

Universal subleading terms in ground-state fidelity from boundary conformal field theory

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The study of the (logarithm of the) *fidelity*, i.e., of the overlap amplitude, between ground states of Hamiltonians corresponding to different coupling constants provides a valuable insight on critical phenomena. When the parameters are infinitesimally close, it is known that the leading term behaves as $O(L^\alpha)$ (L system size), where α is equal to the spatial dimension d for gapped systems, and otherwise depends on the critical exponents. Here we show that when parameters are changed along a critical manifold, a subleading $O(1)$ term can appear. This term, somewhat similar to the topological entanglement entropy, depends only on the system's universality class and encodes nontrivial information about the topology of the system. We relate it to universal g factors and partition functions of (boundary) conformal field theory in $d=1$ and $d=2$ dimensions. Numerical checks are presented on the simple example of the XXZ chain.

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I. INTRODUCTION

Let $|\Psi(\lambda)\rangle$ denote the ground state (GS) of a system with Hamiltonian $H(\lambda)$ depending on a set of parameters λ . We define the ground-state fidelity associated to the pair of parameter points λ and λ' as follows:

$$\mathcal{F}(\lambda, \lambda') := |\langle \Psi(\lambda) | \Psi(\lambda') \rangle|. \quad (1)$$

This quantity might provide valuable different insight for systems exhibiting quantum phase transitions,¹⁻³ in particular when there are no obvious local order parameters, but some sort of topological order.⁴ The strategy advocated in Refs. 5 and 6 is differential geometric in nature. The parameters λ and λ' are chosen infinitesimally close to each other and one focuses on the leading term, the fidelity metric, or susceptibility χ_L , in the expansion of Eq. (1) as a function of $\delta\lambda := \lambda - \lambda'$: $\mathcal{F} \simeq 1 - \delta\lambda^2 \chi_L(\lambda)/2$. Critical lines can be identified as singular points of the fidelity metric (in the thermodynamical limit) (Ref. 5) or by its finite-size scaling.⁶ In particular, in Ref. 6, it has been shown that the leading finite-size term in the fidelity metric is always extensive for gapped systems; whereas, if λ is a critical point, its singular part obeys the scaling $\chi_L(\lambda)/L^d \sim L^{2z+d-2\Delta_\lambda}$, where z is the dynamical exponent and Δ_λ is the scaling dimension of the operator coupled with λ . For sufficiently relevant interactions, one sees that the fidelity metric can display a superextensive behavior that in turn is responsible for the fidelity drops observed at the quantum phase transition (QPT). On the other hand for marginal perturbations $\Delta_\lambda = d+z$, i.e., when one is moving along a manifold of critical points, the above scaling formula does not provide a definite prediction as besides $O(1)$; also loglike terms might appear. Accordingly, moving along a line of gapless points may not give rise to a detectable fidelity drop.^{6,7}

In this Brief Report, we shall demonstrate that the finite-size expansion of the GS fidelity (1), when λ and λ' are critical, features subleading terms of order one that depend only on the universality class of the considered model and

encodes nontrivial information about the system topology. Specifically, expanding the logarithm of Eq. (1) in the linear system size L , we find $\ln(\mathcal{F}) = -fL^d - f_b L^{d-1} + \dots + \ln g + \dots$. The bulk term f and the boundary terms f_b are nonuniversal and depend on the detail of the microscopic model. Instead, if present, the term of order one ($\ln g$) is free both from ultraviolet and infrared cutoffs and depends thus only on the low-energy theory and—as we will show—on the boundary conditions (BCs) on the base space. Given the results for the scaling of the fidelity susceptibility, a good situation for expecting $g \neq 1$ is when λ and λ' correspond to critical states. By establishing connections to boundary conformal field theories (BCFTs),^{8,9} we will show that this is indeed the case. We will compute g for two notable critical theories. We shall first discuss the case where $\Psi(\lambda)$ and $\Psi(\lambda')$ are ground states of the 1+1 free-boson theory. Results obtained for this continuum model will be checked, via exact diagonalization, against one of its many lattice versions: the critical XXZ Heisenberg chain. To give an example in higher dimension, we will consider the 2+1 quantum eight-vertex model.¹⁰ This model is an analog to the 1+1 free bosons, in that it also admits critical manifold with continuously varying critical exponents. Finally, extensions to the case where one of the parameters corresponds to a gapped phase will be discussed and potential connections with entanglement measures will be proposed.

