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Ground-state factorization and correlations with broken symmetry

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Abstract – We show how the phenomenon of factorization in a quantum many-body system is of collective nature. To this aim we study the quantum discord Q in the one-dimensional XY model in a transverse field. We analyze the behavior of Q at both the critical point and at the non-critical factorizing field. The factorization is found to be governed by an exponential scaling law for Q . We also address the thermal effects fanning out from the anomalies occurring at zero temperature. Close to the quantum phase transition, Q exhibits a finite-temperature crossover with universal scaling behavior, while the factorization phenomenon results in a non-trivial pattern of correlations present at low temperature.

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Introduction. – The concepts of symmetry and correlations pervade all the modern many-body physics [1]. A system consisting in a very large number of particles can be found in different phases and the Landau-Ginzburg paradigm of symmetry breaking characterizes the various phases in terms of different symmetries. Different quantum phases are separated by Quantum Phase Transitions (QPTs), which are driven by tuning an external control parameter h across a critical value h_c [2].

Nevertheless, in the past twenty years it has been understood that symmetry cannot explain quite all the phases of matter [3]. Indeed, different patterns of correlations can define different quantum phases featuring unconventional transitions [4]. Examples in many-body physics come from studies on high- T_c superconductors, as well as intermetallic compounds (heavy fermions) and fractional quantum Hall liquids [3,5,6].

Here we analyze quantum correlations in a many-body system addressing the *quantum discord*, beyond the generic notion of “correlations in a quantum system” [7,8]. Quantum correlations are not all captured by entanglement, because a non-vanishing quantum discord results for certain separable (mixed) states [7]. This study addresses some new features of the quantum phases involved in the phenomenon of symmetry breaking. Besides the critical

behavior of the quantum discord at the quantum phase transition, the discord displays dramatic changes also at a non-critical value of the control parameter $h_f \neq h_c$, where quantum correlations vanish, thus producing a factorized classical state [9,10]. Such factorization can even occur within the symmetry-broken phase, and it consists in the sudden reshuffling of quantum correlations, leading to a transition in the entanglement pattern [11,12]. We show that this *correlation transition* at h_f is governed by a new class of scaling laws, thus signaling a collective nature of the phenomenon, even if it is not associated to any symmetry breaking. We speculate that the factorization can be associated to exotic quantum phase transitions that are not described by symmetry breaking but by a reorganization of entanglement patterns without symmetry breaking, like in topological quantum phase transitions [13].

We complete our study by detecting how the quantum critical and the factorization point affect the quantum discord at low-temperature, thus opening the way towards actual observations [14].

Quantum discord in the XY model. – The total amount of correlations in a bipartite (mixed) quantum state $\hat{\rho}_{AB}$ is given by the mutual information $I_{AB} \equiv S(\hat{\rho}_A) + S(\hat{\rho}_B) - S(\hat{\rho}_{AB})$, where $S(\hat{\rho}) = -\text{Tr}[\hat{\rho} \log_2 \hat{\rho}]$ is the von Neumann entropy. On the other hand, classical correlations can be defined in terms of the quantum

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conditional entropy: $S(\hat{\rho}_{AB}|\{\hat{B}_k\}) = \sum_k p_k S(\hat{\rho}_{AB}^{(k)})$, where $\hat{\rho}_{AB}^{(k)} = \frac{1}{p_k} (\hat{I} \otimes \hat{B}_k) \hat{\rho}_{AB} (\hat{I} \otimes \hat{B}_k)$ is the state of the composite system AB , conditioned to the outcome \hat{B}_k (being a set of projectors representing a complete measurement of the subsystem B) of the measurement, with probability $p_k = \text{Tr}[(\hat{I} \otimes \hat{B}_k) \hat{\rho}_{AB} (\hat{I} \otimes \hat{B}_k)]$. The amount of classical correlations C is obtained by finding the set of measurement on B that disturbs the least the part A , *i.e.*, by maximizing $C = \max_{\{\hat{B}_k\}} [S(\hat{\rho}_A) - S(\hat{\rho}_{AB}|\{\hat{B}_k\})]$ (here we restrict to projective measurements) [7,8]. The quantum discord is given by: $Q = I - C$. In a pure state, Q reduces to entanglement. A mixed state though, may contain quantum correlations that are not accounted in the lack of separability (see ref. [7] for examples).

