that in symmetry-breaking ground states and for the Hilbert-Schmidt distance, the pairwise discord of response is dominated by the entanglement of response, thus providing a concrete physical realization of the fact that the Hilbert-Schmidt metrics does not provide a reliable quantification of quantum correlations.

The present paper is organized as follows. In Section I we review the unifying approach to the quantification of quantum correlations based on local unitaries, by recalling the definitions of the entanglement and discord of response. In Section II we recall some features of the one-dimensional XY
model in a transverse field with periodic boundary conditions. In Sections VII and VIII we perform the comparison between the entanglement of response and the discord of response for spin pairs in an infinite XY, respectively in symmetric and symmetry breaking ground states, as well as in thermal states at finite temperature \( T > 0 \). We draw our conclusions in Section VII.

II. ENTAILMENT OF RESPONSE AND DISCORD OF RESPONSE: DEFINITIONS AND RESULTS

Let us first briefly review some basic definitions and results concerning the quantification of entanglement and quantum correlations by local unitary operations. All along the present work, we focus our attention on a quantum system AB composed of two distinguishable subsystems A and B. Such quantum system is associated to an Hilbert space \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \) which is the tensor product of the Hilbert spaces associated with each subsystem, so that \( d \equiv \dim \mathcal{H} = d_A \times d_B \). Moreover, the space of states of AB is characterized by the convex set of density operators on \( \mathcal{H} \), i.e., the set of semi-positive definite and trace one operators on \( \mathcal{H} \), whose extremal points are the trace one projection operators on \( \mathcal{H} \) that represent pure states.

Let us denote by \( \rho_{AB}^{\Phi} \equiv |\Phi^{AB}\rangle \langle \Phi^{AB}| \) and \( \Lambda \), respectively, a generic pure state of the bipartite quantum system AB and the set of local unitary operators \( U_A \equiv U_A \otimes I_B \) such that \( I_B \) is the identity operator on \( \mathcal{H}_B \) and \( U_A \) is any unitary operator on \( \mathcal{H}_A \) whose spectrum is given by the \( d_A \)-th complex roots of unity. The entanglement of response [24, 25] of a bipartite pure state \( \rho_{AB}^{\Phi} \equiv |\Phi^{AB}\rangle \langle \Phi^{AB}| \), \( E(|\Phi^{AB}\rangle) \), is defined by:

\[
E(|\Phi^{AB}\rangle) = \frac{1}{4} \min_{U_A \in \Lambda} D_{Tr} \left( \rho_{AB}^{\Phi}, \rho_{AB}^{\Phi} \right),
\]

where \( \rho_{AB}^{\Phi} \equiv U_A \rho_{AB}^{\Phi} U_A^\dagger \) and \( D_{Tr} \) is the trace distance between the two states. In other words, when the whole quantum system AB is in a pure state \( \rho_{AB}^{\Phi} \), the entanglement of response measures the quantum correlations between parts A and B by considering the distance between \( \rho_{AB}^{\Phi} \) and its image after the least disturbing local unitary transformation of the fixed spectrum of the complex roots of unity.

There are at least two distinct ways to extend the entanglement of response to mixed states: the convex roof extension, which then identifies the entanglement of response of mixed states, and the discord of response defined as the distance from a mixed state and its image under least disturbing unitary operations [27]. On the one hand, the entanglement of response of any bi-partite mixed state \( \rho_{AB} \), \( E(\rho_{AB}) \), is defined as the convex roof extension of the entanglement of response for pure states, i.e.:

\[
E(\rho_{AB}) = \min_{\{\phi_i^{AB}\}, \{p_i\}} \sum_i p_i E(|\phi_i^{AB}\rangle),
\]

where the minimization is performed over all the decompositions of \( \rho_{AB} \) in pure states \( \sum_i p_i |\phi_i^{AB}\rangle \langle \phi_i^{AB}| = \rho_{AB} \), \( p_i \geq 0, \sum_i p_i = 1 \). On the other hand, the discord of response of any bi-partite state \( \rho_{AB} \), \( Q(\rho_{AB}) \), is defined as [27] (see also Ref. [26] for earlier related work):

\[
Q(\rho_{AB}) \equiv \frac{1}{4} \min_{U_A \in \Lambda} D_{Tr} \left( \rho_{AB}, \rho_{AB}^{U_A} \right)^2,
\]

where, as in the case of pure states, \( \rho_{AB}^{U_A} \equiv U_A \rho_{AB} U_A^\dagger \).

