# Quantum Critical Scaling of the Geometric Tensors

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Berry phases and the quantum-information theoretic notion of *fidelity* have been recently used to analyze quantum phase transitions from a geometrical perspective. In this Letter we unify these two approaches showing that the underlying mechanism is the critical singular behavior of a complex tensor over the Hamiltonian parameter space. This is achieved by performing a scaling analysis of this quantum geometric tensor in the vicinity of the critical points. In this way most of the previous results are understood on general grounds and new ones are found. We show that criticality is not a sufficient condition to ensure superextensive divergence of the geometric tensor, and state the conditions under which this is possible. The validity of this analysis is further checked by exact diagonalization of the spin-1/2 *XXZ* Heisenberg chain.

*Introduction.*—Phase transitions at zero temperature are dramatic changes in the ground-state (GS) properties of a system driven by quantum fluctuations. This phenomenon, known as quantum phase transition (QPT), is due to the interplay between different orderings associated with the competing terms in the system's Hamiltonian [1]. Traditionally such a problem is addressed by resorting to notions like order parameter and symmetry breaking, i.e., the Landau-Ginzburg paradigm [2]. In the last few years a big effort has been devoted to the analysis of QPTs from the perspective of quantum information [3], the main tool being the study of different entanglement measures [4].

More recently an approach to QPTs based on the quantum-information concept of *fidelity* has been put forward [5,6]. The strategy there is differential-geometric and information-theoretic in nature: GSs associated to infinitesimally close parameters are compared; i.e., their overlap is evaluated. The intuition behind this is extremely simple: at QPTs, even the slightest move results in a major difference in some of the system's observables, in turn this has to show up in the degree of orthogonality, i.e., fidelity between the corresponding GSs. Systems of quasifree fermions have been analyzed [7,8] as well as QPTs in matrix-product states [9]. Finite-temperature extensions have also been considered, showing the robustness of the approach against mixing with low excited states [10]. Remarkably, the fidelity analysis has been successfully carried over for the superfluid-insulator transition of the Hubbard model [11]; this suggests that this framework, besides its conceptual appeal, can have some practical relevance even for fully interacting systems where a simple description is not possible.

In Ref. [12] it has been shown that the fidelity approach can be better understood in terms of a Riemannian metric tensor *g* defined over the parameter manifold $\mathcal{M}$. Loosely speaking the singularities developed by *g* in the thermodynamic limit correspond to QPTs [12]. Even for finite-size

systems, critical points have a markedly distinct (finite-size scaling) behavior from the regular ones; in all the examples studied so far this difference amounts to an enhanced orthogonalization ratio as a function of the system's size at the QPTs. Another intriguing relation between QPTs and geometrical objects, i.e., Berry phases, was suggested in Refs. [13,14]. There it was argued that loops in the parameter space, encircling a critical line give rise to a non-zero GS Berry phase even for an arbitrary small loop size. This fact indicates that at the critical points the curvature of the Berry connection should display some sort of singularity [14].

In this Letter we shall show that these two approaches share the same origin and can be therefore unified. We will perform a scaling analysis that allows one to understand, from a single perspective, most of the results obtained so far in the fidelity approach and to investigate somewhat unexpected new ones.

*Geometric tensors.*—We now lay down the formal setting. For each element $\lambda$ of the parameter manifold $\mathcal{M}$ there is an associated quantum Hamiltonian $H(\lambda) = \sum_{n=0}^{\dim \mathcal{H}-1} E_n(\lambda)|\Psi_n(\lambda)\rangle\langle\Psi_n(\lambda)|$, $(E_{n+1} \geq E_n)$ acting over a finite-dimensional state-space $\mathcal{H}$; the mapping $\lambda \rightarrow H(\lambda)$ is assumed to be smooth. If $|\Psi_0(\lambda)\rangle$ denotes the unique GS of $H(\lambda)$ then one has the mapping $\Psi_0 : \mathcal{M} \rightarrow \mathcal{H} : \lambda \rightarrow |\Psi_0(\lambda)\rangle$. More properly we will consider this map as a function valued in the projective space $P\mathcal{H}$ of rays. If the spectral gap of $H(\lambda)$ above the GS is bounded away from zero over $\mathcal{M}$ then $\Psi_0$ is smooth [15]. The projective Hilbert space is the base manifold of a $U(1)$ fiber bundle [16] and it is equipped with a complex metric given by $g(u, v) = \langle u, (1 - |\Psi\rangle\langle\Psi|)v\rangle$ ($u$ and $v$ denote tangent vectors in $|\Psi\rangle\langle\Psi|$). Pulling this metric back to $\mathcal{M}$ by $\Psi_0$, i.e., evaluating it on vectors of the form $d/dt\Psi_0[\lambda(t)]$, one obtains the complex Hermitian tensor