II. FIDELITY AND THEORIES WITH BOUNDARY

We would like now to establish, on general grounds, a connection between the GS fidelity (1) and the partition function of a classical statistical-mechanics system with a boundary interface between regions with different couplings λ and λ' . This can be understood in terms of the usual correspondence between quantum mechanics in d dimensions and $d+1$ Euclidean statistical mechanics, where the imaginary-time length L_τ is taken to infinity to assure projection onto the ground state. In particular, one can prove that

$$\mathcal{F}(\lambda, \lambda') = \lim_{L_\tau \rightarrow \infty} \frac{Z(\lambda, \lambda')}{\sqrt{Z(\lambda)Z(\lambda')}}. \quad (2)$$

Here $Z(\lambda)$ is the partition function of the corresponding homogeneous system with imaginary-time axis of length $2L_\tau$, while $Z(\lambda, \lambda')$ is the partition function in the same system with one interface and couplings λ and λ' , respectively, at either side of the interface. Assume that the corresponding Euclidean model is described by a transfer matrix $T(\lambda)$. Then to prove Eq. (2) simply note that, for $L_\tau \rightarrow \infty$, the quantum ground state is given by $|\Psi(\lambda)\rangle = T(\lambda)^{L_\tau} |\Phi\rangle / \sqrt{Z(\lambda)}$ with $|\Phi\rangle$ not orthogonal to the ground state. Here $Z(\lambda) = \langle \Phi | T(\lambda)^{2L_\tau} | \Phi \rangle$ is the partition function of a homogeneous system of imaginary-time length $2L_\tau$ and boundary conditions, which depend on the quantum model and on $|\Phi\rangle$. Note also that $Z(\lambda) = Z(\lambda, \lambda)$. For instance, for $d=1$ and periodic boundary conditions, $Z(\lambda, \lambda')$ is a partition function on an infinitely long cylinder split into two regions with different couplings λ and λ' .

The sort of inhomogeneous system we have in mind is often better seen as a system with a *boundary*. This is easily done by folding. Instead of having fields on both sides of the interface (where the scalar product is evaluated), one can consider fields only on the left side with coordinate $x_\tau \leq 0$ and fold the fields living on $x_\tau > 0$ into the left domain by introducing new species. The problem then becomes a boundary one for a theory with double the number of species and some BC at $x_\tau = 0$.

III. BOUNDARIES AND IMPURITIES

Let us for the moment focus on one-dimensional quantum systems $d=1$. By again using the standard mapping to the two-dimensional (2D) classical system, we have $\ln Z(\lambda, \lambda') = \ln z_L - LL_\tau f$ where f is a nonuniversal bulk term and $\ln z_L$ is a term associated with the boundary itself. One can now go back to a $d=1$ quantum point of view but this time with space along the x_τ axis and L is interpreted as the inverse temperature β . One can write the free energy associated with the boundary as $Lf_b := -\ln z_L = Lu - s$. In the critical case for $L \rightarrow \infty$, the latter term gives rise to a degeneracy $O(1)$ factor $g = e^s$, which is, by scaling, independent of L .¹¹ This boundary degeneracy—or equivalently s , often referred to as the boundary entropy—has played a major role in the analysis of BCFTs. It has been proven in particular that it is *universal* and thus depends only on the universality class of the critical theory and the type of conformal boundary condition:¹² for instance, for the Ising universality class with free boundary conditions $g=1$, while for fixed boundary conditions $g=\frac{1}{2}$. Note that the issue of the scalar product of ground states occurred in this context very early on through the considerations of the Anderson¹³ orthogonality catastrophe.

