Collective behavior in many-body quantum systems is associated with the development of classical correlations, as well as of correlations which cannot be accounted for in terms of classical physics, namely entanglement. Entanglement represents in essence the impossibility of giving a local description of a many-body quantum state. In particular, entanglement is expected to play an essential role at quantum phase transitions, where quantum fluctuations manifest themselves at all length scales. The behavior of entanglement at quantum phase transitions is a very recent topic, so far investigated in a few exactly solvable cases [1, 2, 3, 4]. Moreover, entanglement overwhelming comes into play in quantum computation and communication theory, being the main physical resource needed for their specific tasks [5]. In this respect, the perspective of manipulating entanglement by tunable quantum many-body effects appears very intriguing.

In this letter we show that entanglement estimators give important insight in the physics of spin systems. In particular, we focus on two striking features of anisotropic spin chains in an external field: the occurrence of an anisotropic ground state at a field less than the critical field, and therefore it belongs to the same universality class. The analysis is carried out via Quantum Monte Carlo simulations, based on a modified directed-loop algorithm [13, 14], for chains of various length, from \( L = 40 \) to \( L = 120 \). Ground state properties have been determined by considering inverse temperatures \( \beta = 2L \), in order to capture the \( T = 0 \) behavior.

The ground-state phase diagram of the XYZ model in the \( \Delta_y - h \) plane is shown in Fig. 1. The model displays a field-driven quantum phase transition at a critical field \( h_c(\Delta_y) \), which separates the Néel-ordered phase \((h < h_c)\) from a disordered phase \((h > h_c)\) with short-range antiferromagnetic correlations [8]. The transition line \( h_c(\Delta_y) \) has been determined by a scaling analysis of the correlation length \( \xi^{xx} \), whose linear scaling \( \xi^{xx} \sim L \) marks the quantum critical point. Using the critical scaling of the structure factor \( S_{xx}(q = 0) \sim L^{\gamma/\nu - 2} \), we verified that the transition belongs to the 1D transverse-field Ising universality class \((\gamma/\nu = 7/4 \text{ and } z = 1)\), in agreement with analytical predictions [8].

Besides its quantum critical behavior, a striking feature of the model of Eq. 1 is the occurrence of an exactly solvable XY model in a transverse field [6]. For \( \Delta_z = 0 \) the model does not admit an exact solution [7], and it has been recently studied within approximate analytical and numerical approaches [8, 9, 10]. Interestingly, the general model with finite \( \Delta_z \) is experimentally realized by the \( S = 1/2 \) quantum spin chain \( \text{Cs}_2\text{CoCl}_4 \) [11], with strong planar XZ anisotropy, \( \Delta_y \approx 0.25 \), \( \Delta_z \approx 1 \), and \( J \approx 0.23 \text{ meV} \).

In our study, we concentrate on the case \( 0 \leq \Delta_y \leq 1 \), \( \Delta_z = 1 \), defining the XYZ model in a field [12]. The more general case of the XYZ model in a magnetic field with \( \Delta_z < 1 \) should exhibit the same qualitative behavior, as it shares the same symmetries with the XYX model in a field, and therefore it belongs to the same universality class. The analysis is carried out via Stochastic Series Expansion (SSE) Quantum Monte Carlo (QMC) simulations, based on a modified directed-loop algorithm [13, 14], for chains of various length, from \( L = 40 \) to \( L = 120 \). Ground state properties have been determined by considering inverse temperatures \( \beta = 2L \), in order to capture the \( T = 0 \) behavior.

where \( J > 0 \) is the exchange coupling, \( i \) runs over the sites of the chain, and \( h = g \mu_B H / J \) is the reduced magnetic field. In Eq. 1 we have implicitly performed the canonical transformation \( S_{i,x,y} \rightarrow (-1)^y S_{i,x,y} \) with respect to the more standard antiferromagnetic Hamiltonian. The parameters \( \Delta_y, \Delta_z \geq 0 \) control the anisotropy of the system. In particular, for \( \Delta_z = 0 \) Eq. 1 reduces to the exactly solvable XY model in a transverse field [6]. For \( \Delta_z \neq 0 \) the model does not admit an exact solution [7], and it has been recently studied within approximate analytical and numerical approaches [8, 9, 10]. Interestingly, the general model with finite \( \Delta_z \) is experimentally realized by the \( S = 1/2 \) quantum spin chain \( \text{Cs}_2\text{CoCl}_4 \) [11], with strong planar XZ anisotropy, \( \Delta_y \approx 0.25 \), \( \Delta_z \approx 1 \), and \( J \approx 0.23 \text{ meV} \).