The model we study is the spin-1/2 chain with XY exchange couplings in a transverse field h :

$$\hat{\mathcal{H}} = - \sum_j \left(\frac{1+\gamma}{2} \hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + \frac{1-\gamma}{2} \hat{\sigma}_j^y \hat{\sigma}_{j+1}^y + h \hat{\sigma}_j^z \right), \quad (1)$$

where $\hat{\sigma}_j^\alpha$ ($\alpha = x, y, z$) are the Pauli matrices on site j , $\gamma \in (0, 1]$ denotes the xy anisotropy, while h is the transverse magnetic field strength. The Hamiltonian $\hat{\mathcal{H}}$ is diagonalized by means of a Jordan-Wigner transformation followed by a Bogoliubov rotation in momentum space [15]. In the range of γ we consider hereafter, the system displays a continuous QPT at $h_c = 1$ of the Ising universality class with critical indices $\nu = z = 1$, $\beta = 1/8$. Because of superselection rules, the region $|h| < h_c$ is magnetically ordered and the global Z_2 symmetry is broken in the thermodynamic limit with non-vanishing order parameter $g_x = \langle \hat{\sigma}^x \rangle$; elsewhere the system is a paramagnet. Although the ground state of $\hat{\mathcal{H}}$ is generally entangled, for specific values of γ and h it is completely separable [12]. Besides the trivial cases $h = 0$ and $h \rightarrow \infty$, where $|\psi_{gs}\rangle$ is fully polarized, there is a non-trivial line of factorization $h_f^2 + \gamma^2 = 1$ where, for $\langle \sigma_x \rangle \neq 0$, $|\psi_{gs}\rangle = \prod_j |\psi_j\rangle$ [15], within the findings of [9,10]. This line corresponds to an accidental degeneracy of the Hamiltonian [16,17], while the entanglement pattern swaps from parallel to anti-parallel, with a logarithmically divergent range of bipartite entanglement (“entanglement transition” [11,18]).

In order to compute the classical correlations C_r and the quantum discord Q_r of two spins A and B at distance r , one needs to access the single-spin and the two-spin reduced density matrices $\hat{\rho}_A$ and $\hat{\rho}_{AB}(r)$ (see, *e.g.*, ref. [19] for an explicit expression of the generic two-spin matrix in a system with global phase flip symmetry). Hereafter we focus on the symmetry-broken ground state and on the thermal states of eq. (1). For Z_2 -symmetric states, the non-vanishing entries of $\hat{\rho}_A$ and $\hat{\rho}_{AB}(r)$ can be evaluated analytically in terms of $g_z = \langle \hat{\sigma}^z \rangle$ and $g_{\alpha\alpha}(r) = \langle \hat{\sigma}_j^\alpha \hat{\sigma}_{j+r}^\alpha \rangle$ [15]. In that case we use a fully analytic treatment for the quantum discord, obtaining the *thermal ground state* as the zero temperature limit of such class of states [20]. For symmetry-broken states, $g_{xz}(r)$ and g_x also need to be accessed. Since the expression of $g_{xz}(r)$ is

