Bures metric over thermal state manifolds and quantum criticality

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(Received 24 July 2007; published 20 December 2007)

We analyze the Bures metric over the manifold of thermal density matrices for systems featuring a zero temperature quantum phase transition. We show that the quantum critical region can be characterized in terms of the temperature scaling behavior of the metric tensor itself. Furthermore, the analysis of the metric tensor when both temperature and an external field are varied, allows one to complement the understanding of the phase diagram including crossover regions which are not characterized by any singular behavior. These results provide a further extension of the scope of the metric approach to quantum criticality.

DOI: 10.1103/PhysRevA.76.062318 PACS number(s): 03.67.−a, 05.70.Fh, 68.35.Rh

I. INTRODUCTION

These years are witnessing an increasing research effort at the intersection of quantum information science [1] and more established fields such as theoretical condensed-matter physics [2]. Belonging to this class is the approach to quantum phase transitions (QPT) [3] based on the information geometry of quantum states that has been recently proposed in Refs. [4,5]. Further developments, for specific, yet important, classes of quantum states have been reported in [6–13]. The underlying idea is deceptively simple: the major structural change in the ground-state (GS) properties at the QPT should reveal itself by some sort of singular behavior in the distance function between the GSs corresponding to slightly different values of the coupling constants. This intuition can be made more quantitative by analyzing the leading-order terms in the expansion of the *quantum fidelity* between close GSs.

A general differential-geometric framework encompassing all of these results has been offered in Ref. [14]. There it has been shown that these leading-order terms do correspond to a Riemannian metric g over the parameter manifold. This metric g is nothing but the pullback of the natural metric over the projective Hilbert space via the map associating the Hamiltonian parameters with the corresponding GS. In the thermodynamical limit the singularities of g correspond to QPTs. In Ref. [15] the nature of this correspondence has been further investigated and it has been shown that both the metric approach to QPT and the one based on geometrical phases [16,17] can be understood in terms of the critical scaling behavior of the quantum geometric tensor [18].

The conceptually appealing and potentially practically relevant feature of this strategy consists of the fact that its viability does not rely on any *a priori* knowledge of the physics of the model, e.g., order parameters, symmetry breaking patterns,…, but just on a universal geometrical structure (basically the Hilbert scalar product). Very much in the spirit of quantum information the metric approach is fully based on quantum states rather than Hamiltonians (that might be even unknown), once these are given the machinery can be applied.

In this paper we further extend the scope of this metric approach by considering the manifold of thermal states of a family of Hamiltonians featuring a zero-temperature PT. In [19] it was shown that by studying the mixed-state fidelity [20] between Gibbs states associated with slightly different Hamiltonians one could detect the influence of the zero-temperature quantum criticality over a finite range of temperatures. Here we will refine that analysis and make it more quantitative by resorting to the concept of *Bures* metric between mixed quantum states. This metric provides the natural finite-temperature extension of the metric tensor g studied in the GS case and corresponds again to the leading order in the expansion of the (mixed-state) fidelity between close states, i.e., associated with infinitesimally close parameters. By analyzing the case of the quantum Ising model we shall show how the quantum-critical region above the zero-temperature QPT can be remarkably characterized in terms of the scaling behavior of the Bures metric tensor.

The paper is organized as follows: in Sec. II we introduce the basic concepts about mixed-state metrics and in Sec. III we specialize them to the case of thermal (Gibbs) states. In Sec. IV we provide generalities about quasifree fermion systems and in Sec. V we analyze in detail the Bures metric tensor for the quantum Ising model. Finally, in Sec. VI conclusions and outlook are given.

II. PRELIMINARIES

The Bures distance between two mixed-states ρ and σ is given in terms of the Uhlmann fidelity [20]

$$\mathcal{F}(\rho,\sigma)=\mathrm{tr}\sqrt{\rho^{1/2}\sigma\rho^{1/2}} \tag{1}$$

by $d_B(\rho,\sigma)=\sqrt{2[1-\mathcal{F}(\rho,\sigma)]}$.

The starting point of our analysis is provided by the following expression for the Bures distance between two infinitesimally close density matrices (see, e.g., [21] for a derivation)

$$ds^2(d\rho) := d_B^2(\rho,\rho+d\rho)=\frac{1}{2}\sum_{n,m}\frac{|\langle m|d\rho|n\rangle|^2}{p_m+p_n}, \tag{2}$$

where $|n\rangle$ is the eigenbasis of ρ with eigenvalues p_n, i.e., $\rho=\Sigma_n p_n|n\rangle\langle n|$. Even though in the sum in Eq. (2) p_n and p_m cannot be simultaneously in the kernel of ρ, since $|n\rangle,|m\rangle \in \mathrm{Ker}(\rho)\Rightarrow\langle n|d\rho|m\rangle=0$, one can formally extend the sum to all possible pairs by setting to zero the unwanted terms.

For ρ pure, i.e., $\rho=|\psi\rangle\langle\psi|$, one has $d\rho=|d\psi\rangle\langle\psi|+|\psi\rangle\langle d\psi|$ from which one sees that the diagonal matrix elements of $d\rho$ are vanishing and one is left with $ds_B^2=\sum_{m\in \mathrm{Ker}(\rho)}|\langle d\psi|m\rangle|^2 =\langle d\psi|(1-|\psi\rangle\langle\psi|)|d\psi\rangle$. This expression coincides with the Riemannian metric considered in [14]. The bures metric (2) is tightly connected to the so-called quantum Fisher information and it appears in the quantum version of the celebrated Cramer-Rao bound [22]. This suggests the possible relevance of the results that we are going to present in this paper to the field of quantum estimation [23].