Collective behavior in many-body quantum systems is associated with the development of classical correlations, as well as of correlations which cannot be accounted for in terms of classical physics, namely entanglement. Entanglement represents in essence the impossibility of giving a local description of a many-body quantum state. In particular, entanglement is expected to play an essential role at quantum phase transitions, where quantum fluctuations manifest themselves at all length scales. The behavior of entanglement at quantum phase transitions is a very recent topic, so far investigated in a few exactly solvable cases [1, 2, 3, 4]. Moreover, entanglement overwhelmingly comes into play in quantum computation and communication theory, being the main physical resource needed for their specific tasks [5]. In this respect, the perspective of manipulating entanglement by tunable quantum many-body effects appears very intriguing.

In this letter we show that entanglement estimators give important insight in the physics of spin systems. In particular, we focus on two striking features of anisotropic spin chains in an external field: the occurrence of a factorized ground state at a field \( h_t \) and of a quantum phase transition at \( h_c \). We propose a novel estimator to understand the role of quantum fluctuations in the quantum critical region.

We focus our attention on the 1D XYZ model in a field:

\[
\hat{H} = -J \sum_i \left[ S_i^x S_{i+1}^x + \Delta_y S_i^y S_{i+1}^y - \Delta_z S_i^z S_{i+1}^z + h S_i^z \right]
\]

where \( J > 0 \) is the exchange coupling, \( i \) runs over the sites of the chain, and \( h = g \mu_B H / J \) is the reduced magnetic field. In Eq. 1 we have implicitly performed the canonical transformation \( S_{i,x,y} \rightarrow (-1)^y S_{i,x,y} \) with respect to the more standard antiferromagnetic Hamiltonian. The parameters \( \Delta_y, \Delta_z \geq 0 \) control the anisotropy of the system. In particular, for \( \Delta_z = 0 \) Eq. 1 reduces to the

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In terms of the spin expectation values $M$ it can be easily shown that the vanishing of $\tau$ quantifies the simple form:

$$\tau = 1 - 4 \sum_{\alpha} (M^\alpha)^2.$$  

It can be easily shown that the vanishing of $\tau_1$ implies a factorized ground state, and vice versa.

The concurrence $C_{ij}$ quantifies instead the pairwise entanglement between two spins at sites $i, j$ both at zero and finite temperature. For the model of interest, in absence of spontaneous symmetry breaking ($M^z = 0$) the concurrence takes the form:

$$C_{ij} = 2 \max\{0, C_{ij}^{(1)}, C_{ij}^{(2)}\},$$

where

$$C_{ij}^{(1)} = g_{ij}^{zz} - \frac{1}{4} + |g_{ij}^{xx} - g_{ij}^{yy}|,$$

$$C_{ij}^{(2)} = |g_{ij}^{xx} + g_{ij}^{yy}| - \sqrt{\left(\frac{1}{4} + g_{ij}^{zz}\right)^2 - (M^z)^2},$$

with $g_{ij}^{\alpha\beta} = \langle \hat{S}_i^\alpha \hat{S}_j^\beta \rangle$.

The $T = 0$ QMC results for the model Eq. 10 with $\Delta_y = 0.25$ are shown in Fig. 2 where we plot $\tau_1$, the sum of squared concurrences

$$\tau_2 = \sum_{j \neq i} C_{ij}^2,$$

and the field and space dependence of the concurrence. The following discussion, although directly referred to the results for $\Delta_y = 0.25$, is actually quite general and applies to all the other studied values of $\Delta_y$. 

![Figure 1](image1.png)

**FIG. 1:** Upper panel: ground state phase diagram of the XYX model in a field. Mean-field (MFA) results are taken from Ref. 10, the factorizing field $h_f$ from Ref. 1. Lower panel: quantum critical behavior of $x$– and $z$– magnetizations and correlation length for the model with $\Delta_y = 0.25$, $L = 100$, $\beta = 200$. The factorizing field is indicated by a dashed line. The arrow indicates the quantum critical point (QCP).