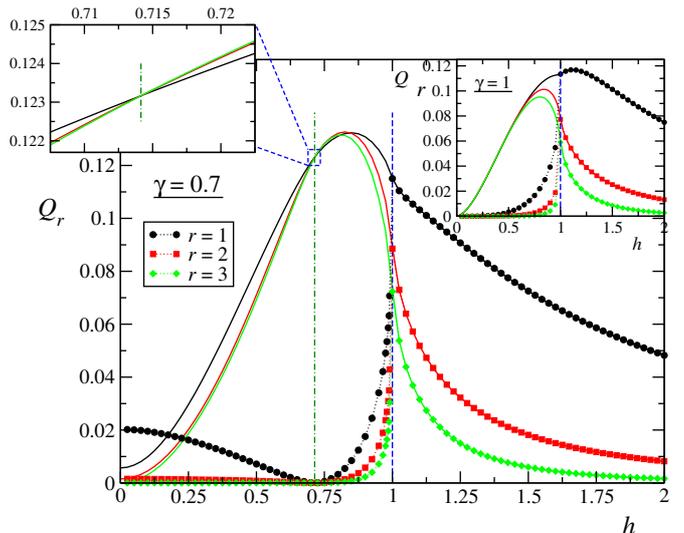


Fig. 1: (Colour on-line) Quantum discord $Q_r(h)$ between two spins at distance r in the XY model at $\gamma = 0.7$ (main plot and left inset) and $\gamma = 1$ (right inset), as a function of the field h . Continuous lines are for the thermal ground state, while symbols denote the symmetry-broken state obtained by adding a small symmetry-breaking longitudinal field $h_x = 10^{-6}$ and it was computed with DMRG in a chain of $L = 400$ spins; simulations were performed by keeping $m = 500$ states and evaluating correlators at the center of the open-bounded chain. For $\gamma = 0.7$ and at $h_f \simeq 0.714$, in the symmetric state all the curves for different values of r intersect, while after breaking the symmetry Q_r is rigorously zero. At the critical point Q_r is non-analytic, thus signaling the QPT. In the paramagnetic phase, there is no symmetry breaking to affect Q_r .

cumbersome [21], in the latter case we resort to the numerical Density Matrix Renormalization Group (DMRG) for finite systems with open boundaries [22].

Ground state. – As displayed in fig. 1, the difference between the quantum discord Q_r for the thermal ground state and for the symmetry-broken state is always finite in the ordered phase (the mutual information I does have the same behavior). Moreover, quantum correlations are typically much smaller deep in the ordered ferromagnetic phase $h < h_c$, rather than in the paramagnetic one $h > h_c$. Nonetheless, as we shall see, they play a fundamental role to drive the order-disorder transition at the QPT, where Q_r exhibits a maximum, as well as the correlation transition at h_f , where Q_r is rigorously zero.

Let us first focus on the quantum critical point, where the QPT is marked by a divergent derivative of the quantum discord (see also [20,23,24]). Such divergence is present at every γ , for the symmetry-broken state; on the other hand, for the thermal ground state, it is not present at $\gamma = 1$. A thorough finite-size scaling analysis is shown in fig. 2 proving that $z = \nu = 1$. For the thermal ground state (in the thermodynamic limit), we found that $\partial_h Q_r$ diverge logarithmically as $\partial_h Q_r \sim \ln|h - h_c|$, within the Ising universality class.

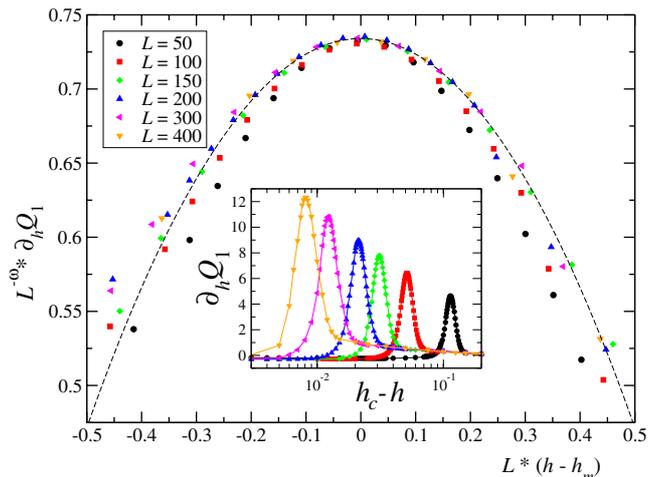


Fig. 2: (Colour on-line) Finite-size scaling of $\partial_h Q_1$ for the symmetry-broken state in proximity of the critical point h_c . Displayed data are for $\gamma = 0.7$. The first derivative of the quantum discord is a function of $L^{-\nu}(h - h_m)$ only, and satisfies the scaling ansatz $\partial_h Q_1 \sim L^\omega \times F[L^{-\nu}(h - h_m)]$, where h_m is the renormalized critical point at finite size L and $\omega = 0.472$. We found a universal behavior $h_c - h_m \sim L^{-1.28 \pm 0.03}$ with respect to γ . Inset: raw data of $\partial_h Q_1$ as a function of the transverse field.