$$Q_{\mu\nu} := \langle\partial_\mu\Psi_0|\partial_\nu\Psi_0\rangle - \langle\partial_\mu\Psi_0|\Psi_0\rangle\langle\Psi_0|\partial_\nu\Psi_0\rangle. \quad (1)$$

Here the indices $\mu$ and $\nu$ are labeling the coordinates of $\mathcal{M}$, i.e., $\mu, \nu = 1, \ldots, \dim \mathcal{M}$. This quantity is the quantum geometric tensor (QGT) [17], both its real and imaginary parts have a relevant physical meaning.

The real part $g_{\mu\nu} := \Re Q_{\mu\nu}$ is a *Riemannian* (real) metric tensor over $\mathcal{M}$ which defines the line element as $ds^2 = \sum_{\mu\nu} g_{\mu\nu} d\lambda_\mu d\lambda_\nu$. This metric has been shown to provide the leading term in the expansion of the fidelity between two GSs associated to slightly different Hamiltonians [12]. More precisely if $\mathcal{F}(\lambda, \lambda') := |\langle \Psi_0(\lambda), \Psi_0(\lambda') \rangle|$ is the fidelity then $\mathcal{F}(\lambda, \lambda + \delta\lambda) \approx 1 - \delta\lambda^2/2 g(d\Psi_0, d\Psi_0) = 1 - ds^2/2$ [i.e., $g_{\mu\nu}$ is the Hessian matrix of $\mathcal{F}(\lambda, \lambda')$ as a function of $\lambda'$ in $\lambda = \lambda'$]. The meaning of this distance function between parameters should be obvious: it is the Hilbert-space one between the corresponding GSs. This latter quantifies the operational distinguishability of two states [18]; therefore, even the induced metric $g$ conveys a definite information-theoretic meaning [12]. The fact that at the QPTs $g$ exhibits singularities is consistent with the intuition that at critical points one has a major change in the GS structure, i.e., it becomes "more different", and makes it quantitative. Now we consider the imaginary part of (1) $F_{\mu\nu} := \Im Q_{\mu\nu}$. Since the terms $\langle \Psi | \partial_\nu \Psi \rangle$ are—from normalization—purely imaginary, one finds $\Im Q_{\mu\nu} = \Im \langle \partial_\mu \Psi | \partial_\nu \Psi \rangle = \langle \partial_\mu \Psi | \partial_\nu \Psi \rangle - \langle \partial_\nu \Psi | \partial_\mu \Psi \rangle = \partial_\mu A_\nu - \partial_\nu A_\mu$, where $A_\mu := \langle \Psi | \partial_\nu \Psi \rangle$ is, for $|\Psi\rangle = |\Psi_0(\lambda)\rangle$, the Berry adiabatic connection [19]. From this one sees that $\Im Q_{\mu\nu}$ is nothing but the curvature 2-form, responsible for the appearance of the Berry geometrical phase [19]. Of course for systems with real GS $F$ is zero and the QGT coincides with its real part $g$.