Therefore, the entanglement and the discord of response measure different aspects of bipartite quantum correlations by two different uses of local unitary operations. The discord of response is obtained by applying local unitaries directly to the density operator \( \rho_{AB} \) describing the state of the global system AB, while the entanglement of response stems from the application of local unitaries to the pure states of the optimal decomposition of \( \rho_{AB} \). By virtue of their common origin, it is possible to perform a direct comparison between entanglement of response and discord of response.

Indeed, the discord of response of any two-qubits state is a computable measure for two-qubit states, even when considering the trace distance [26, 27]. In such case, it relates nicely to the trace based geometric discord [28]. On the contrary, a direct evaluation of the convex roof is still extremely demanding even in this simple case. However, we can prove that the entanglement of response of a two-qubit mixed state is equal to the square of the concurrence [27, 29]. In the following we outline a sketch of the proof, referring to Ref. [27] for all the details. We start our proof considering that, in the case of two-qubit pure states, the entanglement of response coincides with the tangle [24], which is equal to the squared concurrence [30]. Moving to mixed states, it is well known that, for the entanglement of formation, the minimum of the convex roof is achieved by pure states \( |\phi_{AB}^{(i)}\rangle \) of the same concurrence of the mixed [29]. Subsequently, it was noticed that the convex roof extensions of other measures of entanglement, which are convex and monotonically increasing functions of the concurrence, have the same optimal decomposition [31, 32]. Consequently, also the entanglement of response for two-qubit mixed states results to have the same optimal decomposition, implying that the entanglement of response of a mixed state of two qubits is equal to its squared concurrence.

III. XY MODEL

In order to compare entanglement of response and discord of response, let us set the stage by recalling some aspects of the complex quantum systems we shall focus on, that is the one-dimensional anti-ferromagnetic XY models in transverse field with periodic boundary conditions [33-37]. Such quantum spin models consist of a periodic chain of \( N \frac{1}{2} \)-spins, with nearest-neighbor interactions competing with a transverse magnetic field, whose dynamics is governed by the following Hamiltonian:

\[
H = \sum_{i=1}^{N} \left[ \left( \frac{1 + \gamma}{2} \right) \sigma_i^x \sigma_{i+1}^x + \left( \frac{1 - \gamma}{2} \right) \sigma_i^y \sigma_{i+1}^y - h \sigma_i^z \right].
\]

This is the basic model that we will investigate in detail, with different values of the transverse field \( h \), the anisotropy parameter \( \gamma \), and the number of sites \( N \).
Here $\sigma_\alpha^a$, $\alpha = x, y, z$, are the Pauli matrices on site $i$, $\gamma$ is the anisotropy in the $xy$ plane and $h$ is the strength of the transverse magnetic field and the periodic boundary conditions imply that $\sigma_{N+1}^x \equiv \sigma_1^x$. The XY model reduces to the isotropic XX model and to the Ising model, respectively for $\gamma = 0$ and $\gamma = 1$.

Regardless of the value of $\gamma$, in the thermodynamic limit, these models feature a quantum phase transition at $h = h_c = 1$. For $h > h_c = 1$ and for any $\gamma$, the ground state space is non-degenerate and there is a finite gap in the energy spectrum between the ground state and the first excited state. On the other hand, for $h < h_c$, for $\gamma = 0$ the ground state space remains non-degenerate while the energy spectrum becomes gapless, whereas for $\gamma > 0$ the ground state space becomes two-fold degenerate and the energy spectrum is gapped and the system can be characterized by a non vanishing order parameter $m_+ = (-1)^i \langle S_i^z \rangle$. Together with the quantum critical point, there exists another relevant value of the external magnetic field, that is $h_f = \sqrt{1 - \gamma^2}$, the factorizing field. Indeed, at this value of $h$, the system admits at least two completely factorized ground states $|15, 17, 38, 39\rangle$, that collapse into a single state for $\gamma = 0$.