At the factorizing field h_f , all the correlation measures are zero in the state with broken symmetry (see symbols in fig. 1); in particular, we numerically found a dependence $Q_r \sim (h - h_f)^2 \times \left(\frac{1-\gamma}{1+\gamma}\right)^r$ close to it. Such behavior is consistent with the expression of correlation functions close to the factorizing line obtained in ref. [25], and here appears to incorporate the effect arising from the non-vanishing spontaneous magnetization. The factorization phenomenon can be traced also for the thermal ground state [26]: it is the unique value of the field where the same quantum correlations are present at any length scale (left inset of fig. 1). We found a rather peculiar dependence of Q_r on the system size, converging to the asymptotic value $Q_r^{(L \rightarrow \infty)}$ with an exponential scaling behavior (see fig. 3). The picture elucidated here suggests the existence of a non-trivial mechanism leading to the factorization of the ground state. In [11,18], it was shown that h_f marks the transition between two different patterns of entanglement. The factorization is thus a new kind of zero-temperature transition of collective nature, not accompanied by a change of symmetry, and with a scaling law that is new in the panorama of the cooperative phenomena in quantum many-body systems. We emphasize, though, that this transition does not correspond—in this model—to a QPT. The factorization occurs without any non-analyticity in the ground-state wave function $|gs(h)\rangle$ as a function of h , as it is shown by the ground-state fidelity $\mathcal{F}(h) \equiv |\langle gs(h) | gs(h + \delta h) \rangle|$. This quantity (which can detect both symmetry-breaking and non-symmetry-breaking QPTs [13,27]), is a smooth function at h_f . So there is no QPT here. Nevertheless, the

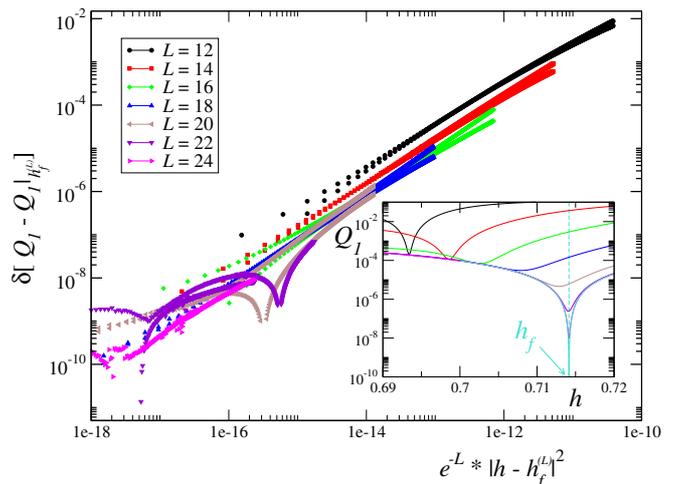


Fig. 3: (Colour on-line) Scaling of Q_1 close to the factorizing field, for $\gamma = 0.7$: we found an exponential convergence to the thermodynamic limit, with a universal behavior according to $e^{-\alpha L}(h - h_f^{(L)})$, $\alpha \approx 1$ ($h_f^{(L)}$ denotes the effective factorizing field at size L , while $\delta(Q_1) \equiv Q_1^{(L)} - Q_1^{(L \rightarrow \infty)}$). Due to the extremely fast convergence to the asymptotic value, already at $L \sim 20$ differences with the thermodynamic limit are comparable with DMRG accuracy. Inset: raw data of Q_1 as a function of h . The cyan line is for $L = 30$ so that, up to numerical precision, the system behaves at the thermodynamic limit.

phenomenon of factorization can accompany a topological QPT [13]. We speculate that the scaling laws associated to topological QPTs are those associated to factorization or other phenomena of entanglement reorganization. At the level of spectral properties of the system, we interpret this result as an effect of certain *competition between* states belonging to different parity sectors for finite L [17]; as these states intersect, the ground-state energy density is diverging *for all finite L* (such divergence, though, vanishes in the thermodynamic limit).