The QGT (1) can be cast in a way useful for later derivations as well as to decrypt its physical meaning. By inserting in Eq. (1) the spectral resolution $\mathbb{1} = \sum_{n=0}^{\dim \mathcal{H}-1} |\Psi_n(\lambda)\rangle\langle\Psi_n(\lambda)|$ and differentiating the eigenvalue equation $H(\lambda)|\Psi_0(\lambda)\rangle = E_0(\lambda)|\Psi_0(\lambda)\rangle$, one finds the identity

$$Q_{\mu\nu} = \sum_{n \neq 0} \frac{\langle \Psi_0(\lambda) | \partial_\mu H | \Psi_n(\lambda) \rangle \langle \Psi_n(\lambda) | \partial_\nu H | \Psi_0(\lambda) \rangle}{[E_n(\lambda) - E_0(\lambda)]^2}. \quad (2)$$

This expression clearly suggests that at the critical points, where one of the $\varepsilon_n(\lambda_c) = E_n(\lambda_c) - E_0(\lambda_c) \geq 0$ vanishes in the thermodynamic limit, the QGT might show a singular behavior. This heuristic argument is the same one proposed in [12] for the Riemannian tensor $g_{\mu\nu}$ and for the Berry curvature $F_{\mu\nu}$ in [14]. One of the aims of this Letter is to establish this argument on more firm grounds. A similar scaling analysis in connection with local measures of entanglement at QPTs has been presented in [20].

We would like first to demonstrate an inequality useful to establish a connection between the tensor $g$ and QPTs. We consider a system with size $L^d$ ($d$ is the spatial dimension). Since $Q(\lambda)$ is a Hermitean non-negative matrix one has $|Q_{\mu\nu}| \leq \|Q\|_\infty = \langle \phi | Q | \phi \rangle$, where $|\phi\rangle = (\phi_\mu)_{\mu=1}^{\dim \mathcal{M}}$

denotes the eigenvector of $Q$ corresponding to the largest eigenvalue. We set $\delta H = \sum_\mu (\partial_\mu H) \phi_\mu$, then from Eq. (2) and the above inequality

$$|Q_{\mu\nu}| \leq \sum_{n>0} \varepsilon_n^{-2} |\langle \Psi_0 | \delta H | \Psi_n \rangle|^2 \leq \varepsilon_1^{-2} \sum_{n>0} |\langle \Psi_0 | \delta H | \Psi_n \rangle|^2$$
$$= \varepsilon_1^{-2} (\langle \delta H \delta H^\dagger \rangle - |\langle \delta H \rangle|^2), \quad (3)$$

where the angular brackets denote the average over $|\Psi_0(\lambda)\rangle$. Now we assume that the operator $\delta H$ is a local one, i.e., $\delta H = \sum_j \delta V_j$; then the last term in Eq. (3) reads $\sum_{i,j} (\langle \delta V_i \delta V_j^\dagger \rangle - \langle \delta V_i \rangle \langle \delta V_j^\dagger \rangle)$. If the GS is translationally invariant this last quantity can be written as $L^d \sum_r K(r) := L^d K$, where $K(r) := \langle \delta V_i \delta V_{i+r}^\dagger \rangle - \langle \delta V_i \rangle \langle \delta V_{i+r}^\dagger \rangle$ is independent of $i$. For gapped systems, i.e., $\varepsilon_1(\infty) := \lim_{L\to\infty} \varepsilon_1(L) > 0$, the correlation function $G(r)$ is rapidly decaying [21] and therefore $K$ is finite and independent on the system size. Using (3), it follows that for these noncritical systems $|Q_{\mu\nu}|$ cannot grow, as a function of $L$, more than extensively. Indeed, one has that $\lim_{L\to\infty} |Q_{\mu\nu}|/L^d \leq K \varepsilon_1^{-2}(\infty) < \infty$. Conversely, if $\lim_{L\to\infty} |Q_{\mu\nu}|/L^d = \infty$, i.e., $|Q_{\mu\nu}|$ grows superextensively, then either $\varepsilon_1(L) \to 0$ or $K$ cannot be finite. In both cases the system has to be gapless [22]. Summarizing: a superextensive behavior of any of the components of $Q$ for systems with local interaction implies a vanishing gap in the thermodynamic limit.

This sort of behavior has been observed in all the systems analyzed in Refs. [5–9] and does amount to the critical fidelity drop at the QPTs. As we will show in the next section, in general the converse result, i.e., QPT → superextensive growth of $ds^2(L)$, does not hold true: $Q_{\mu\nu}/L^d$ can be finite in the thermodynamic limit even for gapless systems. In order to demonstrate this fact we now move to a representation of $Q_{\mu\nu}$ in terms of suitable correlation functions. This key move is an extension of the results of You, Li, and Gu [23], for the so-called fidelity susceptibility, to the whole QGT.

