

Global entanglement and quantum criticality in spin chains

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The entanglement of quantum XY spin chains of arbitrary length is investigated via a recently developed *global* measure suitable for generic quantum many-body systems. This entanglement is determined over the phase diagram and found to exhibit rich structure. In particular, the field derivative of the entanglement density becomes singular along the critical line. The form of this singularity is dictated by the universality class controlling the quantum phase transition.

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INTRODUCTION

Quantum entanglement, a term coined by Schrödinger, has been recognized over the past decade as the central actor in many quantum information processing tasks [1]. More recently, entanglement has emerged on the nearby stage of quantum many-body physics, especially for systems that exhibit quantum phase transitions [2–7], where it can play the role of a diagnostic of quantum correlations. Quantum phase transitions [8] are transitions between qualitatively distinct phases of quantum many-body systems, driven by quantum fluctuations. In view of the connection between entanglement and quantum correlations, one anticipates that entanglement will furnish a dramatic signature of the quantum critical point, where quantum fluctuations are greatly enhanced. From the viewpoint of quantum information, the more entangled a state, the more resources it is likely to possess. It is thus desirable to study and quantify the degree of entanglement near quantum phase transitions. By employing entanglement to diagnose many-body quantum states one may obtain fresh insight into the quantum many-body problem.

To date, progress in quantifying entanglement has taken place primarily in the domain of bipartite systems [9]. For multipartite systems, however, the complete characterization of entanglement requires the consideration of multipartite entanglement, for which a consensus measure has not yet emerged. Much of the previous work on entanglement in quantum phase transitions has been based on bipartite measures, i.e., entanglement either between pairs of parties (via the concurrence) [2,3] or between a part and the remainder of a system (via the von Neumann entropy) [4,6,7]. Singular and scaling behavior of entanglement near quantum critical points was discovered by Osterloh and co-workers [3], who invoked Wootters' *two-qubit* concurrence [10]. Vidal and co-workers [4] have connected the von Neumann entropy to the results of conformal field theory. Gu and co-workers [7] have found further application of the von Neumann entropy in the extended Hubbard model. Despite the success of these two bipartite measures as a probe of quantum phase transitions, body problems, Yang has recently found examples where both measures fail to faithfully reflect the underlying quantum critical points [11].

To characterize the entanglement of a many-body system, a multipartite approach of entanglement is indispensable.

Here we study a recently developed *global* measure of entanglement [12] that provides a *holistic*, rather than bipartite, characterization of the entanglement of quantum many-body systems. It has the merit of being applicable beyond qubit systems, and allows us to study the *thermodynamic* entanglement density. In the present paper we employ the Jordan-Wigner technique and calculate the global entanglement for both the ground and first excited states for arbitrary number of spins. The thermodynamic entanglement density we have obtained provides information on various phases and phase boundaries. Specifically, we observe that it varies in a singular manner near the quantum critical line, and that it vanishes along the disorder line.

GLOBAL MEASURE OF ENTANGLEMENT

To introduce a measure for characterizing the *global* entanglement, consider a general, n -partite, normalized pure state: $|\Psi\rangle = \sum_{p_1 \dots p_n} \Psi_{p_1 p_2 \dots p_n} |e_{p_1}^{(1)} e_{p_2}^{(2)} \dots e_{p_n}^{(n)}\rangle$. If the parties are all spin-1/2 then each can be taken to have the basis $\{|\uparrow\rangle, |\downarrow\rangle\}$. Our scheme for analyzing the entanglement involves considering how well an entangled state can be approximated by some unentangled (normalized) state (e.g., the state in which every spin points in a definite direction): $|\Phi\rangle \equiv \otimes_{i=1}^n |\phi^{(i)}\rangle$. The proximity of $|\Psi\rangle$ to $|\Phi\rangle$ is captured by their overlap; the entanglement of $|\Psi\rangle$ is revealed by the maximal overlap [12],