Finite temperature. – In order to check how the observed phenomena are resilient with respect to thermal fluctuations, we analyze the quantum correlations at finite temperature. The low-temperature behavior is influenced by the proximity to critical and factorizing fields. Close to h_c , the physics is dictated by the interplay between thermal and quantum fluctuations of the order parameter. A V-shaped diagram in the h - T plane emerges, characterized by the cross-over temperature $T_{cross} = |h - h_c|^z$ fixing the energy scale [2]. $T \ll T_{cross}$ identifies two semiclassical regimes. In the quantum critical region $T \gg T_{cross}$, quantum and thermal effects cannot be resolved; here the critical properties dominate the physics of the system, even at finite temperature. Close to h_f and at small T , the bipartite entanglement remains vanishing in a finite non-linear cone in the h - T plane [12,18]. Thermal states, though, are not separable, and entanglement is present in a multipartite form [28]. In this regime the bipartite entanglement results to be non-monotonous, and a re-entrant

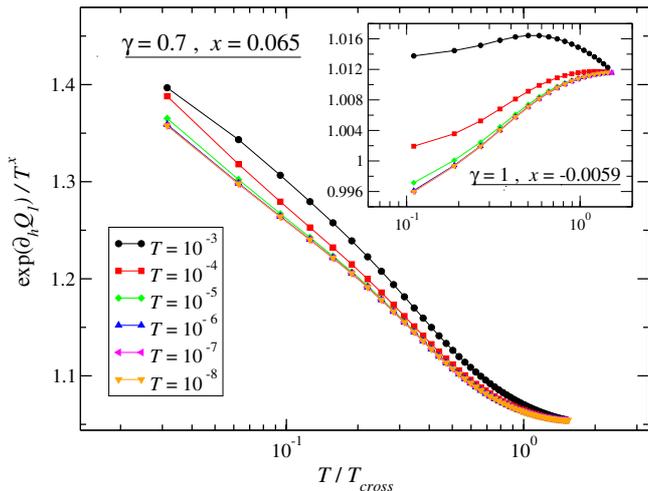


Fig. 4: (Colour on-line) Finite-temperature scaling of the quantum discord for the thermal state close to the critical point. The logarithmic scaling is verified: along the critical line we found $\partial_h Q_1|_{h_c} \sim x \ln(T) + k$, with $x = 0.065$ for $\gamma = 0.7$. The scaling function F shows a data collapse close to the critical point. Inset: same analysis for the Ising case ($\gamma = 1$); we found an analogous scaling behavior with $x = -0.0059$.

swap between parallel and antiparallel entanglement is observed [18].

At any temperature $T > 0$, the state is Z_2 -symmetric. By inspection of fig. 1, and since Q_r is a continuous function of T for finite temperatures, we conclude that Q_r is discontinuous as the temperature is switched on, in all the phase $h < h_c$. Such discontinuity is also observed in the entanglement, even if in that case it is much less pronounced and occurs only for $h < h_f$ [19]. We now analyze how criticality and factorization modify the fabric of purely quantum correlations in the h - T plane.