To begin with we would like to cast Eq. (2) in a form suitable for future elaborations. Let us first differentiate the density matrix $d\rho=\sum_n(dp_n|n\rangle\langle n|+p_n|dn\rangle\langle n|+p_n|n\rangle\langle dn|)$ and consider to begin the matrix element $(d\rho)_{ij}$. We observe that $\langle i|j\rangle=\delta_{i,j}\Rightarrow\langle di|j\rangle=-\langle i|dj\rangle$; whence $\langle i|d\rho|j\rangle =\delta_{i,j}dp_i+\langle i|dj\rangle(p_j-p_i)$. Putting this expression back into Eq. (2) one obtains

$$ds^2=\frac{1}{4}\sum_n\frac{dp_n^2}{p_n}+\frac{1}{2}\sum_{n\neq m}|\langle n|dm\rangle|^2\frac{(p_n-p_m)^2}{p_n+p_m}. \quad (3)$$

This relation is quite interesting since it tells apart the classical and the quantum contributions. Indeed the first term in Eq. (3) is nothing but the *Fisher-Rao* distance between the probability distributions $\{p_n\}_n$ and $\{p_n+dp_n\}_n$, whereas the second term takes into account the generic noncommutativity of ρ and $\rho':=\rho+d\rho$. We will refer to these two terms as the classical and nonclassical one, respectively. When $[\rho',\rho]=0$ the problem becomes effectively classical and the Bures metric collapses to the Fisher-Rao one; this latter being in general just a lower bound [22,24].

Before moving to the analysis of the metric (2) we would like to comment about the connection with the recently established quantum Chernoff bound [25]. This latter, denoted by ξ_{QCB}, is the quantum analog of the Chernoff bound in classical information theory; it quantifies the rate of exponential decay of the probability of error in discriminating two quantum states ρ and σ when a large number n of them is provided and collective measurements are allowed, i.e., $P_{err}\sim\exp(-n\xi_{QCB})$. The Chernoff bound naturally induces a distance function over the manifold of quantum states with a well-defined operational meaning (the bigger the distance between the states the smaller the asymptotic error probability in telling one from the other). In [25] it has been proven that $\exp(-\xi_{QCB})=\min_{0\leq s\leq 1}\mathrm{tr}(\rho^s\sigma^{1-s})\leq\mathcal{F}(\rho,\sigma)$ and that for infinitesimally close states, i.e., $\sigma=\rho+d\rho$, one has

$$ds_{QCB}^2:=1-\exp(-\xi_{QCB})=\frac{1}{2}\sum_{n,m}\frac{|\langle m|d\rho|n\rangle|^2}{(\sqrt{p_m}+\sqrt{p_n})^2}. \quad (4)$$

From this expression we see that the distinguishability metric associated with the quantum Chernoff bound has the same form of the Bures one Eq. (2), but the denominators p_n+p_m are replaced by $(\sqrt{p_m}+\sqrt{p_n})^2$. Using the inequalities $(\sqrt{p_m}+\sqrt{p_n})^2\geq p_n+p_m$ and $2(p_n+p_m)\geq(\sqrt{p_m}+\sqrt{p_n})^2$ one immediately sees that

$$\frac{ds^2}{2}\leq ds_{QCB}^2\leq ds^2. \quad (5)$$

This relation shows that, as far as divergent behavior is concerned, the Bures and the Chernoff bound metric are equivalent, i.e., one metric diverges iff the other does. On the other hand, in the metric approach to QPTs the identification of divergences of the *rescaled* metric tensor and their study plays the central role [14]. Therefore one expects the two distinguishability measures to convey equivalent information about the location of the QPTs. Though most of the calculations that are reported in this paper could be easily extended to the Chernoff bound metric, here we will limit ourselves to the analysis of the Bures metric (2).

III. THERMAL STATES

From now on we specialize our analysis to the case of thermal states. If the Hamiltonian smoothly depends on a set of parameters, denoted by λ, living in some manifold $\mathcal{M}$ one has the smooth map $(\lambda,\beta)\rightarrow\rho(\beta,\lambda):=Z^{-1}e^{-\beta H(\lambda)}$, $(Z=\mathrm{tr}\,e^{-\beta H})$. What we are going to study in this paper is basically the pullback onto the (λ,β) plane of the Bures metric through this map. This is the obvious finite-temperature extension of the ground-state approach of Ref. [14].

We start by studying the Bures distance when $T\neq 0$ is fixed and for infinitesimal variations of the Hamiltonian's parameters λ. Notice first that $\rho=Z^{-1}\sum_n e^{-\beta E_n}|n\rangle\langle n|$, where E_n and $|n\rangle$ are the eigenvalues and eigenvectors of the Hamiltonian operator H. With a standard reasoning, by differentiating the Hamiltonian eigenvalue equation one finds that $\langle i|dj\rangle=\langle i|dH|j\rangle/(E_i-E_j)$. Moreover, one easily sees that $dp_i=d(e^{-\beta E_i}/Z)=-\beta p_i[dE_i-(\sum_j dE_j p_j)]$, therefore the first term in Eq. (3) can be written as $\beta^2/4\sum_i p_i(dE_i^2-\langle dE\rangle)^2$, where $\langle dE\rangle_\beta:=\sum_j dE_j p_j$. This means that the Fisher-Raodistance is expressed by the thermal variance of the diagonal observable $dH_d:=\sum_j dE_j|j\rangle\langle j|$ times the square of the inverse temperature. Summarizing,

$$ds_B^2=\frac{\beta^2}{4}(\langle dH_d^2\rangle_\beta-\langle dH_d\rangle_\beta^2)+\frac{1}{2}\sum_{n\neq m}\left|\frac{\langle n|dH|m\rangle}{E_n-E_m}\right|^2\frac{(e^{-\beta E_n}-e^{-\beta E_m})^2}{Z(e^{-\beta E_n}+e^{-\beta E_m})}. \quad (6)$$