IV. FIDELITY AND BCFT

We consider first the archetypal problem of a two-dimensional free boson with two different values of the coupling constants. We write the action as $S = \sum_{i=1}^2 \frac{\lambda_i}{2} \int_{D_i} (\partial_\mu \varphi_i)^2$, where $D_{1,2} = R^\pm \times [0, L]$. The only condition we put at the “interface” $x_\tau = 0$ is that the fields are continuous (this corre-

sponds to taking the scalar product of wave functions).

We first recall that for a single free boson with coupling λ , compactified on a circle $\varphi \equiv \varphi + 2\pi$, the g factors are $g_D = 2^{-1/2}(\pi\lambda)^{-1/4}$ and $g_N = (\pi\lambda)^{1/4}$, for Dirichlet (D) and Neumann (N) boundary conditions, respectively. Assuming now both bosons compactified on a circle of circumference 2π , and using the equations of motion to fold the system in half, gives rise to an equivalent problem of *two orthogonal* species of bosons with the same compactification radius; one seeing N boundary conditions with coupling $\lambda_N = \lambda_1 + \lambda_2$, the other seeing D boundary conditions with coupling $\lambda_D = \frac{\lambda_1 \lambda_2}{(\lambda_1 + \lambda_2)}$. The total g factor is thus

$$g = g_D(\lambda_D)g_N(\lambda_N) = \frac{1}{\sqrt{2}} \left(\frac{\lambda_N}{\lambda_D} \right)^{1/4} = \sqrt{\frac{\lambda_1 + \lambda_2}{2\sqrt{\lambda_1 \lambda_2}}}. \quad (3)$$

Of course we recover that $g=1$ when $\lambda_1 = \lambda_2$. Moreover, because one field sees D and the other N , it is clear that in fact the final result does not depend on the compactification radius (and is homogeneous in λ 's).

It is instructive to recover this result via a direct computation (see also Ref. 14). First note that in this noninteracting case, one can show that $Z(\lambda_1, \lambda_2) = Z(\frac{\lambda_1 + \lambda_2}{2})$. Second, since all modes contribute identically to the ratio of partition functions (one is simply dealing with Gaussians), the full fidelity is $F(\lambda_1, \lambda_2) = \prod_{k \neq 0} \sqrt{\frac{2\sqrt{\lambda_1 \lambda_2}}{\lambda_1 + \lambda_2}}$ where the product is taken over the Brillouin zone. This means $L-1$ modes—the zero mode is missing—and thus we have $F = e^{-fL}g$, with g the same as Eq. (3) of course. While in this calculation f , the bulk term is identical to $\ln g$, we emphasize that, unlike g , f is not universal and depends in general on the details of the model.

It is interesting to check our prediction against some quick numerical calculations. We thus consider XXZ spin chains defined on a circle of length L with anisotropy Δ . Going over the standard fermionization and bosonization steps¹⁵ and matching the results with the Bethe ansatz, one finds that the continuum limit corresponds to

$$\lambda = \frac{1}{2\pi^2} [\pi - \arccos \Delta] \equiv \frac{1}{4\pi K}. \quad (4)$$

Here we used the conventions where the spin σ_i^z of the spin chain is described by $\partial_x \varphi$, and K is an alternative coupling constant often used in the condensed-matter literature. In Fig. 1 we report the results obtained for the lattice XXZ model together with the theoretical predictions based on BCFT Eqs. (3) and (4); the agreement is very good. We note that the g factor does depend on boundary conditions. For instance, it is possible, by breaking the $O(2)$ symmetry of the XXZ chain, to induce antiperiodic conditions on the fields ϕ in the x direction; a quick calculation shows then that the term $O(1)$ in the fidelity disappears, i.e., $g=1$ in this case, again in agreement with our numerics.