$$\Lambda_{\max}(\Psi) \equiv \max_{\Phi} |\langle \Phi | \Psi \rangle|; \quad (1)$$

the larger Λ_{\max} is, the less entangled is $|\Psi\rangle$. If the entangled state consists of two separate entangled pairs of subsystems, Λ_{\max} is the product of the maximal overlaps of the two. Hence, it makes sense to quantify the entanglement of $|\Psi\rangle$ via the following *extensive* quantity [12,13]:

$$E_{\log_2}(\Psi) \equiv -\log_2 \Lambda_{\max}^2(\Psi), \quad (2)$$

This normalizes to unity the entanglement of EPR-Bell and N -parity Greenberger-Horne-Zeilinger (GHZ) states, as these states have $\Lambda_{\max} = 1/\sqrt{2}$ [12], as well as gives zero for unentangled states. To characterize the properties of the quantum critical point we use the thermodynamic quantity \mathcal{E} defined by

$$\mathcal{E} \equiv \lim_{N \rightarrow \infty} \mathcal{E}_N, \quad \mathcal{E}_N \equiv N^{-1} E_{\log_2}(\Psi). \quad (3)$$

QUANTUM XY SPIN CHAINS AND ENTANGLEMENT

We consider the family of models governed by the Hamiltonian

$$\mathcal{H}_{XY} = - \sum_{j=1}^N \left(\frac{1+r}{2} \sigma_j^x \sigma_{j+1}^x + \frac{1-r}{2} \sigma_j^y \sigma_{j+1}^y + h \sigma_j^z \right), \quad (4)$$

where r measures the anisotropy between x and y couplings, h is the transverse external field along the z direction, and we impose periodic boundary conditions. At $r=0$ we have the isotropic XY limit (also known as the XX model) and at $r=1$, the Ising limit. All anisotropic XY models ($0 < r \leq 1$) belong to the same universality class, i.e., the Ising class, whereas the isotropic XX model belongs to a different universality class. XY models exhibit three phases (see Fig. 1): oscillatory (O), ferromagnetic (F) and paramagnetic (P) [14].

As is well known [8,14,15], the energy eigenproblem for the XY spin chain can be solved by a Jordan-Wigner transformation, via which the spins are recast as fermions, followed by a Bogoliubov transformation, which diagonalizes the quadratic Hamiltonian. Having found the eigenstates, Λ_{\max} of Eq. (1), and hence the entanglement, can be found. To do this, we parametrize the separable states via

$$|\Phi\rangle \equiv \otimes_{i=1}^N [\cos(\xi_i/2) |\uparrow\rangle_i + e^{i\phi_i} \sin(\xi_i/2) |\downarrow\rangle_i], \quad (5)$$

where $|\uparrow\rangle$ ($|\downarrow\rangle$) denote spin states parallel (antiparallel) to the z axis. Instead of maximizing the overlap with respect to the $2N$ real parameters $\{\xi_i, \phi_i\}$, for the lowest two states it is adequate to appeal to the translational symmetry and the reality of the wave functions. Thus taking $\xi_i = \xi$ and $\phi_i = 0$ we make the ansatz: $|\Phi(\xi)\rangle \equiv e^{-i\xi/2 \sum_{j=1}^N \sigma_j^y} |\uparrow \uparrow \dots \uparrow\rangle$ for searching the maximal the overlap $\Lambda_{\max}(\Psi)$ [16]. This form shows that this separable state can be constructed as a global rotation of the ground state at $h=\infty$, viz., the state $|\uparrow \uparrow \dots \uparrow\rangle$. The energy eigenstates are readily expressed in terms of the Jordan-Wigner fermion operators, and so too are the ansatz states $|\Phi(\xi)\rangle$. By working in this fermion basis we are able to evaluate the overlaps between the two lowest states and the ansatz states. With $|\Psi_0\rangle$ ($|\Psi_1\rangle$) denoting the lowest state in the even (odd) fermion-number sector, we arrive at the overlaps