The two terms correspond to the first and second term of Eq. (3), respectively, and they depend on β and on the other parameters of the Hamiltonian. For example, when a single parameter h is considered, the Bures distance defines a simple metric that can be expressed in term of the classical and nonclassical part,

$$g_{hh}(h,\beta)=g_{hh}^c(h,\beta)+g_{hh}^{nc}(h,\beta), \quad (7)$$

such that $ds_B^2=g_{hh}(h,\beta)dh^2$. Let us now explore the behavior of the Bures distance in presence of infinitesimal variations of both the temperature (β variations) and a field h in the Hamiltonian. It is easy to see that the variation of β only affects the Fisher-Rao classical term in Eq. (3). In fact the variation dH in Eq. (6), or analogously the variations $|dm\rangle$ in Eq. (3), are taken with respect to h only. The calculations can be summarized as follows. We first have to expand the dp_n as $dp_n=(\partial_\beta p_n)d\beta+(\partial_h p_n)dh$. We have that

$$(\partial_\beta p_n)d\beta = p_n[\langle H\rangle - E_n]d\beta$$

and

$$(\partial_h p_n)dh = \beta p_n[\langle \partial_h H_d\rangle - \partial_h E_n]dh,$$

where $E_n=E_n(h)$. The complete classical term of the Bures distance can be written expanding $(dp_n)^2=(\partial_h p_n dh)^2+(\partial_\beta p_n d\beta)^2+2\partial_\beta p_n \partial_h p_n d\beta dh$, and summing over n. We thus have three different contributions:

$$\frac{1}{4}\sum_n \frac{(dp_n)^2}{p_n} = \frac{1}{4}\{[\langle H^2\rangle - \langle H\rangle^2]d\beta^2 + \beta^2[\langle[(\partial_h H)_d]^2\rangle - \langle(\partial_h H)_d\rangle^2]dh^2 + 2\beta[\langle H(\partial_h H)_d\rangle - \langle(\partial_h H)_d\rangle\langle H\rangle]d\beta dh\}. \quad (8)$$

These terms correspond to the elements of the metric $g_{\beta,\beta}$, $g_{h,\beta}$, $g^c_{h,h}$, respectively. The full metric can be written once one calculates the nonclassical term in Eq. (3). The infinitesimal Bures distance can then be written in terms of the 2×2 metric tensor g as

$$ds^2 = (dh,d\beta)g\begin{pmatrix} dh \\ d\beta \end{pmatrix}, \quad g = \begin{pmatrix} g_{hh} & g_{h\beta} \\ g_{h\beta} & g_{\beta\beta} \end{pmatrix}, \quad (9)$$

where again $g_{hh}(h,\beta)=g^c_{hh}(h,\beta)+g^{nc}_{hh}(h,\beta)$.

It is at this point interesting to check whether, for $\beta\to\infty$, one recovers the known results for ground-state (pure) fidelity and metric tensor. In order to do that we will consider separately the classical and nonclassical term in Eq. (3). In fact $\|\rho(\beta)-\rho(\infty)\|_1=(1-p_0)+\Sigma_{n>0}p_n \le 2\Sigma_{n>0}e^{-\beta(E_n-E_0)}$, from which one sees that, for finite-dimensional systems, the thermal density matrix converges (in trace norm) exponentially fast to the projector over the ground state $|0\rangle$. Then it follows that all the expectations values will converge exponentially fast to their zero-temperature limits: $|\mathrm{tr}[A\rho(\beta)]-\mathrm{tr}[A\rho(\infty)]| \le \|A\|\|\rho(\beta)-\rho(\infty)\|_1$, this in turn guarantees that the covariances of diagonal operators in the Fisher-Rao term (8) are vanishing (since, e.g., dH_d is diagonal $\langle dH^2\rangle_\infty=\langle dH\rangle^2_\infty$) in the zero-temperature limit. In the infinite dimensional case the convergence to zero of this term will typically be only algebraic in the region where the smallest excitation gap is small compared to the temperature, whereas it will be exponential elsewhere. The overall convergence behavior of the classical term for $\beta\to\infty$ depends now on the detailed interplay between the decay of covariances we just discussed in Eq. (8) and the divergence of the powers of β in front of them. An analysis of the zero-temperature limit of these terms will be provided later for the quantum Ising model. We will see that all the classical terms vanish in the zero temperature limit but at the critical value of the parameter. As far as the second nonclassical term in Eq. (3) is concerned one has just to notice that from $\lim_{\beta\to\infty} p_n(\beta)=\delta_{n,0}$ it follows that the only contributions will come from the elements involving the ground state, i.e., $\langle 0|dj\rangle=\langle 0|dH|j\rangle/(E_j-E_0)$. This completes the remark.

Before moving to the next sections, where we will specialize the previous results to the particular case of the quantum Ising model, we would like to note that the variation of the Bures distance with temperature only, given by the element $g_{\beta\beta}$ of the metric, is precisely proportional to the *specific heat* c_v [14], i.e.,

$$ds_B^2 = \frac{d\beta^2}{4}(\langle H^2\rangle_\beta - \langle H\rangle_\beta^2) = \frac{d\beta^2}{4}T^2 c_v.$$

This simple fact was already observed in [14] and [9] and provides, we believe, a neat connection between quantum-information theoretic concept, geometry, and thermodynamics.