Since our goal is to compare the two-spin entanglement of response and discord of response, we need to determine the pairwise reduced density matrix $\rho_{ij}$ either in a symmetric ground state, in a symmetry-broken ground state, or in a thermal state at temperature $T > 0$. The pairwise reduced density matrix $\rho_{ij}$ is defined as the partial trace of the state of the whole chain with respect to all spins except those at sites $i$ and $j$. While the ground state of the entire chain is a pure state, the reduced state of a pair of spins, in general, is a mixed state but at the factorization point. The two-site density matrix can be expanded in operators as follows $^{40}$:

$$\rho_{ij} = \frac{1}{4} \sum_{\alpha, \beta = 0}^3 \langle \sigma_i^\alpha \sigma_j^\beta | \sigma_i^\alpha \sigma_j^\beta \rangle$$

where $\sigma_i^0 = |I_i, 0\rangle$ and $\langle \sigma_i^\alpha \sigma_j^\beta | \sigma_i^\alpha \sigma_j^\beta \rangle$ represent the two body correlation functions between $\sigma_i^\alpha$ and $\sigma_j^\beta$. The operator expansion in eq. (5) depends on 16 different correlation functions. However, this number can be reduced by appealing to the symmetries of the Hamiltonian. Translational invariance of the lattice means that the reduced density matrix depends only on the distance $r = |i - j|$ between the spins. Also, since the Hamiltonian is real, $\rho_{ij} = \rho_{ji}^\dagger$. Finally, except for the symmetry broken ground state, the global phase-flip symmetry implies that $\langle \sigma_i^x \sigma_j^x | \rho_{ij} \rangle = 0$. Therefore the symmetries of the Hamiltonian imply that, for both the symmetric ground state and the thermal state, the only correlation functions different from zero are $\langle \sigma_i^x \sigma_j^x \rangle$ and $\langle \sigma_i^\alpha \sigma_j^\alpha \rangle$ for $\alpha = x, y, z$. Such correlation functions can be obtained from the literature or generalizing the approach of Ref. $^{33, 34}$ at non vanishing external field for the finite size system, or directly from Refs. $^{35, 36}$ in the thermodynamic limit.

On the other hand, when we are dealing with the symmetry-broken ground state, that requires that the lattice is at the thermodynamic limit, the external field is below the quantum critical point and $\gamma > 0$, also other correlation functions can be different from zero. Such correlation functions are $\langle \sigma_i^x \sigma_j^x \rangle$ and $\langle \sigma_i^\alpha \sigma_j^\alpha \rangle$. The expression of the first can be found in Refs. $^{36}$ while to obtain $\langle \sigma_i^\alpha \sigma_j^\alpha \rangle$ we generalize the approach used in the previous reference to obtain $\langle \sigma_i^\alpha \rangle$.

IV. RESULTS FOR THE SYMMETRIC GROUNDSTATE

Let us start our comparison reporting and commenting the results for the entanglement of response and discord of response obtained in the symmetric ground state in the thermodynamic limit. In Fig. 1, we plot the behavior of this two quantities for two neighboring spins for different values of $\gamma$. With the exception of the two limiting cases, the pairwise entanglement exhibits a very similar dependence on the external field for any value of $\gamma$. In fact, starting from high values of $h$ and going to the left, we see that the entanglement increases until it reaches a maximum before the quantum critical point. Soon after it starts to decrease until it completely vanishes at the factorization point. It then increases again reaching a new maximum at $h = 0$. In the Ising case $\gamma = 1$ this second maximum is absent because the factorization point goes to zero, while the isotropic XX model does not show the first maximum because its ground state, for any $h \geq h_c$, is the tensor
product of local pure states and hence all measures of entanglement must vanish. On the other hand, regardless of the value of $\gamma$, the pairwise discord shows a single local maximum that, depending on $\gamma$, can be either in the ordered phase $h < h_c$ or in the disordered phase $h > h_c$ and shifts towards higher values of $h$ when $\gamma$ increases. It is worth remarking that, except for the two limiting cases $\gamma = 0, 1$, the discord of the symmetric ground state never vanishes at the factorization point. This can be easily understood taking into account that for any $\gamma \neq 0, 1$ the symmetric ground state can be seen as the sum of the two completely factorized ground states and hence, while the entanglement vanishes, in agreement with the convex roof extension, the discord remains finite.