$$\begin{aligned} \langle \Psi_a(r, h) | \Phi(\xi) \rangle &= f_N^{(a)}(\xi) \prod_{m=1-a}^{m < (N-1)/2} [\cos \theta_m^{(a)}(r, h) \cos^2(\xi/2) \\ &\quad + \sin \theta_m^{(a)}(r, h) \sin^2(\xi/2) \cot(k_{m,N}^{(a)}/2)], \\ k_{m,N}^{(a)} &\equiv \frac{2\pi}{N} \left(m + \frac{a}{2} \right), \end{aligned}$$

$$\tan 2\theta_m^{(a)}(r, h) \equiv r \sin k_{m,N}^{(a)} / (h - \cos k_{m,N}^{(a)});$$

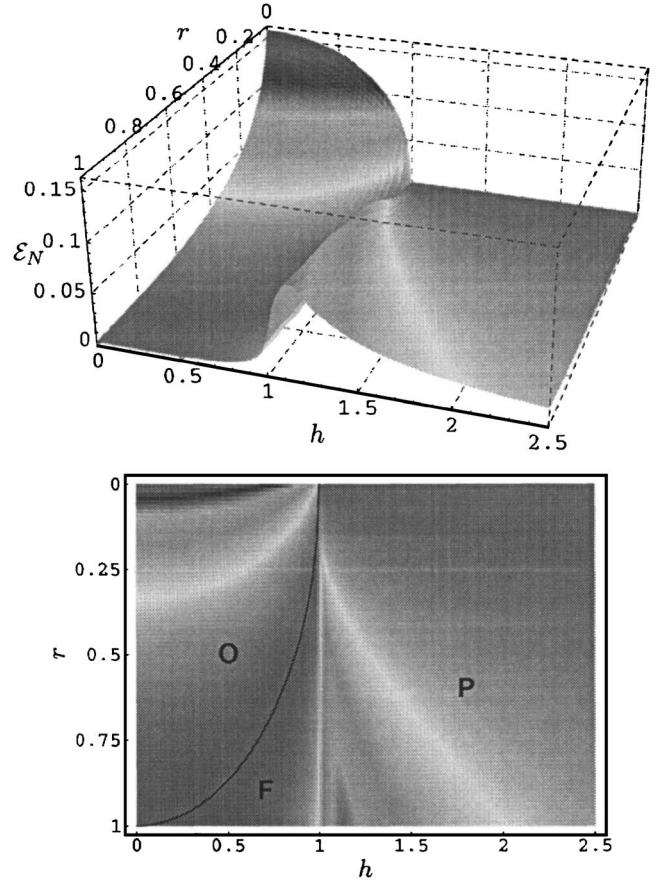


FIG. 1. (Color online) Entanglement density \mathcal{E}_N (upper) and phase diagram (lower) vs (r, h) for the XY model with $N=10^4$ spins, which is essentially in the thermodynamic limit. There are three phases: O : ordered oscillatory, for $r^2+h^2 < 1$ and $r \neq 0$; F : ordered ferromagnetic, between $r^2+h^2 > 1$ and $h < 1$; P : paramagnetic, for $h > 1$. As is apparent, there is a sharp rise in the entanglement across the line $h=1$, which signifies a quantum phase transition. The arc $h^2+r^2=1$, along which the entanglement density is zero (see also Fig. 2), separates phases O and F . Along $r=0$ lies the XX model, which belongs to a different universality class from the anisotropic XY model.