IV. QUASIFREE FERMIONS

In this section we specialize the study of the behavior of the Bures metric to systems of quasifree fermions when one has the variation of one parameter h of the Hamiltonian and of the temperature T. The results that we present here are a finite-temperature generalization of those given in Refs. [6,7] and directly related to the mixed-state fidelity ones reported in [19].

The quasifree Hamiltonians we consider are given, after performing a suitable Bogoliubov transformation, by

$$H = \sum_\nu \Lambda_\nu \eta_\nu^\dagger \eta_\nu, \quad (10)$$

where $\Lambda_\nu > 0$ and η_ν denote the quasiparticle energies and annihilation operator respectively. One has that ν is a suitable quasiparticle label, that for translationally invariant systems amounts to a linear momentum; the ground state is the vacuum of the η_ν operators, i.e., $\eta_\nu|GS\rangle=0,\ \forall\ \nu$. The dependence on the parameter h is both through the Λ_ν's and the η_ν's.

We now derive the explicit general form of the Bures distance (2) starting from the classical part (8). We observe that the (many-body) Hamiltonian eigenvalues are given by $E_j=\Sigma_\nu n_\nu \Lambda_\nu$ where the n_ν's are fermion occupation numbers, i.e., $n_\nu=0,1$. Therefore we have that $dE_j=\Sigma_\nu n_\nu d\Lambda_\nu$ and $\langle dE_j\rangle_\beta=\Sigma_\nu\langle n_\nu\rangle_\beta d\Lambda_\nu$, where the averages are easy to compute since the probability distribution of the dE_j factorizes over the ν's. Furthermore, $\langle n_\mu n_\nu\rangle_\beta-\langle n_\mu\rangle_\beta\langle n_\nu\rangle_\beta =\delta_{\mu\nu}\langle n_\nu\rangle_\beta(1-\langle n_\nu\rangle_\beta)$ and we can thus write

$$\frac{1}{4}\sum_n \frac{(dp_n)^2}{p_n} = \frac{1}{4}\sum_k \langle n_k\rangle(1-\langle n_k\rangle) \times \{\Lambda_k^2 d\beta^2 + \beta^2(\partial_h\Lambda_k)^2 dh^2 + 2\beta\Lambda_k\partial_h\Lambda_k d\beta dh\}. \quad (11)$$

The term in dh^2 is the classical term due to the infinitesimal variations of the parameters of the Hamiltonian at fixed T and it corresponds to the variance, see Eq. (6), $\mathrm{var}(H_d) =\Sigma_\nu\langle n_\nu\rangle_\beta(1-\langle n_\nu\rangle_\beta)d\Lambda_\nu^2$. Since we are dealing with independent free fermions one has that $\langle n_\nu\rangle_\beta=[\exp(\beta\Lambda_\nu)+1]^{-1}$, whence

$$ds_c^2 = \frac{\beta^2}{16}\sum_\nu \frac{(\partial_h \Lambda_\nu)^2}{\cosh^2(\beta\Lambda_\nu/2)} dh^2. \tag{12}$$

In order to compute the nonclassical part of Eq. (3), one has to explicitly consider the eigenvectors of Eq. (10). Following the notation of Ref. [6] one has $|m=\{\alpha_\nu,\alpha_{-\nu}\}_{\nu>0}\rangle =\otimes_{\nu>0}|\alpha_\nu,\alpha_{-\nu}\rangle$, where,

$$|0_\nu 0_\nu\rangle = \cos(\theta_\nu/2)|00\rangle_{\nu,-\nu} - \sin(\theta_\nu/2)|11\rangle_{\nu,-\nu},$$

$$|0_\nu 1_{-\nu}\rangle = |01\rangle_{\nu,-\nu}, \quad |1_\nu 0_{-\nu}\rangle = |10\rangle_{\nu,-\nu},$$

$$|1_\nu 1_\nu\rangle = \cos(\theta_\nu/2)|11\rangle_{\nu,-\nu} + \sin(\theta_\nu/2)|00\rangle_{\nu,-\nu}.$$

We assume now that parameter dependence is only in the angles θ_ν's (this assumption holds true for all the translationally invariant systems). It is easy to see from the above factorized form that the only nonvanishing matrix elements $\langle n|dm\rangle$ are given by $\langle 0_\nu 0_{-\nu}|d|1_\nu 1_{-\nu}\rangle = d\theta_\nu/2$ and that the thermal factor $(p_n-p_m)^2/(p_n+p_m)$ has the form $\sinh^2(\beta\Lambda_\nu)/\{[\cosh(\beta\Lambda_\nu)+1][\cosh(\beta\Lambda_\nu)]\} =[\cosh(\beta\Lambda_\nu)-1]/\cosh(\beta\Lambda_\nu)$. Putting all together one finds

$$ds_{nc}^2 = \frac{1}{4}\sum_{\nu>0} \frac{\cosh(\beta\Lambda_\nu)-1}{\cosh(\beta\Lambda_\nu)} (\partial_h\theta_\nu)^2 dh^2. \tag{13}$$

We finally note that the two elements (12) and (13) define the metric element (7). The results of this section can be applied to any quasifree fermionic model (10).