*Correlation function representation.*—Let us consider the following imaginary time (connected) correlation functions

$$G_{\mu\nu}(\tau) = \theta(\tau)(\langle \partial_\mu H(\tau) \partial_\nu H(0) \rangle - \langle \partial_\mu H(0) \rangle \langle \partial_\nu H(0) \rangle), \quad (4)$$

where $X(\tau) := e^{\tau H} X e^{-\tau H}$. Using again the spectral resolution of the identity associated to $H(\lambda)$ one finds $G_{\mu\nu}(\tau) = \theta(\tau) \sum_{n>0} e^{-\varepsilon_n(\lambda)\tau} X_{n\mu} X_{n\nu}^*$, where $X_{n\mu} := \langle \Psi_0(\lambda) | \partial_\mu H | \Psi_n(\lambda) \rangle$. Notice that if $H(\lambda) = H_0 + \lambda V$ then $G(\tau)$ is nothing but the dynamic response function associated to the "perturbation" $V$. We now move to the frequency domain $\tilde{G}_{\mu\nu}(\omega) = \int_{-\infty}^{+\infty} d\tau e^{-i\omega\tau} G_{\mu\nu}(\tau) = \sum_{n>0} X_{n\mu} X_{n\nu}^* (i\omega + \varepsilon_n)^{-1}$. By comparing this equation with (2) it is immediate to see that

$$Q_{\mu\nu} = -i \frac{d}{d\omega} \tilde{G}_{\mu\nu}(\omega)\Big|_{\omega=0} = \int_{-\infty}^{+\infty} d\tau \tau G_{\mu\nu}(\tau). \quad (5)$$

This equation is an integral representation of the QGT in

terms of the (imaginary time) correlation functions of the operators $\partial_\mu H$. Equation (4) is remarkable in that it connect the tensors $g_{\mu\nu}$ and $F_{\mu\nu}$ directly (and nonperturbatively) to the dynamical response of the system to the interactions $\partial_\mu H$'s. In this way geometrical and information-theoretic objects $F$ and $g$ are expressed in terms of standard quantities in response theory and their physics content is so further clarified. Equations (4) and (5) provide the starting point for our scaling analysis.

*Scaling behavior.*—First we assume that the operators $\partial_\mu H$ are local ones, i.e., $\partial_\mu H = \sum_x V_\mu(x)$. We also rescale the QGT (1) by the system size $Q_{\mu\nu} \rightarrow q_{\mu\nu} = L^{-d} Q_{\mu\nu}$ in order to obtain well-defined quantities in the thermodynamic limit. Now we consider the scaling transformations $x \rightarrow \alpha x$, $\tau \rightarrow \alpha^\zeta \tau$, $(\alpha \in \mathbf{R}^+)$. Assuming that, in the vicinity of the critical point $\lambda_c$, the operators $V_\mu$ have well-defined scaling dimensions [24] one has $V_\mu \rightarrow \alpha^{-\Delta_\mu} V_\mu$; these relations along with Eqs. (4) and (5) imply

$$q_{\mu\nu} \rightarrow \alpha^{-\Delta^Q_{\mu\nu}} q_{\mu\nu}; \qquad \Delta^Q_{\mu\nu} := \Delta_\mu + \Delta_\nu - 2\zeta - d. \quad (6)$$

For simplicity we assume now that there is only one driving parameter $\lambda$ and drop the indices $\mu$ and $\nu$ in $\Delta^Q_{\mu\nu}$.