$$f_N^{(1)}(\xi) \equiv 1, \quad f_N^{(0)}(\xi) \equiv \sqrt{N} \sin(\xi/2) \cos(\xi/2), \quad (N \text{ even});$$

$$f_N^{(1)}(\xi) \equiv \cos(\xi/2), \quad f_N^{(0)}(\xi) \equiv \sqrt{N} \sin(\xi/2), \quad (N \text{ odd}); \quad (6)$$

where $a=0, 1$ and $m \in [0, N-1]$ is an integer. The above results are exact for arbitrary N , obtained with periodic boundary conditions on spins rather than the so-called c -cyclic approximation [15]. Given these overlaps, we can readily obtain the entanglement of the ground state, the first excited state, and any linear superposition, $\cos \alpha |\Psi_0\rangle + \sin \alpha |\Psi_1\rangle$ of the two lowest states, for arbitrary (r, h) and N , by maximizing the magnitude of the overlap with respect to the single real parameter ξ .

The formulas that we have just established contain all the results that we explore in the present paper. By analyzing the structure of Eq. (6), we find that the global entanglement

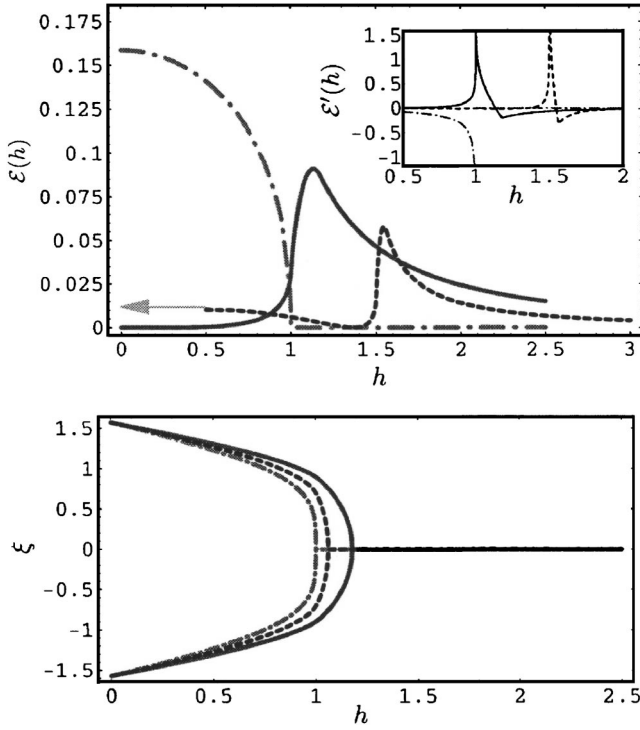


FIG. 2. (Color online) Upper panel: Entanglement density and its h derivative (inset) for the ground state of three systems at $N = \infty$. Solid blue line: Ising ($r=1$) limit; dashed black line: anisotropic ($r=1/2$) XY model; dash-dotted red line: ($r=0$) XX model. For the sake of clarity, the XY-case curves are shifted to the right by 0.5, indicated by the green arrow. For the $r=1/2$, at $h^2+r^2=1$ the entanglement density vanishes, which is a general property for the anisotropic XY model. Note that whilst the entanglement itself has a nonsingular maximum at $h \approx 1.1$ (Ising), $h \approx 1.04$ (XY $r=1/2$), $h=0$ (XX), respectively, it has a singularity at the quantum critical point at $h=1$, as revealed by the divergence of its derivative. Lower panel: The solutions of the single rotation parameter ξ for the ansatz state vs h .

does provide information on the phase structure and critical properties of the quantum spin chains. In addition to arbitrary number results, two of our key results, as captured in Figs. 1 and 2, are that: (i) although the entanglement itself is, generically, not maximized at the quantum critical line in the (r, h) plane, *the field derivative of the entanglement diverges as the critical line $h=1$ is approached*; and (ii) the entanglement *vanishes* at the disorder line $r^2+h^2=1$, which separates the oscillatory and ferromagnetic phases.