This kind of calculation admits many variants. Instead of having both Hamiltonians involved in the fidelity critical, we can decide to have only one. In this case, the massive side induces a conformal boundary condition on the critical side in the calculation of $Z(\lambda, \lambda')$, and the term of $O(1)$ in the fidelity is given by the corresponding g factor. We can simulate this situation by turning again to the XXZ model, but this

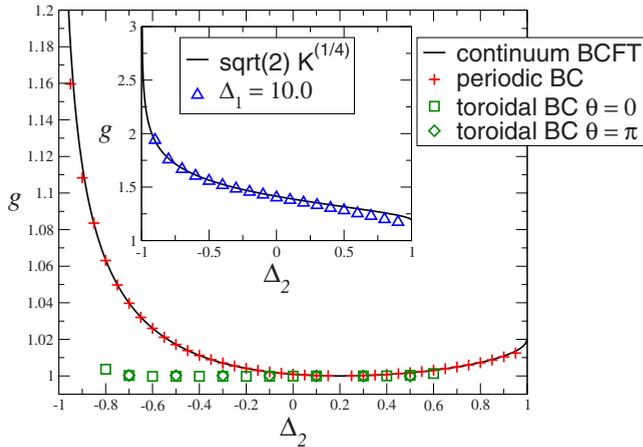


FIG. 1. (Color online) Universal g factor in the fidelity for the XXZ model together with BCFT predictions. The fidelity is computed between ground states with different anisotropies $\Delta_{1,2}$ in the critical region ($|\Delta_{1,2}| < 1$), and we fixed $\Delta_1 = 0.20$. Plus signs are extrapolations of data obtained with Lanczos diagonalization on very small lattices (length $L \leq 22$) and periodic boundary conditions. These data agree perfectly with BCFT predictions [Eq. (3)] together with Eq. (4). Instead, toroidal BCs given by $\sigma_{L+1}^{\pm} = e^{\pm i\theta} \sigma_1^{\pm}$ and $\sigma_{L+1}^z = -\sigma_1^z$ induce antiperiodic BCs on the field ϕ and consequently there is no term of order one in this case (i.e., $g = 1$). Note that such BC [they belong to conjugacy class (IV) of Ref. 16] breaks the conservation of total magnetization. In the inset, the fidelity is computed when one ground state is critical and the other is deep; the massive (Néel) phase $\Delta_1 \gg 1$. Solid line gives the BCFT prediction. The small discrepancy around $\Delta_2 \approx 1$ is due to finite-size effects which are more pronounced near the Kosterlitz-Thouless point $\Delta = 1$.

time choosing one of the Δ 's to be much greater than one. In this case, the massive side is in the ordered phase, corresponding to two possible ground states, described in terms of spins as $\sigma_i^z = (-1)^i$ and $\sigma_i^z = (-1)^{i+1}$, respectively. Each of these ground states induces Dirichlet boundary conditions for the field ϕ on the massless side. For each of these Dirichlet cases, we have $g_D = K^{1/4}$. Meanwhile, the massive side is a superposition of the two orthogonal ground states with equal coefficients $\frac{1}{\sqrt{2}}$, so we get in the end $g = 2 \times \frac{1}{\sqrt{2}} \times K^{1/4} = \sqrt{2} K^{1/4}$. Again these predictions are well confirmed by finite-size Lanczos calculation (see inset of Fig. 1).¹⁶

V. TERMS OF ORDER ONE IN THE 2+1 CASE: THE QUANTUM EIGHT-VERTEX MODEL

We turn to consider $O(1)$ terms in the GS fidelity of 2+1 models whose quantum critical points have dynamical critical exponent $z=2$. For these models at criticality, ground-state functionals are conformal invariant in the 2D physical space, and equal-time correlators coincide with correlations in a 2D conformal field theory (CFT). We will now show that the fidelity involves universal terms of $O(1)$ in this case as well and that this time they are related to partition functions of CFTs on Riemann surfaces.