If $\xi$ is the correlation length one has $\xi = |\lambda - \lambda_c|^{-\nu}$ (here $\nu$ is the correlation length critical exponent) and, if $\Delta_\lambda$ is the scaling dimension of the driving parameter $\lambda$, $\nu = \Delta_\lambda^{-1}$. Putting all this together and following standard arguments in scaling analysis one obtains that (in the off-critical region, $L \gg \xi$) the singular part of the—intensive—QGT behaves as

$$q_{\mu\nu}(\lambda \approx \lambda_c) \sim |\lambda - \lambda_c|^{\Delta_Q/\Delta_\lambda}. \quad (7)$$

Instead, at the critical point, i.e., $\xi = \infty$, where the only length scale is provided by the system size itself, one gets

$$q_{\mu\nu}(\lambda = \lambda_c) \sim L^{-\Delta_Q}. \quad (8)$$

Equations (7) and (8) represent the main result of this Letter. From Eq. (7) one sees that close to the critical point the QGT $q_{\mu\nu}$ is diverging for $\Delta_Q/\Delta_\lambda < 0$; on the other hand, when one is sitting exactly at the critical point one finds that, besides an extensive contribution coming from the regular part, the singular part contributes to $Q_{\mu\nu}$ in a manner which is (i) superextensive if $\Delta_Q < 0$, (ii) extensive if $\Delta_Q = 0$, and (iii) subextensive for $\Delta_Q > 0$. Hence, we observe that $q_{\mu\nu}$ can be finite at the critical point, even in a gapless system, provided $\Delta_Q > 0$. An explicit example of this phenomenon will be discussed in the sequel; before doing that we show that this analysis allows one to understand in a unified manner the results found for quasifree fermionic models in [7,8]. In quasifree fermionic models the most relevant operator admissible has a scaling dimension equal to one; therefore, from Eqs. (7) and (8) one finds, close to $\lambda_c$, $Q_{\mu\nu} = g_{\mu\nu} \sim L|\lambda - \lambda_c|^{-1}$ and $Q_{\mu\nu} \sim L^2$ at the QPT. Notice that if $\Delta_Q < -1$ one expects superquadratic behavior.

*XXZ chain.*—We provide now a further test for the ideas presented in this Letter: the $S = 1/2$ *XXZ* Heisenberg

chain. The model is defined by $H = J\sum_i[S^x_i S^x_{i+1} + S^y_i S^y_{i+1} + \lambda S^z_i S^z_{i+1}]$. It is well known (see, e.g., [25]) that in the regime $\lambda \in (-1, 1)$ the model is in the universality class of a $c = 1$ conformal field theory ($d = \zeta = 1$) displaying gapless excitations and power low correlations. For $\lambda > 1$ the model enters a phase with Ising-like antiferromagnetic order and a nonzero gap. Finally, the isotropic point $\lambda = 1$ is a Berezinskii-Kosterlitz-Thouless transition point. The low energy effective continuum theory is given by the sine-Gordon model: $H = \int d^2x\{\frac{u}{2}[\Pi^2 + (\partial_x\Phi)^2] - \frac{v\lambda}{(a\pi)^2}\cos(\sqrt{16\pi K}\Phi)\}$, where $v$ is the bare Fermi velocity, $u$ the renormalized one, $K$ is related to the compactification radius of the field $\Phi$, and $a$ is the lattice spacing (we use the notations of [25]).

We now analyze the behavior of the fidelity when the anisotropy parameter $\lambda$ is varied. Correspondingly, we are interested in the operator $V(x) = S^z_x S^z_{x+1}$ and its scaling exponents. In the continuum limit the operator $V(x)$ contributes with a marginal operator—$(\partial_x\Phi)^2$—with scaling exponent $\Delta_V = 2$, plus a term which is precisely the cosine in the sine-Gordon Hamiltonian. The cosine term is irrelevant for $|\lambda| < 1$, marginal at $\lambda = 1$ and relevant for $\lambda > 1$, where it is responsible for the opening of a mass gap. Its scaling dimension is precisely equal to $4K$. The parameter $K$ can be fixed by the long distance asymptotic of the correlation functions obtained by Bethe ansatz, and one gets, for $\lambda \in (-1, 1]$ $K = \pi/2(\pi - \arccos(\lambda))^{-1}$.
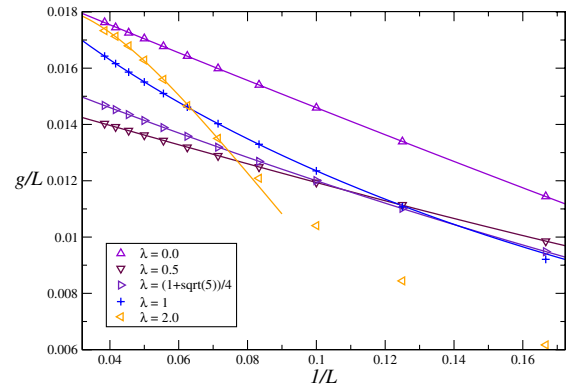


