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Ground-state fidelity in one-dimensional gapless models

Min-Fong Yang
Department of Physics, Tunghai University, Taichung, Taiwan
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A general relation between quantum phase transitions and the second derivative of the fidelity (or the "fidelity susceptibility") is proposed. The validity and the limitation of the fidelity susceptibility in characterizing quantum phase transitions are thus established. Moreover, based on the bosonization method, general formulas of the fidelity and the fidelity susceptibility are obtained for a class of one-dimensional gapless systems known as the Tomonaga-Luttinger liquid. Applying these formulas to the one-dimensional spin-1/2 *XXZ* model, we find that quantum phase transitions, even of the Beresinskii-Kosterlitz-Thouless type, can be signaled by the fidelity susceptibility.

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In order to obtain fresh insight into the quantum many-body problem, a great deal of effort has been devoted to the application of concepts emerging from quantum information science[1] to the analysis of quantum phase transitions (QPTs).[2] QPTs are characterized by a drastic change in the ground states of quantum many-body systems, driven solely by quantum fluctuations. Since entanglement measures the strength of quantum correlations between subsystems of a compound system, it is natural to expect that entanglement will be a reliable indicator of QPTs. Much attention has been focused on the role of entanglement in characterizing QPTs in the last few years (e.g., Refs. 3–6 and references therein). More recently, another approach to identify QPTs based on the ground-state fidelity has been proposed[7] and applied to various many-body systems.[8–20] Because the fidelity is a measure of similarity between states, one anticipates that the fidelity should drop abruptly at critical points, as a consequence of the dramatic changes in the structure of the ground states, regardless of what type of internal order is present in quantum many-body states. A perhaps more effective indicator is given by the singularity in the second derivative of the fidelity (or the so-called fidelity susceptibility).[7–11,13–17,21] The main advantage of this approach lies in the fact that, since the fidelity is a purely Hilbert-space geometrical quantity, no *a priori* knowledge of the structure (order parameter, correlations driving the QPTs, topology, etc.) of the considered system is required for its use. The fidelity approach has been examined in various systems, including the Dicke model,[7] one-dimensional *XY* model in a transverse field,[7,19]general quadratic fermionic Hamiltonians,[8,9] and Bose-Hubbard model.[11,12] The success in analyzing QPTs in these models shows the generality of this procedure. The ground-state fidelity is usually difficult to calculate, due to the lack of knowledge of the exact ground-state wave functions. Therefore, investigations so far are restricted to some particular many-body models. Conceivably, in order to understand its validity and limitation, a general connection between the fidelity and QPTs is highly desired.

In this paper, we discuss, in a general framework, how the fidelity can be related to a QPT characterized by nonanalyticities in the derivative of the ground-state energy. It is found that, under certain conditions mentioned below, the fidelity susceptibility is indeed an effective tool in detecting the critical points of first-order QPTs (1QPTs) and second-order QPTs (2QPTs), as illustrated before in several concrete models. However, it fails to determine the order of the transition, and may not detect higher-order QPTs. We stress that, although the fidelity susceptibility cannot always detect higher-order QPTs, it is possible to signal the Beresinskii-Kosterlitz-Thouless (BKT) transition[22] in one-dimensional many-body systems, which is a QPT of infinite order. To demonstrate this, analytic formulas for the fidelity and the fidelity susceptibility are derived for the single-component Luttinger model, which describes a large class of one-dimensional systems possessing a gapless spectrum. The fidelity susceptibility is shown to be finite in the thermodynamic limit even for these gapless systems. Besides, it is a smooth function of the controlling parameter driving QPTs [see Eq. (12) below], as long as the system lying in the critical Luttinger-liquid phase. By using these formulas, the fidelity and the fidelity susceptibility can be easily calculated for a large class of gapless systems, as long as the relation between the Luttinger-liquid parameters and the controlling parameter driving QPTs is known. Employing our general formulas to the one-dimensional spin-1/2 *XXZ* model, we show that the BKT transition therein can indeed be signaled by the singularity in the fidelity susceptibility. Though we restrict our attention to the *XXZ* spin chain, according to the general expressions of the fidelity and the fidelity susceptibility, one can expect that the same results should apply to all the BKT-type QPTs of one-dimensional models.