To make things concrete, let us specialize to the 2+1 analog of the free boson—the quantum Lifshitz model—for which a convenient lattice realization is provided by the

quantum vertex model.¹⁰ The Hilbert space of this model is spanned by an orthonormal basis $\{|C\rangle\}$ in a one-to-one correspondence with the configurations \mathcal{C} of the classical eight-vertex model. The Hamiltonian is defined on a two-dimensional lattice (say a rectangle $L_1 \times L_2$ with certain BCs) and has the form $H = \sum_i Q_i$, with Q_i positive operators, chosen such that H annihilates the following state: $|\Psi(c^2)\rangle = \sum_{\{C\}} c^{\hat{n}_c(C)} |C\rangle / \sqrt{Z_{2D}(c^2)}$, where we have chosen, for simplicity, $a=b=1$ and $d=0$ so the only remaining parameter is c , which is the equivalent here of λ in Secs. I–IV (see Ref. 17 for details and conventions on the eight-vertex model). $\hat{n}_c(C)$ are the number operators for the c -type vertices, for the configuration \mathcal{C} , and the normalization factor is given by the partition function of the classical eight-vertex model defined on the same geometry of the quantum problem $Z_{2D}(c^2) = \sum_{\{C\}} c^{2\hat{n}_c(C)}$. The ground-state phase diagram for the quantum model is identical to the classical one, but given in terms of c^2 . The scalar product of ground states is given by

$$\langle \Psi | \Psi' \rangle = \frac{Z_{2D}(cc')}{\sqrt{Z_{2D}(c^2)Z_{2D}[(c')^2]}}. \tag{5}$$

As usual we are interested in the infinite volume limit $L_1, L_2 \rightarrow \infty$. Now consider the case where the weights obey $c^2 \leq 2$, $(c')^2 \leq 2$, and $|cc'| \leq 2$. In that case, we are dealing with partition functions of two-dimensional critical vertex models, which are described in the continuum limit by Euclidian free bosons in 2D.⁸ With *periodic boundary conditions*, for instance, these partition functions behave as $Z_{2D} = e^{-fL_1L_2} Z_{\text{CFT}}(L_1/L_2)$, where Z_{CFT} is the modular invariant partition function of the conformal invariant field theory.

The important point is that the scalar product (5) will have a term behaving like an exponential of the area $\exp\{-L_1L_2\{f(cc') - f(c^2)/2 - f[(c')^2]/2\}\}$ and a term of order one $Z_{\text{CFT}}(\Lambda)Z_{\text{CFT}}^{-1/2}(\lambda)Z_{\text{CFT}}^{-1/2}(\lambda')$, where λ is formally the same coupling constant as before [see Eq. (4)] and Λ is the coupling associated with the product $cc' : \Delta = \frac{c^4}{2} - 1 = -\cos 2\pi^2\lambda, \frac{(c')^4}{2} - 1 = -\cos 2\pi^2\lambda', \frac{(cc')^2}{2} - 1 = -\cos 2\pi^2\Lambda$. The conformal partition function itself reads as $Z_{\text{CFT}}(\lambda) = [\eta(q)\eta(\bar{q})]^{-1} \mathcal{I}(\lambda)$, where $q = \bar{q} = \exp(-2\pi L_1/L_2)$ parametrizes the torus, $\mathcal{I}(\lambda) = \sum_{n,m=-\infty}^{\infty} q^{1/4(n/\sqrt{2\pi\lambda} + m/\sqrt{2\pi\lambda})^2} \bar{q}^{1/4(n/\sqrt{2\pi\lambda} - m/\sqrt{2\pi\lambda})^2}$ and $\eta(q) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n)$.⁸ While the prefactor and the η terms disappear in the ratio, the instanton sums \mathcal{I} remain, leading to a rather complicated expression $\mathcal{I}(cc') / \sqrt{\mathcal{I}(c^2)\mathcal{I}[(c')^2]}$ for the term $O(1)$. An example of the behavior of this term is given in Fig. 2.