Increasing the distance $r$ between the two spins, we can see that the behaviors of entanglement and discord become more and more diverging. Indeed, for what concerns entanglement, from the lower panel of Fig. (2) one can see that it rapidly vanishes as $r$ increases, except in a small region around $h_f$ that becomes smaller and smaller as the distance between the two spins increases, in agreement with the results of Ref. [11]. On the contrary, in the anti-ferromagnetic phase, the discord survives also in the limit of infinite $r$, as shown in the upper panel of Fig. (2). In the paramagnetic and critical phases, the discord vanishes when $r$ increases. This is due to the fact that in these regions, in the limit of infinite $r$, for a symmetric ground state, all one-body expectation values and two-body correlation functions vanish, with the exception of $\langle S_i^z \rangle$ and $\langle S_i^z S_{i+r}^z \rangle$. As a result, in these regions, the pairwise density matrix can be seen as a classical mixture of eigenvectors of $S_i^z S_{i+r}^z$. On the contrary, the ordered phase is associated to the presence of a non vanishing two-body correlation function along $x (\langle S_i^z S_{i+r}^z \rangle)$ for any $r$, while the expectation value of $S_i^z$ is identically zero due to the fact that the symmetry of the Hamiltonian is preserved in the symmetric ground state. These two facts together prevent the two-body reduced den-
FIG. 4: Finite size scaling of the first derivative of nearest-neighbor discord (a) and entanglement (b) for a symmetric ground state in the case of $\gamma = 0.5$. The inset shows the first derivative of nearest-neighbor discord (a) and entanglement (b) for a symmetric ground state as a function of $\log |h_c - h|$ near the critical point, in the thermodynamic limit, for $\gamma = 0.5$.

As a consequence of the scaling ansatz relative to the case of logarithmic divergence \[44\], $\nu$ is nothing but the opposite of the ratio between the pre-factors of the logarithms in Eq. \[7\] and Eq. \[6\], respectively. As a result we obtain $\nu = 1$, in agreement with the known fact that for any $\gamma \in [0, 1]$ the $XY$ model belongs to the Ising universality class.

The precision of the finite size scaling just performed is analyzed in Fig. (4), where it is shown how, by proper scaling the data of the first derivative of both $E_1$ and $Q_1$ with respect to the external field when the length of the chain diverges (see inset of Fig. (4)),

$$\partial_h E_1^{(N)}{\bigg|}_{h_m} = 0.15 \ln N + \text{const},$$
$$\partial_h Q_1^{(N)}{\bigg|}_{h_m} = -0.59 \ln N + \text{const}. \quad (6)$$

Eq. \[6\] shows the logarithmic divergence of $\partial_h E_1^{(N)}{\bigg|}_{h_m}$ and $\partial_h Q_1^{(N)}{\bigg|}_{h_m}$ as the length of the chain increases and approaches the thermodynamic limit, as a consequence of the fact that $h_m$ tends to $h_c$ (see upper insets in Fig. (3)).

On the other hand, we have the dependence on $\log |h_c - h|$ of the first derivative of $E_1$ and $Q_1$ with respect to the external field when the length of the chain diverges, which is given by

$$\partial_h E_1^{(\infty)} = -0.15 \ln |h_c - h| + \text{const},$$
$$\partial_h Q_1^{(\infty)} = 0.59 \ln |h_c - h| + \text{const}. \quad (7)$$

By performing the finite size scaling analysis, one can show that both $\partial_h E_1$ and $\partial_h Q_1$ allow for an accurate description of the quantum phase transition occurring at $h_c = 1$, providing an information about the critical exponent $\nu$ \[19,43-45\]. To obtain the critical exponent $\nu$ we need to compare two different behaviors. On the one hand, for finite-size chains of length $N$, there is the dependence on $N$ of the maximum value, for nearest neighbor entanglement, and of the minimum value, for nearest neighbor discord, attained by the first derivative as a function of the external field $h$. For instance, in the case $\gamma = 0.5$, from the data showed in the lower insets in Fig. (3) we obtain

$$\partial_h E_1^{(\infty)} = -0.15 \ln |h_c - h| + \text{const},$$
$$\partial_h Q_1^{(\infty)} = 0.59 \ln |h_c - h| + \text{const}. \quad (7)$$