We now begin to show the general relation between quantum phase transitions and the fidelity susceptibility. Only QPTs characterized by nonanalytic behavior in the derivatives of the ground state energy are considered here. According to the conventional classification, a 1QPT is characterized by a finite discontinuity in the first derivative of the ground state energy. Similarly, a 2QPT is characterized by a finite discontinuity, or divergence, in the second derivative of the ground state energy, assuming the first derivative is continuous. Following the notations in Ref. 4, the most general Hamiltonian of N distinguishable particles governed by up to two-body interactions can be written as

$$H = \sum_{i\alpha\beta} \epsilon^{i}_{\alpha\beta} |\alpha_i\rangle\langle\beta_i| + \sum_{ij\alpha\beta\gamma\delta} V^{ij}_{\alpha\beta\gamma\delta} |\alpha_i\rangle|\beta_j\rangle\langle\gamma_i|\langle\delta_j|,$$

where $\{|\alpha_i\rangle\}$ is the basis for the local Hilbert space of particle i. For these systems, it has been shown that the derivatives of the ground state energy per particle $\mathcal{E}$ can be written as[4]

$$\frac{\partial \mathcal{E}}{\partial \lambda} = \frac{1}{N}\sum_{ij} \mathrm{tr}\left(\frac{\partial \mathbf{U}(ij)}{\partial \lambda}\rho^{ij}\right), \quad (1)$$

$$\frac{\partial^2 \mathcal{E}}{\partial \lambda^2} = \frac{1}{N}\sum_{ij}\left[\mathrm{tr}\left(\frac{\partial^2 \mathbf{U}(ij)}{\partial \lambda^2}\rho^{ij}\right) + \mathrm{tr}\left(\frac{\partial \mathbf{U}(ij)}{\partial \lambda}\frac{\partial \rho^{ij}}{\partial \lambda}\right)\right], \quad (2)$$

where λ is a controlling parameter of the system's Hamiltonian and tr denotes the trace over the degrees of freedom for two particles. $\mathbf{U}(ij)$ denotes a matrix with matrix elements $U_{\alpha\beta,\gamma\delta}(ij) = \epsilon^i_{\alpha\gamma}\delta^j_{\beta\delta}/N_i + V^{ij}_{\alpha\beta\gamma\delta}$, where $\delta^j_{\beta\delta}$ is the Kronecker symbol on particle j, and N_i is the number of particles that particle i interacts with. $\rho^{ij} = \mathrm{Tr}_{\hat{i}\hat{j}}\rho_0(\lambda)$ is the two-particle reduced density matrix, which is obtained by taking a partial trace $\mathrm{Tr}_{\hat{i}\hat{j}}$ over all degrees of freedom except particles i and j. Here $\rho_0(\lambda) \equiv |\Psi_0(\lambda)\rangle\langle\Psi_0(\lambda)|$ is the density matrix of the ground state with $|\Psi_0(\lambda)\rangle$ being the normalized ground state. $\mathbf{U}(ij)$ includes all the single- and two-body terms of the Hamiltonian associated with particles i and j. We assume that $\mathbf{U}(ij)$ is a smooth function of the Hamiltonian parameter λ. From Eqs. (1) and (2), one finds that the origin of a 1QPT (2QPT) is due to the fact that one or more of the matrix elements of ρ^{ij} ($\partial_\lambda \rho^{ij}$) are discontinuous or divergent at the transition point $\lambda = \lambda_c$.[4]

The quantum fidelity (or the modulus of the overlap) F of two normalized ground states $|\Psi_0(\lambda+\delta\lambda)\rangle$ and $|\Psi_0(\lambda)\rangle$ corresponding to neighboring Hamiltonian parameters is given by $F(\lambda+\delta\lambda,\lambda) = |\langle\Psi_0(\lambda+\delta\lambda)|\Psi_0(\lambda)\rangle|$.[7] To detect QPTs, a more effective indicator is provided by the peak in the "density" of the second derivative of the fidelity (or the so-called fidelity susceptibility) $\mathcal{S}(\lambda)$,[7–11,13–17,21] which is free from the arbitrariness of the small parameter $\delta\lambda$. In the thermodynamic limit (i.e., both the particle number N and the number of lattice sites L approach to infinity, while N/L keeps finite), $\mathcal{S}(\lambda)$ can be written as[23]

$$\mathcal{S}(\lambda) = \lim_{\delta\lambda\to 0}\lim_{L\to\infty}\frac{-2\ln F(\lambda+\delta\lambda,\lambda)}{L\delta\lambda^2}. \quad (3)$$

To make comparison with the expressions of the derivatives of the ground-state energy, we rewrite the quantum fidelity and the fidelity susceptibility in terms of the density matrix $\rho_0(\lambda)$ of the ground state. Notice that

$$F(\lambda+\delta\lambda,\lambda)^2 = \mathrm{Tr}[\rho_0(\lambda)\rho_0(\lambda+\delta\lambda)]. \quad (4)$$