V. QUANTUM ISING MODEL

We are now going to discuss in some detail the behavior of the metric tensor for a paradigmatic example in the class of quasifree fermionic models, the one-dimensional (1D) Ising model in transverse field. The model is defined by the Hamiltonian

$$H = -\sum_j \sigma_j^x\sigma_{j+1}^x + h\sigma_j^z. \tag{14}$$

At $T=0$ this system undergoes a quantum phase transition for $h=1$. For $h<1$ the system is in an ordered phase as the correlator $\langle\sigma_1^x\sigma_r^x\rangle_{T=0}$ tends to a nonzero value: $\lim_{r\to\infty}\langle\sigma_1^x\sigma_r^x\rangle_{T=0}=(1-h^2)^{1/4}$. The excitations in this region are domain walls in the σ^x direction. Instead for $h>1$ the magnetic field dominates, and excitations are given by spin flip over a paramagnetic ground state. The transition point $h=1$ is described by a $c=1/2$ conformal field theory, which implies that the dynamical exponent $z=1$; the correlation function exponent is $\nu=1$. As is well known [3], a signature of the ground state phase diagram remains at positive temperature. In the *quasiclassical* region $T\ll\Delta$, where $\Delta=|1-h|$ is the lowest excitation gap, the system can be described by a diluted gas of thermally excited quasiparticles, even if the nature of the quasiparticles is different at the different sides of the transition. Instead in the *quantum critical* region $T\gg\Delta$ the mean interparticle distance becomes of the order of the quasiparticle de Broglie wavelength and thus quantum critical effects dominate and no semiclassical theory is available. In each of the above-described regions of the (h,T) plane the system displays very different dynamical as well thermodynamical properties. For example, in the quantum critical region the specific heat approaches zero linearly with the temperature (this is in fact a general feature of all conformal field theories), whereas in the quasiclassical regions the approach is exponentially fast.

A. Bures metric tensor in the (h,T) plane

We now investigate whether the signature of the physically different regions can be revealed by analyzing the elements of the metric tensor defined by the Bures distance. We begin by studying the temperature dependence of the metric tensor when only the external field is varied, i.e., the term $g_{hh}(h,T)$, see Eq. (7). The Hamiltonian (14) is equivalent to a quasifree fermionic model, and following our previous notation one has $\epsilon_k=\cos(k)-h$, $\Delta_k=\sin(k)$, $\Lambda_k=\sqrt{\epsilon_k^2+\Delta_k^2}$, and $\tan(\vartheta_k)=\Delta_k/\epsilon_k$. Using formulas (12) and (13) it is straightforward to write (7). After rescaling $g\to g/L$ and passing to the thermodynamic limit we obtain

$$g_{hh}^c = \frac{\beta^2}{16\pi}\int_{-\pi}^{\pi} \frac{1}{\cosh(\beta\Lambda_k)+1}\frac{\epsilon_k^2}{\Lambda_k^2}dk,$$

$$g_{hh}^{nc} = \frac{1}{8\pi}\int_{-\pi}^{\pi} \frac{\cosh(\beta\Lambda_k)-1}{\cosh(\beta\Lambda_k)}\frac{\Delta_k^2}{\Lambda_k^4}dk.$$

The integrals are better evaluated by transforming momentum integration to energy integration in a standard way. As previously noticed, on general grounds, the classical term g_{hh}^c vanishes when the temperature goes to zero. In the quantum-critical region $\beta\Delta\approx 0$, and one obtains the following low temperature expansion:

$$g_{hh}^c = \frac{\pi}{96h^2}T + O(T^2).$$

In the quasiclassical region where $\beta\Delta\gg 1$, the fall-off to zero is exponential. With a saddle-point approximation one obtains

$$g_{hh}^c = \sqrt{\frac{\Delta}{32\pi h}}T^{-3/2}e^{-\Delta/T} + \text{lower order}.$$

We now analyze the scaling behavior of the nonclassical term of the metric g. From the results of [4,6] it is known that the geometric tensor at zero temperature diverges as Δ^{-1} when $\Delta\to 0$. The nonclassical term matches this ground-state behavior from positive temperature. Indeed, in the quantum-critical region the integral is well approximated by

$$g_{hh}^{nc} \approx \frac{1}{8\pi h^2}\int_0^{2\beta} \frac{\cosh(x)-1}{\cosh(x)}\frac{\sqrt{(4\beta^2-x^2)}}{x^2}dx.$$

For large β (low temperatures) this expression can be Laurent expanded and the resulting integrals can be summed using residue theorem, giving

$$g_{hh}^{nc} = \frac{1}{h^2}\left[\frac{\mathcal{C}}{\pi^2}T^{-1} - \frac{1}{16} + O(T)\right], \tag{15}$$

where $\mathcal{C}$ is Catalan's constant $\mathcal{C}=0.915\,966\ldots$.

We would like to point out that the behavior of the metric tensor in the quasicritical region can be inferred from dimensional scaling analysis in much the same spirit as was done in [15] for the zero temperature metric tensor. From Eq. (6) we see that the scaling dimension of g_{hh}^{nc} is $\Delta_{nc} = 2\Delta_V - 2z - d$, where Δ_V is the scaling dimension of the operator dH, z is the dynamical exponent, and d is the spatial dimensionality. Following [15] (β now plays the role of the length) we obtain

$$g_{hh}^{nc} \sim T^{\Delta_{nc}/z}. \tag{16}$$

In the present case, $z=d=\Delta_V=1$ (the scaling dimension of σ_i^z—a free fermionic field—is one) which agrees with Eq. (15).