Similarly as for the 1+1 case, the term of $O(1)$ depends heavily on the *topology* and boundary conditions of the base space. One can, for instance, imagine defining the 2D quantum models on higher genus Riemann surfaces¹⁸ or on surfaces with boundaries and curvature. To give a very simple example, the logarithm of the free-boson partition function on a rectangle of sizes L_1 and L_2 with *free boundary conditions* (either D on all sides or N on all sides) is given by $\ln Z_{2D} = f_1 L_1 L_2 + f_2(L_1 + L_2) + \frac{1}{4} \ln L_2 - \frac{1}{2} \ln[\eta(q)]$, where f_1 and f_2 are nonuniversal terms. The logarithmic term meanwhile is universal and comes from the general formula for the free energy of a critical region A of linear size $L_2 \propto L_1$, Euler characteristic χ , and a boundary with a discrete set of singu-

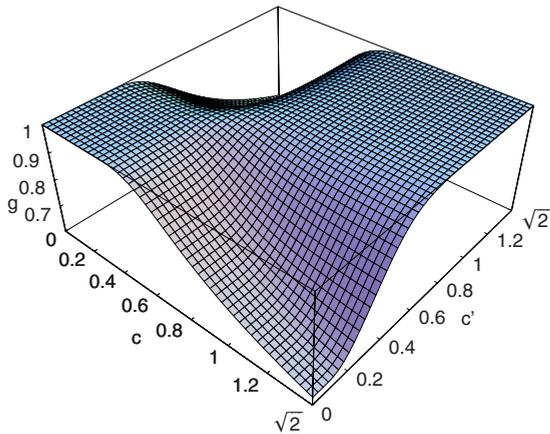


FIG. 2. (Color online) Universal g factor in the fidelity of the quantum eight-vertex model with periodic BC when all the theories are in the disordered region, i.e., $c^4 < 4$, $(c')^4 < 4$, and $(cc')^2 < 4$. We fixed the ratio $L_1/L_2=1$. The g factor is smooth at the border of the region $c, c' \rightarrow 0$, c , and $c' \rightarrow \sqrt{2}$.

larities. Now, when forming the ratio in Eq. (5), the $O(1)$ term cancels out exactly. It follows that if we were to calculate the scalar product of ground states in this situation, there would be just no term of order one.

VI. CONNECTIONS WITH QUANTUM ENTANGLEMENT

Before concluding we would like briefly to comment about the possible connections between the fidelity approach pursued in this Brief Report and quantum entanglement. First, let us notice that BCFT arguments have been used in

the calculations by Kitaev and Preskill to motivate their expression for the topological entanglement entropy (TEE).¹⁹ Their derivation shows that TEE is a $O(1)$ subleading universal term that is strictly analogous to those for the fidelity in this Brief Report. This is even more apparent if one expresses the degeneracy g factors in terms of the modular S matrix of the CFT (Ref. 11) and compares it with the TEE $S_{\text{topo}} = \log|S_{11}^a|$. Moreover there is a striking similarity between our formulas for the logarithm of the fidelity in Sec. V and formulas in Ref. 20 for the entanglement entropy at conformal quantum critical points: $S = \log[Z_F / (Z_D^A Z_D^B)]$. Both involve logarithms of conformal partition functions, and it is clear that by taking the ground states of the quantum vertex model with different couplings in different regions, one could obtain entanglement entropy through a term of $O(1)$ in the fidelity. How general and useful this observation might be is an open question.

VII. CONCLUSIONS

Using BCFT techniques, we have shown that the fidelity between critical states contains a term of order $O(1)$ which depends only on the universality class and on the topology of the base space. As such, it bears similarity to the topological entanglement entropy or the central charge appearing in the expansion of the ground-state energy. The use of methods of CFT in information theory should go much beyond the consideration of these terms of $O(1)$. For example, the same techniques can be used to extract information about the Loschmidt echo.²¹

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