![Figure 2](image2.png)

**FIG. 2:** (a) One-tangle $\tau_1$ and sum of squared concurrences $\tau_2$ as a function of the applied field for the $S = 1/2$ XYX model with $\Delta_y = 0.25$, $L = 100$ and $\beta = 200$. Inset: contributions to the concurrence between $j$–th neighbors. Full symbols stand for $C_{ij}^{(1)}$, open symbols for $C_{ij}^{(2)}$. The dashed line marks the critical field $h_c$. (b) Concurrence as a function of spin-spin distance. Parameters as in the previous figure.
FIG. 3: Entanglement ratio $\tau_2/\tau_1$ as a function of the field for $\Delta_y = 0.25$ and $\beta = 2L$. Inset: entanglement ratio for the 1D Ising model in a transverse field. The dashed line is the $L \to \infty$ extrapolation result.

Unlike the standard magnetic observables plotted in Fig. 1 the entanglement estimators display a marked anomaly at the factorizing field, where they clearly vanish as expected for a factorized state. When the field is increased above $h_f$, the ground-state entanglement has a steep recovery, accompanied by the quantum phase transition at $h_c > h_f$. For $\Delta_y = 0.25$, e.g., $h_c = 1.605(3)$ and $h_f = 1.5811$. The system realizes therefore an interesting entanglement switch effect controlled by the magnetic field.

As for the concurrence, Fig. 2(b) shows that its range is always finite at and around the critical point, and it never extends farther than the fourth neighbor. Moreover, the factorizing field divides two field regions with different expressions for the concurrence:

\[
C_{ij}^{(1)} < 0 < C_{ij}^{(2)} \quad \text{for} \quad h < h_f ,
\]

\[
C_{ij}^{(2)} < 0 < C_{ij}^{(1)} \quad \text{for} \quad h > h_f ,
\]

whereas $C_{ij}^{(1)} = C_{ij}^{(2)} = 0$ at $h = h_c$.

In presence of spontaneous symmetry breaking occurring for $h < h_c$, the expression of the concurrence is generally expected to change with respect to Eqs. (1), (2), as extensively discussed in Ref. 19. For the model under investigation, this happens when the condition $\Delta_y = 0$, occurring at the critical field $h_c = 1/2$. Work is in progress to test the universality of such novel signature of quantum critical behavior for completely independent quantum phase transitions.

In turn, we propose the minimum of the entanglement ratio $R$ as a novel estimator of the quantum critical point, fully based on entanglement quantifiers. This result appears general for the whole class of models described by the hamiltonian of Eq. (1). Inset (b) of Fig. 3 shows in fact that an analogous dip in the entanglement ratio signals the quantum phase transition in the Ising model in a transverse field ($\Delta_y = \Delta_z = 0$), occurring at the critical field $h_c = 1/2$. Work is in progress to test the universality of such novel signature of quantum critical behavior for completely independent quantum phase transitions.

The use of the QMC method enables us to naturally monitor the fate of entanglement when the temperature is raised above zero. In this regime the concurrence is the only well-defined estimator of entanglement, whereas the one-tangle has not yet received a finite-temperature generalization. Fig. 3(a) shows the nearest-neighbor (n.n.) concurrence as a function of the field for different temperatures in the XYX model with $\Delta_y = 0$. We observe that $C_{i,i+n} < C_{i,i+1}$ for $n > 0$, and at high enough temperature ($T \gtrsim 0.1J$) only the n.n. concurrence survives. The most prominent feature is the persistence of a field value (or an interval of values) at which the concurrence is either zero (for $T \gtrsim 0.05J$) or $\sim 10^{-3}$ (for $0 < T \lesssim 0.05J$). In particular, the field values for which the concurrence vanishes are temperature-dependent, so that two-spin en-
Entanglement can be switched on and off tuning both the field and the temperature. Fig. 4(b) shows a highly non-trivial temperature dependence of the two-spin entanglement at \( h = h_f = \sqrt{2} \). Although vanishing at \( T = 0 \), the n.n. concurrence has a quick thermal activation due to thermal mixing of the factorized ground state with entangled excited states. Although the spectrum over the ground state displays a gap of order 0.1 \( J \) in one dimension strong fluctuations induce thermal entanglement \( \approx \) already at temperatures which are an order of magnitude lower. The appearance of thermal entanglement is directly related to the increasing behavior of the correlators \( g^{yy} = g^{yy}_{i,i+1} \) and \( g^{zz} = g^{zz}_{i,i+1} \) entering the expression of the \( C^{(1)} \) component, Eq. (4) (also shown in Fig. 4(b)). In particular the appearance of a finite \( g^{yy} \) is a purely quantum effect, since \( \Delta_y = 0 \). Because of the non-monotonous behavior of the correlators, at higher temperatures thermal entanglement disappears and reappears again, revealing an intermediate temperature region where two-spin entanglement is absent.