We now pass to analyze the behavior of g_{hh}^{nc} in the quasiclassical region, i.e., when $\beta\Delta \gg 1$. In this case the "temperature" part of the integral is never effective, i.e., one has $\frac{\cosh(\beta\Lambda)-1}{\cosh(\beta\Lambda)} \approx 1$, so it is quite clear that, in first approximation, one recovers the zero temperature result first given in [4] which we rewrite here as an energy integral

$$g_{hh}^{nc} = \frac{1}{8\pi h^2}\int_{|1-h|}^{|1+h|} \frac{\sqrt{[(h-1)^2-\omega^2][\omega^2-(1+h)^2]}}{\omega^3} d\omega, \tag{17}$$

and we assumed $h>0$. For small values of the gap—hence we are in a situation where we consider first the limit $T\to 0$ and then $\Delta\to 0$—we observe the following divergence

$$g_{hh}^{nc}(T=0,\Delta\to 0) \approx \frac{1}{16\Delta},$$

which is a result also reported in [4,6]. Instead when the gap is large—so that we are necessarily on the $h>1$ side—we can approximate the radical in Eq. (17) with an ellipse centered at $(h,0)$ with semiaxes $r_x=1$ and $r_y=2h$, that amounts to write $\sqrt{[(h-1)^2-\omega^2][\omega^2-(1+h)^2]} \approx 2h\sqrt{1-(\omega-h)^2}$. In this case the integral gives

$$g_{hh}^{nc}(T=0,\Delta \gg 1) \approx \frac{1}{8h^{5/2}(h-1)^{3/2}} \approx \frac{1}{8\Delta^4}.$$

Again, by doing a saddle-point approximation one realizes that the zero-temperature results are approached exponentially fast with the temperature, more precisely one has

$$g_{hh}^{nc}(\beta\Delta \gg 1) = g_{hh}^{nc}(T=0) - \text{const} \times T^{3/2}e^{-\Delta/T}.$$

We now extend our analysis to the other terms of the metric tensor (9). When we consider the case in which both the temperature and the field h are varied, two new matrix elements come into play,

$$g_{TT} = \frac{\beta^4}{16\pi}\int_{-\pi}^{\pi} \frac{\Lambda_k^2}{\cosh(\beta\Lambda_k)+1}dk,$$

$$g_{hT} = \frac{\beta^3}{16\pi}\int_{-\pi}^{\pi} \frac{\epsilon_k}{\cosh(\beta\Lambda_k)+1}dk.$$

Let us first comment on the behavior observed at very low temperature. In the quasi-classical region ($\Delta \gg T$) all matrix elements of g tend to zero except for g_{hh}^{nc}. This is a general feature and is due to the fact that these terms are absent in the zero-temperature expression. As previously stated the falloff to zero is exponential, and in particular, for the model in exam, we have that

$$g_{Th} \approx T^{-5/2}e^{-\Delta/T}, \quad T \ll \Delta,$$

$$g_{TT} \approx T^{-7/2}e^{-\Delta/T}. \tag{18}$$

Let us now look at the quantum critical region $T \gg \Delta$, small temperature. The mixed term tends to a constant,

$$g_{hT} = \frac{\pi}{48} + O(T^2). \tag{19}$$

Instead g_{TT} must diverge at zero temperature, as it has to match with the diverging behavior observed in the ground state [4]. For the diagonal term g_{TT} one has

$$g_{TT} = \frac{T^{-2}}{4}c_v = \frac{\pi}{24}\frac{1}{T} + O(T), \quad T \gtrsim \Delta. \tag{20}$$

We note in passing that this result agrees with the one for the specific heat obtained for general conformal theories [26] $c_v = (\pi c T)/(3v)$, as $T\to 0$, since in our case the velocity v is one and the conformal charge c is one half. We thus see that, in the present case, both g_{hh} and g_{TT} diverge as T^{-1}. This is not to be the case in general, indeed at any quantum critical point described by a conformal field theory, g_{TT} will diverge as T^{-1}, whereas the behavior of g_{hh}^{nc} is dictated by Eq. (16).

In this section we have analyzed the behavior of all the elements of the geometric tensor g. The result of this analysis allows one to conclude that indeed, at least for the specific model studied, *the quantum critical and quasiclassical regions can be clearly identified in terms of the markedly different temperature behavior of the geometric tensor* g.

B. Directions of maximal distinguishability

The analysis carried out in the previous section can be further deepened by studying some useful quantities that can be derived from the analysis of the metric tensor g. Indeed, we will see that these quantities allow one to give a finer description of the behavior of the system in the plane (h,T) and to reveal unexpected features. We first start by noticing that at each point (h,T) the eigenvectors of the metric tensor g define the directions of maximal and minimal growth of the line element ds_B^2. Hence the vector field $\vec{v}_M(h,T)$ given by the eigenvector of g related to the highest eigenvalue λ_M, defines at each point of the (h,T) plane the direction along which the fidelity decreases most rapidly: the latter represents the direction of highest distinguishability between two nearby Gibb's states.

We now focus our analysis on the study of the vector field $\vec{v}_M(h,T)$ in the specific case of the quantum Ising model, see

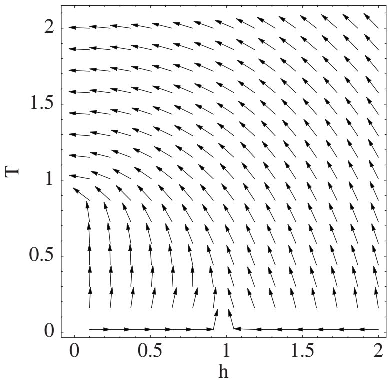

FIG. 1. Vector field of the eigenvector associated to the highest eigenvalue of g, in the plane (h,T) for the Ising model in transverse field.