ENTANGLEMENT AND QUANTUM CRITICALITY

From Eq. (6) it follows that the thermodynamic limit of the entanglement density is given by

$$\mathcal{E}(r, h) = -\frac{2}{\ln 2} \max_{\xi} \int_0^{1/2} d\mu \ln[\cos \theta(\mu, r, h) \cos^2(\xi/2) + \sin \theta(\mu, r, h) \sin^2(\xi/2) \cot \pi \mu], \quad (7)$$

where $\tan 2\theta(\mu, r, h) \equiv r(\sin 2\pi\mu)/(h - \cos 2\pi\mu)$.

Figure 2 shows the thermodynamic limit of the entanglement density $\mathcal{E}(r, h)$ and its h derivative in the ground state, as a function of h for three values of r , i.e., three slices through the surface shown in Fig. 1. As the $r=1$ slice shows, in the Ising limit the entanglement density is small for both small and large h . It increases with h from zero, monotonically, albeit very slowly for small h , then swiftly rising to a maximum at $h \approx 1.13$ before decreasing monotonically upon further increase of h , asymptotically to zero. The entanglement maximum *does not* occur at the quantum critical point. However, the derivative of the entanglement with respect to h *does* diverge at the critical point $h=1$, as shown in the inset. The slice at $r=1/2$ shows qualitatively similar behavior, except that it is finite (although small) at $h=0$, and starts out by decreasing to a shallow minimum of zero at $h = \sqrt{1-r^2}$. By contrast, the slice at $r=0$ (XX) starts out at $h=0$ at a maximum value of $1-2\gamma_C/(\pi \ln 2) \approx 0.159$. (where γ_C is the *Catalan* constant), the globally maximal value of the entanglement over the entire (r, h) plane. For larger h it falls monotonically until it vanishes at $h=1$, remaining zero for larger h .

Inspecting the behavior of entanglement, we find that along the line $r^2+h^2=1$ the entanglement density vanishes in the thermodynamic limit. In fact, this line exactly corresponds to the *crossover* boundary separating the O and F phases; the boundary can be characterized by a set of separable ground states [17] with all spins pointing in the direction

$$(x, y, z) = (\pm \sqrt{2r/(1+r)}, 0, \sqrt{(1-r)/(1+r)}). \quad (8)$$

Hence the total entanglement is at most of order unity, and thus of zero entanglement density. The entanglement density is also able to track the phase boundary ($h=1$) between the F and P phases. Associated with the quantum fluctuations accompanying the transition, the entanglement density shows a drastic variation across the boundary and the field derivative diverges all along $h=1$. The two boundaries separating the three phases coalesce at $(r, h)=(0, 1)$, i.e., the XX critical point. Figures 1 and 2 reveal all these features. The different nature of the two boundaries is reflected in the different behavior of entanglement across the boundary.

The singular behavior of the entanglement density (7) can be analyzed in the vicinity of the quantum critical line, and we find the asymptotic behavior (for $r \neq 0$)

$$\frac{\partial \mathcal{E}}{\partial h} \approx -\frac{1}{2\pi r \ln 2} \ln|h-1|, \quad \text{for } |h-1| \ll 1. \quad (9)$$

From the arbitrary- N results (6) we analyze the approach to the thermodynamic limit, in order to further understand connections with quantum criticality. We focus on the exponent ν , which governs the divergence at criticality of the correlation length: $L_c \sim |h-1|^{-\nu}$. To do this, we compare the divergence of the slope $\partial \mathcal{E}_N / \partial h$ (i) near $h=1$ (at $N=\infty$), given above, and (ii) for large N at the value of h for which the slope is maximal (viz., $h_{\max, N}$), i.e., $\partial \mathcal{E}_N / \partial h|_{h_{\max, N}} \approx 0.230 r^{-1} \ln N + \text{const.}$, obtained by analyzing Eq. (6) for various values of r . Then, noting that $(2\pi \ln 2)^{-1} \approx 0.2296$ and that the logarithmic scaling hypothesis [18] identifies ν

with the ratio of the amplitudes of these divergences, $0.2296/0.230 \approx 1$, we recover the known result that $\nu=1$.