As we have just unveiled, moving from the quantum critical to the factorization point $h \equiv h_f = \sqrt{1 - \gamma^2}$ \[15,16,38\] the difference between discord and entanglement increases because the first, in the thermodynamic limit, stays finite and attains the same value for any distance $r$ of the spin pair, the second vanishes for all $r$. Nevertheless, as is displayed in Fig. (5), at the factorization point $h_f$ the finite size scalings of both the two quantities are extremely similar. In fact, both entanglement and discord decrease with an exponential law with respect to the size $N$ of the chain that is independent on the distance between the two spins and that becomes faster and faster as the anisotropy $\gamma$ increases. More interestingly, for any fixed value of the anisotropy $\gamma$, the decay rate of $E^{(N)}_{h_f}$ to $E^{(\infty)}_{h_f}$ is twice the corresponding rate for the discord.

sity matrix to reduce to a mixture of classical states. The fact that the pairwise discord does not vanish in the limit of infinite $r$ has different relevant consequences. First, it signals that for the discord there is no relation equivalent to the entanglement monogamy \[30,42\]. Secondly, a finite value of the discord between two far-away spins reveals the unavoidable quantum nature of the symmetric ground state in the ordered phase, that can be seen as a Schrödinger cat made by the two different ordered ground states.

Let us now focus on the analysis of the behaviors of entanglement and discord close to the quantum critical point $h \equiv h_c = 1$. For what concerns the entanglement, as expected, due to its relation with the concurrence \[7,43\], it shows a logarithmic positive divergence, for any $\gamma \in [0, 1]$, in its first derivative for two neighboring spins, $\partial_h E_1$. At the same time, as we can see from the upper panel of Fig. (3), also the first derivative of the nearest-neighbor discord, $\partial_h Q_1$, signals the critical point $h_c$ with a logarithmic divergence. However, the latter can now be either positive or negative, depending on the value of $\gamma$ via the position of the maximum of $Q_1$ with respect to $h_c$ (see Fig. (1)).

By performing the finite size scaling analysis, one can show that both $\partial_h E_1$ and $\partial_h Q_1$ allow for an accurate description of
V. SYMMETRY BREAKING GROUND STATE

Let us now move from the symmetry preserving ground states to the symmetry breaking ones that characterize the thermodynamic system for $h < h_c$ and $\gamma > 0$. In the disordered phase, $h > h_c$, the symmetry breaking ground state is not allowed and consequently both entanglement and discord must attain the same value and show the same behavior discussed in the previous section. The difference between symmetric and symmetry breaking ground states occurs in the ordered phase, $h < h_c$, and manifests itself in the non vanishing order parameter $\langle \sigma^z \rangle$ and two-spin correlation functions $\langle \sigma_i^z \sigma_j^z \rangle$ evaluated in the symmetry breaking ground state. In this case, as reported in Fig. (6), for any $\gamma \in [0, 1]$, the critical point $h_c$ corresponds to the value of the external field $h$ in which either the nearest-neighbor discord $Q_1$ shows a discontinuity or the first derivative of nearest-neighbor entanglement $\partial_h E_1$ diverges logarithmically. This difference between the behavior of discord and entanglement (for neighboring spins) is a due of the fact that only the discord is affected by breaking of the Hamiltonian symmetries at the critical point $h_c$. Indeed, according to Ref. [46], the concurrence and, as a consequence, also the pairwise entanglement, attain the same value for any $h \geq h_f$ both in symmetric and symmetry breaking ground states. For some $h < h_f$, there is a slight enhancement in the pairwise entanglement of the symmetry breaking ground state with respect to the symmetric one. Conversely, in general, pairwise discord $Q_1$ undergoes a decrement in the entire ordered phase $h < h_c$ moving from symmetric to symmetry breaking ground states. In other words, for symmetry breaking ground states, the quantum correlations between two neighboring spins in the overall ground state fall down in the ordered phase and are dominated almost entirely by entanglement. In particular, for symmetry breaking ground states, the factorization point $h_f$ represents a point in which simultaneously both the entanglement and the discord vanish, meaning that the purely classical mean field solution represents an exact solution of the system.