The first aspect we consider is the thermal scaling close to the QPT. The scaling ansatz $\partial_h Q_r = T^x F(T/T_{cross})$, where $T_{cross} \equiv |h - h_c|^{\nu z}$ [2], is verified in fig. 4 for $r = 1$. Remarkably, the discord scales also in the Ising case $\gamma = 1$, despite $\partial_h Q$ is not diverging at $T = 0$ [20]. We then discuss the interplay between classical and quantum correlations. In fig. 5(a) we show $\partial_T [Q_1/C_1]$ in the h - T plane, namely the sensitivity of the relative strength between quantum and classical correlations to thermal fluctuations. We found a V-shaped diagram, where the ratio is constant along the critical line $h = 1$ in the quantum critical region $T \gg |h - 1|$, while it explores the largest changes along the crossover region. We remark the asymmetry of fig. 5(a) between $\Delta < 0$ and $\Delta > 0$, taking into account that the mechanism leading to the two corresponding semiclassical regimes traces back to quantum ($\Delta > 0$) or thermal ($\Delta < 0$) fluctuations [2].

We now move to h_f , where, for the thermal ground state, factorization is marked by the fixed point in Q_r (see left inset of fig. 1). This originates a non-trivial pattern of correlations: $Q_r(T) \simeq Q_{r'}(T)$ for any r, r' . We quantify this behavior by analyzing the average displacement between

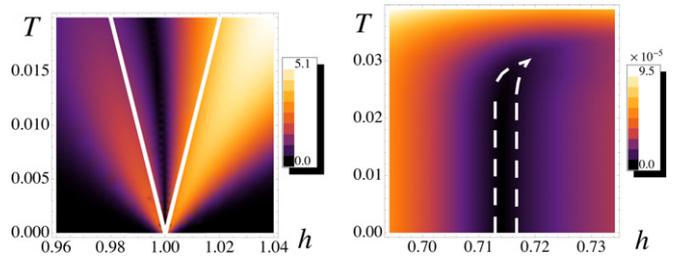


Fig. 5: (Colour on-line) a) Density plot in the h - T plane of $\partial_T [Q_1/C_1]$ close to h_c ; along the critical line the ratio Q_1/C_1 is constant with respect to the temperature. The solid straight line ($T = |h - h_c|$) marks the boundary of the quantum critical region. b) Average quantum discord displacement: $\overline{\Delta Q_r} = 2 \sum_{i,j=1}^m |Q_{r_i}(T) - Q_{r_j}(T)| / m(m-1)$ for $m = 5$ fanning out from the factorizing point $h_f \sim 0.714$, where all correlations coincide at any length scale r , as evidenced in fig. 1, left inset. Dashed line is for guiding eyes. Here $\gamma = 0.7$.

different Q_r fanning out from the fixed point in the thermal ground state at $h = h_f$ (see $\overline{\Delta Q_r}$ in fig. 5(b)).

Outlook and perspectives. – We studied purely quantum correlations quantified by the quantum discord Q_r in the quantum phases involved in a symmetry-breaking QPT. Even if Q_r results relatively small in the symmetry-broken state as compared to the thermal ground state, it underlies key features in driving both the order-disorder transition across the QPT at h_c , and the correlation transition across the factorizing field h_f . The critical point is characterized by a non-analyticity of Q_r found in the Ising universality class. Close to h_f , Q_r displays uniquely non-trivial properties: in the thermal ground state quantum correlations are identical at all scales; for the symmetry-broken state we identified a novel exponential scaling, specific for the factorization phenomenon occurring in the ground state of the system. We remark that this can occur without changing the symmetry of the system, as a signature of the fact that quantum phases and entanglement are more subtle than what the symmetry-breaking paradigm says. Although in model eq. (1) the factorization happens deep in the symmetry-broken phase, its behavior is also particularly relevant in the context of QPTs involving topologically ordered phases [29], which are believed to occur because of a change of the global pattern of entanglement [13] instead of symmetry.

At finite temperatures a discontinuity of Q_r with T is evidenced in the whole ordered phase $h < h_c$. We expect such discontinuity to be present also for models with finite T_c . We proved that Q_r displays universal features, and it exhibits a crossover behavior; in particular the quantum critical region is identified by the condition $Q(T)/C(T) = Q(0)/C(0)$ along the critical line. We have found that a non-trivial pattern of quantum correlations fans out from the factorization of the ground state (where $\overline{\Delta Q_r} = 0$), opening the way to experimental detection of the phenomenon.

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