Now, expanding $\rho_0(\lambda+\delta\lambda)$ in powers of $\delta\lambda$, and using the identity $\partial_\lambda[\langle\Psi_0(\lambda)|\Psi_0(\lambda)\rangle] = 0$, which implies $\mathrm{Tr}[\rho_0(\lambda)\partial_\lambda\rho_0(\lambda)] = 0$, one can easily show that

$$F(\lambda+\delta\lambda,\lambda) \simeq 1 - \frac{\delta\lambda^2}{4}\mathrm{Tr}\left(\frac{\partial\rho_0(\lambda)}{\partial\lambda}\frac{\partial\rho_0(\lambda)}{\partial\lambda}\right), \quad (5)$$

and thus

$$\mathcal{S}(\lambda) = \lim_{L\to\infty}\frac{1}{2L}\mathrm{Tr}\left(\frac{\partial\rho_0(\lambda)}{\partial\lambda}\frac{\partial\rho_0(\lambda)}{\partial\lambda}\right). \quad (6)$$

As mentioned before, 1QPTs (2QPTs) must come from discontinuity in (discontinuity in or divergence of) one or more matrix elements of ρ^{ij} ($\partial_\lambda\rho^{ij}$). Since the matrix elements of the reduced density matrix ρ^{ij} are linear functions of those of ρ_0, 1QPTs and 2QPTs will be associated with nonanalyticity in the matrix elements of $\partial_\lambda\rho_0$, and therefore imply the singularity in $\mathcal{S}(\lambda)$. That is, the singular behavior of the fidelity susceptibility is able to signal 1QPTs and 2QPTs. This explains the success of the fidelity approach discovered in the previous investigations. Note that the above conclusion is valid only if the discontinuous or divergent quantities do not accidentally all vanish or cancel with other terms in Eqs. (5) and (6) [i.e., assumptions (b) and (c) in Ref. 4]. However, some limitations of this approach are discussed in order. First, even though $\mathcal{S}(\lambda)$ can be a good indicator of 1QPTs and 2QPTs, it fails to distinguish between them, in contrast to the entanglement measurements discussed in Refs. 4 and 5. Second, from Eq. (6), we find that $\mathcal{S}(\lambda)$ cannot detect the higher-order QPTs resulting from the nonanalyticities in $\partial^2_\lambda\rho_0$ and even higher-order derivatives. Nevertheless, it does not mean that $\mathcal{S}(\lambda)$ always fails to signal the higher-order QPTs. Reminding that the two-particle reduced density matrix ρ^{ij} is calculated by taking a partial trace of ρ_0, it is thus possible that the nonanalyticities in the matrix elements of $\partial_\lambda\rho_0$ cancel one another in obtaining $\partial_\lambda\rho^{ij}$. That is, while the discontinuity or divergence in ρ^{ij} and $\partial_\lambda\rho^{ij}$ does imply the nonanalyticities in $\partial_\lambda\rho_0$, the reverse is not true. In this case, $\partial^2_\lambda\mathcal{E}$ can be continuous even though $\mathcal{S}(\lambda)$ is singular, and therefore such a higher-order QPT can indeed be detected by $\mathcal{S}(\lambda)$. One such example is provided by the BKT transition in the one-dimensional spin-1/2 *XXZ* model, where a critical anisotropy separates a gapless phase from a gapful phase. As demonstrated in Ref. 24, the ground-state energy and all of its derivatives with respect to the anisotropy are continuous at the critical point. That is, it is a QPT of infinite order. However, as discussed below, $\mathcal{S}(\lambda)$ does become singular despite the regularity of the ground state energy at this critical point.

It is known that many one-dimensional gapless systems, which may undergo the BKT transition, can be described by a single-component Luttinger model.[25] They include the spin-1/2 *XXZ* spin chain and the spin-1/2 *J*-*J*′ spin chain in their spin fluid phases, and the Bose-Hubbard model in its superfluid phase, etc. Before specifying to the *XXZ* spin chain, we first derive analytic formulas of the fidelity and the fidelity susceptibility for the single-component Luttinger model. By using the bosonization method, the Luttinger model can be described by the following effective Hamiltonian:[25,26]

$$H_{\mathrm{eff}} = \frac{u}{2}\int dx\left(K\Pi(x)^2 + \frac{1}{K}(\partial_x\Phi)^2\right). \quad (7)$$