Increasing the distance between the two spins, as one can see from the upper panel of Fig. (7), pairwise quantum correlations lose their long range nature when moving from symmetric to symmetry breaking ground states. Indeed both pairwise entanglement and pairwise discord, in the symmetry breaking ground state, do not survive when the distance between the two spins is sufficiently large. While this result for the entanglement is associated to its monogamy properties [30, 42], for the discord it is related to the fact that in the symmetry breaking ground state, not only the two body correlation function along $x$, i.e. $\langle S_i^z S_{i+r}^z \rangle$, but also the expectation values of $S_i^x$ and $S_i^z S_{i+r}^z$ do not vanish in the limit of infinite $r$. This fact allows to identify the two-spin reduced density matrix as a classical mixture of eigenvectors of $O_i O_{i+r}$, where $O_i$ is an Hermitian operator defined on the $i$-th site as $O_i = \cos \beta S_i^x + \sin \beta S_i^z$ with $\beta$ given by $\tan \beta = \frac{\gamma}{\sqrt{\gamma^2 - 1}}$. Nevertheless, the pairwise discord of response is always larger than or equal to the pairwise entanglement of response for any value of $h$, $\gamma$ and $r$ also in the symmetry breaking ground state, as expected from a good measure of total quantum correlations. Accidentally, we note that this feature is lost when, instead of considering the trace distance,
VI. THERMAL STATE

Up to this point we have focused our analysis on the ground state of our system. We will now consider our system in equilibrium with a thermal bath at generic finite temperature, $T > 0$.

The general behavior of $E_1, Q_1$ and their first derivative as functions of the external field, for different temperatures $T$, is showed in Fig. (8) and Fig. (9). With the appearance of thermal effects, the first derivative of both nearest-neighbor entanglement and discord is no longer singular at the critical point $h_c$, in agreement with the fact that criticality occurs exactly only at zero temperature. In particular, as one can see in the lower panel of Fig. (9), as soon as the temperature $T$ rises from zero to some finite value, the zero temperature singularity of $\partial_{h}E_1$ at the critical point $h_c$ is smoothed into a maximum of $\partial_{h}E_1$ localized at a value of the external field $h$ higher than $h_c$. Moreover, the more the temperature increases, the more this maximum moves away from the critical point $h_c$ and the corresponding absolute value of $\partial_{h}Q_1$ decreases. Similarly, as is shown in the upper panel of Fig. (9), for what concern $\partial_{h}Q_1$, the divergence at the critical point $h_c$ is replaced with either a minimum or a maximum of $\partial_{h}Q_1$ (depending on $\gamma$) at a value of the external field $h$ lower than $h_c$. In addition, the higher $T$, the more this extremal point moves away from the critical point $h_c$ and the corresponding absolute value of $\partial_{h}Q_1$ decreases.

On the other hand, being factorization a phenomenon that affects only the ground state of the system, as soon as the temperature is taken into account, the factorization point $h_f$ loses its particular role. Indeed, as reported in the lower panels of Fig. (8), $h_f$ is no longer the unique point at which the nearest-neighbor entanglement $E_1$ vanishes, but rather it is either the “center” of a region in which $E_1$ is identically zero and whose dimension increases with the temperature, or it is not even a zero of $E_1$. In full agreement with this observation, at any non vanishing value of $T$ the discord does no longer attain the same value for any distance $r$ between the two spins, as it can be seen from Fig. (10).