FIG. 1 (color online). Scaling behavior of metric $g$. The points are the data obtained via Lanczos diagonalization of periodic chains of length $L$ up to 26, using equation $\mathcal{F}(\lambda, \lambda + \delta\lambda) \approx 1 - g\delta\lambda^2/2$ with $\delta\lambda = 1.0 \times 10^{-3}$. The points at $|\lambda| < 1$ are well fitted (solid lines) with $g/L = A_1 + A_2 L^{-1} + A_3 L^{3-2\Delta^{(2)}_V}$. The contribution $A_3$ comes from the irrelevant operator with scaling dimension $\Delta^{(2)}_V = 4K$. As this operator becomes rapidly irrelevant for $|\lambda| < 1$, its contribution can be hardly observed. At $\lambda = 1$ a better a fit is obtained with logarithmic corrections as expected at the isotropic point. In the massive regime we expect that the thermodynamic limit is approached exponentially fast. We obtain a good agreement by fitting our data with the phenomenological formula $g/L = A_1 + A_2 e^{-L/\xi} L^{-1/2}$, where $\xi$ is the correlation length as given by the Bethe ansatz [26]. As $\xi(\lambda = 2) = 8.35\ldots$ we used only points with $L \geq 14$.

When one considers the finite-size scaling of $q$ in the gapless region $|\lambda| < 1$, the leading contribution is dictated by the most relevant component of $V(x)$ which in this case is the marginal one, i.e., $\Delta_V = 2$. Correspondingly, using Eq. (8) we obtain $\Delta_Q = 1$, so that, in the whole region $|\lambda| < 1$, the finite-size dependence of the (rescaled) QGT tensor is $q = A_1 + A_2 L^{-1}$, where $A_{1,2}$ are constants which depend only on $\lambda$. Note that the term $A_1$ is the contribution coming from the regular part. This kind of scaling has to be contrasted with the one observed in quasifree fermionic systems, where one has $q = A_1' + A_2' L$. We would like to stress again that in general one expects a superextensive behavior of $Q$, and a corresponding fidelity drop when $d + 2\zeta - 2\Delta_V > 0$, i.e., when the operator associated to the varying parameter is sufficiently relevant. When this condition is not fulfilled the rescaled QGT tensor does not diverge in the thermodynamic limit at critical points. Nevertheless, a proper finite-size scaling analysis allows one to identify the critical region. To check this latter feature as well as the predicted scaling behavior we have performed exact Lanczos diagonalizations. The agreement between numerical data and the theoretical prediction is shown in Fig. 1.

*Conclusions.*—The mapping between a quantum Hamiltonian and the corresponding ground state endows the parameter manifold with a complex tensor $Q$. The real part of $Q$ is a Riemannian metric $g$, while the imaginary part is the curvature form giving rise to a Berry phase. The metric tensor $g$ is closely related to the quantum fidelity between different ground states; in the thermodynamical limit it has been shown to be singular at the critical point for several models featuring quantum phase transitions, e.g., quasifree fermionic models. The same kind of singularity has been argued to exist for the form $F$ and the associated Berry phases as well. In this Letter we demonstrated that (i) the components $Q_{\mu\nu}$ of $Q$ have an integral representation in terms of response functions (ii) a superextensive behavior of any of the $Q_{\mu\nu}$'s implies, for local models, gaplessness (iii) the singular part of the $Q_{\mu\nu}$ fulfills scaling relations which explicitly connect their singular behavior with the universality class of the transition, i.e., critical exponents. In particular, these relations show that gaplessness is a necessary but not sufficient condition for a superextensive scaling of the metric tensor, i.e., enhanced orthogonalization rate. The theoretical analysis has been further supported by a numerical study of the finite-size scaling of the fidelity for the *XXZ* spin 1/2 chain. The main message of this Letter is that apparently unrelated results can be understood in unified fashion by unveiling the underlying common differential-geometric structure and analyzing its quantum-critical behavior.

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