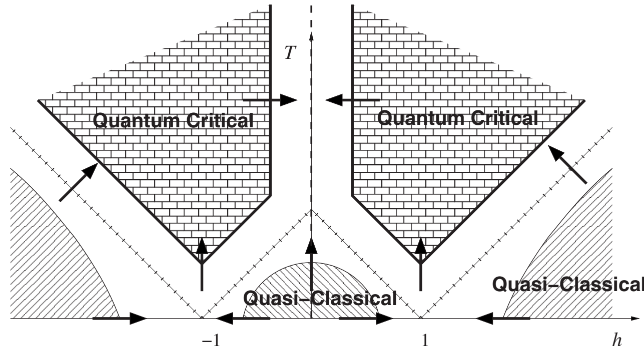

FIG. 2. Phase diagram of the Ising model in transverse field taking into account both critical points at $h=\pm 1$ and the purely classical Ising line $h=0$. The arrows indicate the direction of highest fidelity decrease (the direction of the arrows is conventional, but fixed once for all).

Fig. 1. We first observe that there clearly are some interesting features for small temperatures that reflect the analysis previously carried out on the metric elements of g. On one hand, in the quasiclassical region, when $h \simeq 0$ we have that the direction of highest fidelity drop is parallel to the h axis. This reflects the fact that, in this region, all the elements of g tend to zero except for the term g_{hh}^{nc}. On the other hand, in the quasicritical region, the direction of highest fidelity drop is parallel to the T axis. Again, this feature can be linked to the previous analysis of the terms (15) and (20). Both g_{hh} and g_{TT} diverge as T^{-1}, but, as $(\mathcal{C}/\pi^2)/(\pi/24)=0.70\ldots<1$, g_{TT} eventually becomes bigger and thus the direction of highest distinguishability turns parallel to the T axis.

We proceed in our description of the phase diagram through the introduced vector field by examining what happens at the $h=0$ axis. Here one has the impression that a kind of singular point appear around $T \approx 1$. The reason for this is that at $h=0$ the system becomes the purely classical Ising model, which possess only classical behavior at any temperature. This implies that the quantum-critical region cannot extend over this line. As the dispersion Λ_k is flat, it is straightforward to write down the metric tensor on the $h=0$ line. It turns out that g is completely diagonal meaning that eigenvectors are parallel to the (h,T) axes. One sees that for $0.852<T<\infty$, $g_{hh}>g_{TT}$ then for $0.101<T<0.852$, $g_{TT}>g_{hh}$, and then finally, at very small temperature, the term g_{hh}^{nc} dominate and for $0<T<0.101$, $g_{hh}>g_{TT}$. These "singular points" of $\vec{v}_M$in $h=0$ are related to the level crossing of g: its two eigenvalues become equal at those points but no physical transition or crossover occur.

The appearance of the purely classical Ising line at $h=0$, which forbids the quantum critical phase extend over this line, is related to the fact that the model (14) is invariant under the $\mathbb{Z}_2$ symmetry $h \to -h$. This in turns implies that the phase diagram is mirror symmetric around the $h=0$ line and that there is another quantum critical point at $h=-1$. The physical consequence is that the semiclassical ordered region is much smaller than one would think and the actual phase diagram is very similar to the one in Fig. 2.

Finally we now discuss another feature that can be observed by studying $\vec{v}_M(h,T)$. As one can see in Fig. 1, along the line $T=h \gtrsim 1$ the vector field becomes parallel to the vector $\vec{w}=(-1,1)$. It turns out that this feature can be understood analytically by studying the behavior of the metric tensor g when $|h| \gg 1$. Indeed, by evaluating the dominant part of the various metric elements on the line $T=h=t \gg 1$, one sees that all the Fisher-Rao terms decay as t^{-2} while $g_{hh}^{nc} \sim t^{-4}$, and, what is most surprising, all matrix elements tend to have the same value in magnitude. This feature can be understood by simply observing that when $|h| \gg 1$ it is only the classical term proportional to the external magnetic field of the quantum Ising Hamiltonian that survives, i.e., $H \simeq h\Sigma_i \sigma_i^z$. The density matrix of the system can be written as $\rho(h,T)=\exp(-h\Sigma_i\sigma_i^z/T)/Z$; in this approximation the only nonzero terms of the metric are the Fisher-Rao ones and allthe covariances that define these terms, see Eq. (8), coincide with $\mathrm{var}(H)$. Thus, in the limit $|h| \gg 1$ the Bures distance reads $ds_B^2=\mathrm{var}(H)[dT^2/T^2-hdTdh/T^3+h^2dh^2/T^4]$. If now one chooses the particular case $T=h=t$ and evaluates the density g/L one finds that

$$g(t,t)=\frac{t^{-2}}{16\cosh^2(1/2)}\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}+O(t^{-3}).$$

Thus, one has that on the line $T=h \gg 1$ the only nonzero eigenvalue is $2\,\mathrm{var}(H)/(Lt^2)$ and it corresponds to the eigenvector $\vec{w}=(-1,1)$. In this approximation, that amounts to neglecting the term $g_{hh}^{c} \sim t^{-4}$, when moving along the line $T=h \gg 1$, i.e., along the direction defined by $\vec{w}^{\perp}$, no changes in the state of the system occur.