From Fig. (8) it also emerges that, as the temperature $T$ increases, the peaks corresponding to the nearest-neighbor entanglement $E_1$ and discord $Q_1$ tend to flatten to zero quite differently. Specifically, pairwise discord is more robust than
FIG. 9: First derivative of nearest-neighbor discord (a) and entanglement (b) in the thermal state as functions of the external field $h$, in the thermodynamic limit, in the case of $\gamma = 0.9$, for different values of the temperature $T$: solid/blue line $T = 0$; dashed/red line $T = 0.001$; dot-dashed/green line $T = 0.002$; double-dot-dashed/black line $T = 0.005$ and dotted/orange line $T = 0.01$.

entanglement with respect to thermal effects. Interestingly, as displayed in Fig. 11 and Fig. 12, for any anisotropy $\gamma$ there also exist some particular values of the external field $h$ such that either the pairwise entanglement or the pairwise discord increase when the temperature $T$ rises from zero to some low finite value. This is in contrast to the common perception according to which thermal effects can cause only a deterioration of the quantum features. Furthermore, from Fig. 11 and Fig. 12, one can see that this surprising behavior manifests itself mostly in the case of pairwise discord. Indeed the latter increases with the temperature for any anisotropy $\gamma$, for relatively large ranges of values of the external field $h$ and any sufficiently small inter-spin distance $r$, while thermal pairwise entanglement displays this behavior only for a relatively small range of values of $h$ and mostly for $r = 1$. More precisely, for sufficiently large values of $\gamma$, $Q_1$ increases with the temperature for all values of the external field $h$ except those belonging to a small interval containing the critical point $h_c = 1$, in which $Q_1$ is monotonically non increasing. Viceversa, for sufficiently small values of $\gamma$, again $Q_1$ increases with the temperature for all values of the external field $h$ except those belonging to a particular interval, but this time this interval does not contain the critical point $h_c = 1$ and shifts towards lower values of $h$, until at $\gamma = 0$ this interval shrinks to its lower bound at $h = 0$. Consequently, there is no correspondence between the increase in the pairwise discord with the temperature and the occurrence of a gap in the energy spectrum between the ground state and the first excited state.