In summary, making use of efficient QMC techniques we have provided a comprehensive picture of the entanglement properties in a class of anisotropic spin chains of relevance to experimental compounds. We have shown that the occurrence of a classical factorized state in these systems is remarkably singled out by entanglement estimators, unlike the more conventional magnetic observables. Moreover we find that entanglement estimators are able to detect the quantum critical point, marked by a narrow dip in the pairwise-to-global entanglement ratio. Therefore we have shown that entanglement estimators provide precious insight in the ground-state properties of lattice \( S = 1/2 \) spin systems. Thanks to the versatility of QMC, the same approach can be used for higher-dimensional systems. In this respect, investigations of the occurrence of factorized states in more than one dimension are currently in progress. Finally, the proximity of a quantum critical point to the factorized state of the system gives rise to an interesting field-driven entanglement-switch effect. This demonstrates that many-body effects driven by a macroscopic field are a powerful tool for the control of the microscopic entanglement in a multi-qubit system, and stand as a profitable resource for quantum computing devices.

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**References**

1. A. Osterloh et al., *Nature* (London) **416**, 608 (2002).
2. T.J. Osborne et al., *Phys. Rev. A* **66**, 032110 (2002).
3. G. Vidal et al., *Phys. Rev. Lett.* **90**, 227902 (2003).
4. F. Verstraete et al., *Phys. Rev. Lett.* **92**, 027901 (2004); *ibid.* **92** 087201 (2004).
5. M. A. Nielsen and I. L Chuang, *Quantum Computation and Quantum Information*, Cambridge Univ. Press, 2000.
6. E. Barouch et al., *Phys. Rev. A* **2**, 1075 (1970); *ibid.* **3**, 786 (1971).
7. J. Kurnmann et al., *Physica A* **112**, 235 (1982).
8. D. V. Dmitriev et al., *J. Exp. Th. Phys.* **95**, 538 (2002).
9. F. Capraro and C. Gros, *Eur. Phys. J B* **29**, 35 (2002).
10. J.-S. Caux et al., *Phys. Rev. B* **68**, 134431 (2003).
11. M. Kenzelmann et al., *Phys. Rev. B* **65**, 144432 (2002).
12. T. Delica and H. Leschke, *Physica A* **168**, 736 (1990).
13. O. F. Syljuåsen et al., *Phys. Rev. E* **66**, 046701 (2002).
14. The original directed-loop algorithm was designed to treat models with a continuous rotational symmetry in the plane transverse to the field. We have generalized it to our less symmetric model introducing further vertices not conserving the \( z \)-magnetization, associated with the operators \( S^z_i S^z_{i+1} \) and \( S^z_i S^z_{i+1} \) appearing in our hamiltonian with quantization axis along \( z \). We then minimize the bounce probability as in the original scheme of Ref. 1.
15. Details of the algorithm will be presented elsewhere.
16. C. H. Bennett et al., *Phys. Rev. A* **54**, 3824 (1996).
17. V. Coffman et al., *Phys. Rev. A* **61**, 052306 (2000).
18. L. Amico et al., *Phys. Rev. A* **69**, 022304 (2004).
19. W.K. Wootters, *Phys. Rev. Lett.* **80**, 2245 (1998).
20. O.F. Syljuåsen, *Phys. Rev. A* **68**, 060301 (2003).
21. M.C. Arnesen et al., *Phys. Rev. Lett.* **87**, 017901 (2001).