C. Crossover and metric tensor g

We finally present some preliminary results related to the intriguing possibility of determining the crossover lines between the quasiclassical and quasicritical region (14) through the analysis of the elements of the metric tensor g and the induced Gaussian curvature [27] in the plane (h,T). The capability of the highest (in modulus) eigenvalue of g and of the Gaussian curvature induced by the metric to capture, in terms of divergencies or discontinuities, the existence of QPTs has been already tested in [7] and [14]. Here we would like to test whether these quantities are able to identify the

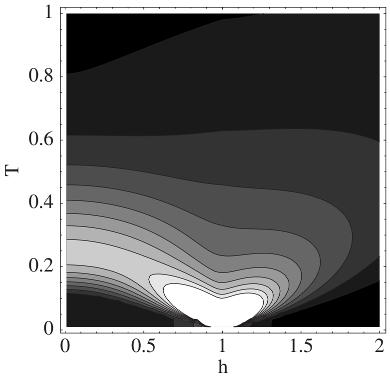

FIG. 3. Contour plot of the highest eigenvalue of g, in the plane (h,T) for the Ising model in transverse field.

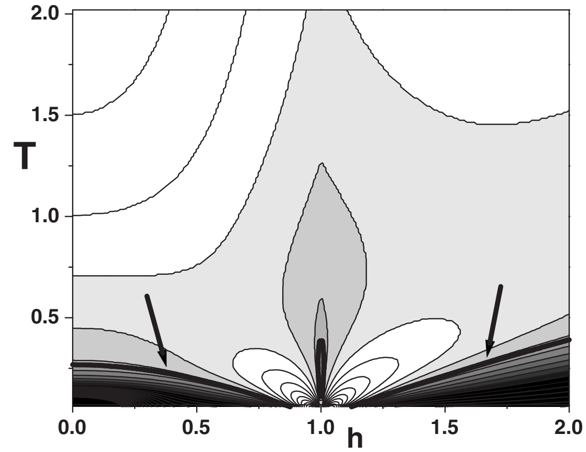

FIG. 4. Contour plot of the Gaussian curvature of g, in the plane (h,T) for the Ising model in transverse field. The arrows indicate the zero curvature lines.

crossover between the quasiclassical and quantum-critical region. Notice that the curvature of the Bures metric in the case of squeezed states has been studied in [28] and an operational interpretation attempted. It is also worthwhile to stress that the so-called thermodynamical curvature plays a central role in the geometrical theory of classical phase transition developed by Ruppeiner and co-workers [29].

As already pointed out, at each point (h,T) the vector field $\vec{v}_M(h,T)$ defines the direction of highest distinguishability between two nearby Gibb's states. The degree of distinguishability along this direction is quantified by the maximal eigenvalue $\lambda_M(h,T)$. Since the quasiclassical and quantum-critical regions are characterized by significantly different physical properties, it is natural to investigate whether the change of the latter, in spite of not involving a phase transition, could be revealed by our measures of statistical distinguishability and by the related functionals.

We now give a descriptive analysis of the raw data. In Fig. 3, we have plotted the contour plot of the maximal eigenvalue of g. The main feature is the presence for $T>0$ of two patterns of high distinguishability (white) that separate the regions $(h<1, T\lesssim 0.25)$ and $(h>1, T\lesssim 0.25)$ from the rest of the diagram. Thus, the first information that can be drawn is that a change of parameters inside these regions implies a small change in the statistical properties of the corresponding ground states. On the contrary, if one varies h and T and moves from these regions towards the center of the diagram, for example, moving along the integral lines of $\vec{v}_M(h,T)$, the statistical properties of the state necessarily have to significantly change. One can see that the "transition" lines between the different regions can be extrapolated numerically by tracing the "ridge" lines of the two patterns of high distinguishability. It turns out that the *same* result can be achieved by looking at the lines where the Gaussian curvature of g changes sign, see Fig. 4. For example, when $h>1$, one can see that along the determined transition line, T has a linear dependence on $h-1$. As Fig. 4 clearly shows, the Gaussian curvature exhibits a fairly complex (lobed-shaped) behavior in particular in the region above $h=1$; this behavior is not fully understood and deserves further investigations.

Nevertheless, this preliminary descriptive analysis seems thus to indicate that a neat distinction between the quasiclassical regions (characterized by a negative curvature) and the quantum-critical (characterized by a positive curvature) can be made on the basis of study of the metric g. The use of the fidelity, and of the related functionals, allows one to identify the crossover between two distinct phases.

VI. CONCLUSIONS

In this paper we have analyzed the relation between quantum criticality, finite temperature, and the differential geometry of the manifold of mixed quantum states. We studied the Bures metric over the set of thermal quantum states associated with Hamiltonians featuring a zero-temperature quantum phase transition, i.e., quasifree fermionic systems. In particular we focused on the study of the quantum Ising model for which we provided a fully analytical characterization of the Bures metric tensor g. Quantum critical and semiclassical regions in the temperature, magnetic field plane can be easily identified in terms of different scaling behavior of the components of g as a function of the temperature. Crossover lines between the different regions can be found just by looking at the shape of the graph of the largest eigenvalue of the metric as a function of temperature and magnetic field. Remarkably these crossover lines seem to be associated also with the change of sign of the Gaussian curvature of the metric g.

The results presented in this paper provide further support to the validity of the statistical-metric approach to phase transitions [14] and clearly show that the scope of this geometrical method can be extended to finite temperatures. The physical significance of the curvature of the metric as well as the study of the thermal states geometry associated with other distinguishability distances, e.g., the quantum Chernoff bound metric, are topics deserving further investigations.

ACKNOWLEDGMENTS

The authors would like to thank R. Ionicioiu and M. Paris for useful discussions.

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