Here the bosonic phase field operators Φ and Π are given by[27]

$$\Phi(x) \sim -\frac{i\sqrt{\pi}}{L}\sum_{k\neq 0}\left(\frac{L|k|}{2\pi}\right)^{1/2}\frac{1}{k}e^{-ikx}(a^\dagger_k + a_{-k}),$$

$$\Pi(x) \sim \frac{\sqrt{\pi}}{L}\sum_{k\neq 0}\left(\frac{L|k|}{2\pi}\right)^{1/2}\frac{k}{|k|}e^{-ikx}(a_k^{\dagger}-a_{-k}),$$

where a_k and $a_{k'}^{\dagger}$ obey canonical boson commutation relations: $[a_k,a_{k'}^{\dagger}]=\delta_{k,k'}$. We note that the Luttinger liquid parameters K and u are functions of the controlling parameter λ of the original Hamiltonian. When $K=1$, the effective Hamiltonian reduces to the free-boson model, whose ground state $|\Psi_0(K=1)\rangle$ is nothing but the vacuum $|0\rangle$ of the canonical bosons satisfying $a_k|0\rangle=0$ for all $k\neq 0$. When $K\neq 1$, the effective Hamiltonian contains the unpleasant terms $a_k a_{-k}$ and $a_k^{\dagger}a_{-k}^{\dagger}$. These terms can be diagonalized by a Bogoliubov transformation on the bosons such that

$$\alpha_{-k}=\cosh\theta a_{-k}+\sinh\theta a_k^{\dagger},$$

$$\alpha_k^{\dagger}=\sinh\theta a_{-k}+\cosh\theta a_k^{\dagger},$$

with $\cosh\theta=(1+K)/2\sqrt{K}$ and $\sinh\theta=(1-K)/2\sqrt{K}$. We note that, in the present case, the parameter θ is independent of the momentum k. The transformed Hamiltonian becomes a free-boson model in terms of the new set of canonical bosons α_k. That is, the effective model in Eq. (7) can be considered as a "quasifree" boson model, where the ground states $|\Psi_0(K)\rangle$ for general values of K are the vacuum of α_k satisfying $\alpha_k|\Psi_0(K)\rangle=0$ for all $k\neq 0$. Thus the (not normalized) ground states become

$$|\Psi_0(K)\rangle=\exp\left(-\frac{\sinh\theta}{\cosh\theta}\sum_{k\neq 0}a_k^{\dagger}a_{-k}^{\dagger}\right)|0\rangle. \quad (8)$$

With these exact expressions of the ground states, now one can calculate the ground-state fidelity. From its definition, the ground-state fidelity F of two (not normalized) ground states $|\Psi_0(K')\rangle$ and $|\Psi_0(K)\rangle$ becomes $F(K',K)=Z(K',K)/\sqrt{Z(K',K')Z(K,K)}$, where $Z(K',K)\equiv|\langle\Psi_0(K')|\Psi_0(K)\rangle|$. By using the expressions of the ground states in Eq. (8), it can be shown that

$$Z(K',K)=\prod_{k\neq 0}\left(1-\frac{\sinh\theta'\sinh\theta}{\cosh\theta'\cosh\theta}\right)^{-1}, \quad (9)$$

and therefore a general expression of the fidelity is reached,

$$F(K',K)=\prod_{k\neq 0}\frac{1}{\cosh(\theta'-\theta)}=\prod_{k\neq 0}\frac{2}{\sqrt{K/K'}+\sqrt{K'/K}}. \quad (10)$$

Here the prime denotes the corresponding variables taking their values at K'. Obviously, $F=1$ if $K'=K$. Generically, $1/\cosh(\theta'-\theta)<1$. Therefore, for systems with a large but finite size L, the fidelity in Eq. (10) scales as $[\cosh(\theta'-\theta)]^{-L}$, and decays very fast when K' separates from K. That is, the fidelity of two different ground states becomes zero in the thermodynamic limit, despite the two states being in the same phase. Therefore, in this case, it is difficult to signal a precursor of the QPT simply by seeking a drop in the fidelity. As mentioned before, a more effective indicator is provided by the fidelity susceptibility given in Eq. (3). From the analytic expression of the fidelity in Eq. (10), it can be shown that

$$\lim_{L\to\infty}\frac{\ln F(K+\delta K,K)}{L}\simeq-\frac{1}{8}\left(\frac{1}{K}\frac{dK}{d\lambda}\right)^2\delta\lambda^2, \quad (11)$$

and one finally obtains the general formula for the fidelity susceptibility

$$\mathcal{S}(\lambda)=\frac{1}{4}\left(\frac{1}{K}\frac{dK}{d\lambda}\right)^2. \quad (12)$$

Thus we show that $\mathcal{S}(\lambda)$ can be finite in the thermodynamic limit even for gapless systems. This result agrees with the findings in Ref. 14 based on the scaling arguments. In the present work, we further provide the analytic expression of $\mathcal{S}(\lambda)$. From this expression, we find that $\mathcal{S}(\lambda)$ becomes singular only when $dK/d\lambda$ diverges. It is noted that, in terms of the Luttinger liquid parameter K, the general expressions of F and $\mathcal{S}(\lambda)$ in Eqs. (10) and (12) apply to all one-dimensional systems in their Luttinger liquid phases. The precise location of the singularity in $\mathcal{S}(\lambda)$ can be determined, once the exact relation between the Luttinger liquid parameter K and the controlling parameter λ driving QPTs is known.