VII. CONCLUSIONS

In this paper, we have compared the trace-distance based discord of response and the trace-distance based entanglement of response, which are, respectively, related to the trace-distance geometric discord and the squared concurrence. We have considered the pairwise quantities for spin pairs in an infinite $XY$ chain which is either in a symmetric ground state, a symmetry breaking ground state, or a thermal state at finite temperature $T > 0$. When the entire $XY$ chain is in a symmetric ground state, it has been found that there exists a considerable amount of total quantum correlations between any two spins, as quantified by the pairwise discord of response, especially in the ordered phase $h < h_c$ for sufficiently small anisotropy $\gamma$, and near the critical point $h_c$ for sufficiently large $\gamma$. Moreover, in general, entanglement captures only a relatively small part of these quantum correlations, particularly at the factorization point or when the distance between the two spins is sufficiently large, in which case only
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[1] H. Ollivier and W. H. Zurek, Phys. Rev. Lett. 88, 017901 (2001).
[2] L. Henderson and V. Vedral, J. Phys. A 34, 6899 (2001).
[3] M. Piani, P. Horodecki, and R. Horodecki, Phys. Rev. Lett. 100, 090502 (2008).
[4] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information, Cambridge University Press, 2000.
[5] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, Rev. Mod. Phys. 81, 865 (2009).
[6] B. P. Lanyon, M. Barbieri, M. P. Almeida, and A. G. White, Phys. Rev. Lett. 101 200501 (2008).
[7] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. 80, 517 (2008).
[8] M. S. Sarandy, T. R.de Oliveira, and L. Amico, Int. J. Mod. Phys. B 27, 1345030 (2013).
[9] T. Werlang, G. A. P. Ribeiro, and G. Rigolin, Int. J. Mod. Phys. 27, 6899 (2013).
[10] H.-C. Jiang, Z. Wang, and L. Balents, Nature Physics 8, 902 (2012).
[11] A. Kitaev and J. Preskill, Phys. Rev. Lett. 96, 110404 (2006).
[12] M. Levin and X.-G. Wen, Phys. Rev. Lett. 96, 110405 (2006).
[13] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003).
[14] J. I. Latorre, E. Rico and G. Vidal, Quantum Inf. Comp. 4, 48 (2004).
[15] S. M. Giampaolo, G. Adesso, and F. Illuminati, Phys. Rev. Lett. 100, 197201 (2008).
[16] S. M. Giampaolo, G. Adesso, and F. Illuminati, Phys. Rev. B 79, 224434 (2009).
[17] S. M. Giampaolo, G. Adesso and F. Illuminati, Phys. Rev. Lett. 104, 207202 (2010).
[18] S. M. Giampaolo, S. Montaner, F. dell’Anno, S. de Siena and F. Illuminati Phys. Rev. B, 88, 125142 (2013).
[19] S. M. Giampaolo and B. C. Hiesmayr, Phys. Rev. A 88, 052305 (2013).
[20] M. Hofmann, A. Osterloh, and O. Gühne, Scaling of genuine multiparticle entanglement at a quantum phase transition, [arXiv:1309.2217] (2013).
[21] B. Tomasello, D. Rossini, A. Hamma, and L. Amico, Europhys. Lett. 96, 27002 (2011).
[22] S. Campbell, J. Richens, N. Lo Gullo, and T. Busch, “Criticality, factorization and long-range correlations in the anisotropic XY-model”, [arXiv:1309.1052] (2013).
[23] J. Batle, and M. Abdel-Aty, Quant. Inf. Rev. 2, No. 1, 9-13 (2014).
[24] S. M. Giampaolo and F. Illuminati, Phys. Rev. A 76, 042301 (2007).
[25] A. Monras, G. Adesso, S. M. Giampaolo, G. Gualdi, G. B. Davies, and F. Illuminati, Phys. Rev. A 84, 012301 (2011).
[26] S. M. Giampaolo, A. Streltsov, W. Roga, D. Bruss, and F. Illuminati, Phys. Rev. A 87, 012313 (2013).
[27] W. Roga, S. M. Giampaolo, and F. Illuminati, J. Phys. A: Math. Theor. 47, 365301 (2014).
[28] F. Ciccarello, T. Tufarelli and V. Giovannetti, [arXiv:1304.6879] (2013).
[29] W. K. Wootters, Phys. Rev. Lett. 60, 2245 (1998).
[30] V. Coffman, J. Kundu, and W. K. Wootters, Phys. Rev. A 61, 052306 (2000).
[31] Tzu-Chieh Wei and P. M. Goldbart, Phys. Rev. A 68, 042307 (2003).
[32] A. Streltsov, H. Kampermann and D. Bruß, New J. Phys. 12, 123004 (2010).
[33] E. Lieb, T. Schultz, and D. Mattis, Ann. of Phys. 16, 407 (1961).
[34] P. Plefuty, Annals of Phys. 57, 79 (1970).
[35] E. Barouch, B. M. McCoy, and M. Dresden, Phys. Rev. A 2, 1075 (1970).
[36] E. Barouch and B. M. McCoy, Phys. Rev. A 3, 786 (1971).
[37] J. D. Johnson and B. M. McCoy, Phys. Rev. A 4, 2314 (1971).
[38] J. Kurman, H. Thomas and G. Muller, Physica A 112, 235 (1982).
[39] T. Roscilde, P. Verrucchi, A. Fubini, S. Haas, and V. Tognetti, Phys. Rev. Lett. 94, 147208 (2005).
[40] T. J. Osborne and M. A. Nielsen, Phys. Rev. A 66, 032110 (2002).
[41] L. Amico, F. Baroni, A. Fubini, D. Patané, V. Tognetti and P. Verrucchi Phys. Rev. A 74, 022322 (2006).
[42] T. J. Osborne, F. Verstraete, Phys. Rev. Lett. 96, 220503 (2006).
[43] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature 416, 608 (2002).
[44] M. N. Barber, Finite size scaling, in Phase Transitions and Critical Phenomena, Domb C. and Leibovitz J. L. Eds., Vol. 8 146–259, (Academic Press, London, 1983).
[45] S. Sachdev, Quantum Phase Transitions, Cambridge Univ. Press, Cambridge (2000).
[46] A. Osterloh, G. Palacios and S. Montangero, Phys. Rev. Lett. 97, 257201 (2006).
[47] M. Piani, Phys. Rev. A 86, 034101 (2012).