Compared with $r \neq 0$ case, the nature of the divergence of $\partial\mathcal{E}/\partial h$ at $r=0$ belongs to a different universality class,

$$\frac{\partial}{\partial h}\mathcal{E}(0,h) \approx -\frac{\log_2(\pi/2)}{\sqrt{2\pi}} \frac{1}{\sqrt{1-h}}, \quad (h \rightarrow 1^-). \quad (10)$$

From this divergence, the scaling hypothesis, and the assumption that the entanglement density is intensive, we can infer the known result that the critical exponent $\nu=1/2$ for the XX model. In keeping with the critical features of the XY -model phase diagram, for any small but nonzero value of the anisotropy, the critical divergence of the entanglement derivative is governed by Ising-type behavior. It is only at the $r=0$ point that the critical behavior of the entanglement is governed by the XX universality class. For small r , XX behavior ultimately crosses over to Ising behavior.

As is to be expected, at finite N the two lowest states $|\Psi_0\rangle$ and $|\Psi_1\rangle$ featuring in Eq. (6) do not spontaneously break the Z_2 symmetry. However, in the thermodynamic limit they are degenerate for $h \leq 1$, and linear combinations are also ground states. The question then arises as to whether linear combinations that explicitly break Z_2 symmetry, i.e., the physically relevant states with finite spontaneous magnetization, show the same entanglement properties. In fact, we see from Eq. (6) that, in the thermodynamic limit, overlaps for both $|\Psi_0\rangle$ and $|\Psi_1\rangle$ are identical, up to the prefactors $f_N^{(0)}$ and $f_N^{(1)}$. These prefactors do not contribute to the entanglement density, and the entanglement density is therefore the same for both $|\Psi_0\rangle$ and $|\Psi_1\rangle$. It follows that, in the thermodynamic limit, the results for the entanglement density are insensitive to the replacement of a symmetric ground state by a broken-symmetry one, as is the case of concurrence [19].

CONCLUDING REMARKS

In summary, we have quantified the global entanglement of the quantum XY spin chain. This model exhibits a rich phase structure, the qualitative features of which are reflected by this entanglement. Perhaps the most interesting aspect is the divergence of the field derivative of the entanglement as the critical line ($h=1$) is crossed. Furthermore, the thermodynamic entanglement density vanishes on the disorder line ($r^2+h^2=1$). The structure of the entanglement surface over the entire phase diagram is surprisingly rich.

We close by pointing towards a deeper connection between the global entanglement and the correlations among quantum fluctuations. The maximal overlap $\Lambda_{\max}^2(\Psi)$ (1) can be decomposed in terms of correlation functions [20],

$$\frac{1}{2^N} + \max_{|\vec{r}|=1} \frac{N}{2^N} \left\{ \langle \vec{r} \cdot \vec{\sigma}_1 \rangle + \frac{1}{2} \sum_{j=2}^N \langle \vec{r} \cdot \vec{\sigma}_1 \otimes \vec{r} \cdot \vec{\sigma}_j \rangle + \dots \right\},$$

where translational invariance is assumed and the Cartesian coordinates of \vec{r} can be taken to be $(\sin \xi, 0, \cos \xi)$, and the average is taken with respect to the state $|\Psi\rangle$. The two-point correlations appearing in the decomposition are related to the concurrence, which also shows similar singular behavior [3]. It would be interesting to establish the connection between the global entanglement and correlations more precisely, e.g., by identifying which correlators are responsible for the singular behavior in the global entanglement and how they relate to the better known critical properties.

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- [20] To obtain this result one invokes the facts that: (i) A one-qubit pure state can be expressed in terms of density matrix as $(1 + \vec{r} \cdot \vec{\sigma})/2$, with $|\vec{r}|=1$; (ii) an N -qubit separable pure state is thus a product of N such terms (with generally different r 's).