Now we consider the case of the XXZ spin chain, which can be taken as a special case in the Luttinger-liquid description. The Hamiltonian of the one-dimensional spin-1/2 XXZ model is written as

$$H=\sum_{j=1}^{L}(S_j^xS_{j+1}^x+S_j^yS_{j+1}^y+\lambda S_j^zS_{j+1}^z). \quad (13)$$

Here S_j^x, S_j^y, and S_j^z are the spin-1/2 operators at the jth lattice site. The parameter λ denotes an anisotropy in the spin-spin interaction. The XXZ spin chain is an exactly solvable model.[24] It is known that there is a critical point of 1QPT at $\lambda=-1$, which corresponds to the isotropic ferromagnetic Heisenberg model. At the isotropic antiferromagnetic point $\lambda=1$, a BKT transition occurs, which is described by a divergent correlation length but without true long-range order.

After applying the Jordan-Wigner transformation and bosonization procedure for the spin-1/2 operators, when $-1<\lambda\leq 1$, the Hamiltonian in Eq. (13) can be mapped to the bosonized effective Hamiltonian in Eq. (7).[25] That is, the XXZ spin chain can be considered as a quasifree boson model. For general values of λ (obeying $-1<\lambda\leq 1$), the Luttinger liquid parameters K and u can be obtained by comparison with the Bethe-ansatz solution. They are given by $K=(\pi/2)/[\pi-\arccos(\lambda)]$ and $u=\pi\sqrt{1-\lambda^2}/(2\arccos\lambda)$.[28] For $\lambda=0$, we have $K=1$; while $K\neq 1$ for $\lambda\neq 0$. Substituting the above exact relation between the Luttinger-liquid parameter K and the anisotropy parameter λ to Eqs. (10) and (12), the expressions of $F(\lambda',\lambda)$ and $\mathcal{S}(\lambda)$ can be obtained. Here we discuss $\mathcal{S}(\lambda)$ only, which becomes

$$\mathcal{S}(\lambda)=\frac{1}{4[\pi-\arccos(\lambda)]^2}\frac{1}{1-\lambda^2}. \quad (14)$$

Therefore, the fidelity susceptibility $\mathcal{S}(\lambda)$ diverges as $\lambda\to\pm 1$. That is, the singular behavior in $\mathcal{S}(\lambda)$ is able to signal either the 1QPT at $\lambda=-1$ or the BKT transition at $\lambda=1$. According to our previous analysis, the singularity in $\mathcal{S}(\lambda)$ at $\lambda=1$ indicates that one or more of the matrix elements of $\partial_\lambda \rho_0$ should be divergent at this BKT transition. Since the BKT transition is a QPT of infinite order, nonanalyticities in the density matrix of the ground state, ρ_0, must accidentally all vanish or cancel with other terms, such that the ground-state energy and all of its derivatives with respect to the anisotropy are continuous at this critical point. Therefore, the BKT transition in the *XXZ* spin chain does provide an example, where the higher-order QPTs can be detected by the singularity in the fidelity susceptibility.

In summary, according to the proposed general relation between QPTs and the fidelity susceptibility, the validity and the limitation of the fidelity susceptibility in characterizing QPTs are discussed. Employing our analytic formulas of the fidelity and the fidelity susceptibility for the one-dimensional Luttinger model, it is shown that the fidelity susceptibility can be finite even for critical systems, which agrees with the result in Ref. 14 based on the scaling analysis. Moreover, while the fidelity susceptibility may not detect higher-order QPTs in general, we demonstrate that the BKT transition, a QPT of infinite order, in the spin-1/2 *XXZ* chain can indeed be signaled by the singularity in the fidelity susceptibility. Though we restrict our attention to the *XXZ* spin chain, we believe that the same results will apply to all the BKT-type QPTs of one-dimensional models, such as the transition from spin fluid to dimerized phase in the *J*-*J*′ model, and the superfluid-insulator transition in the Bose-Hubbard model at integer filling, etc.

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