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Reexamination of entanglement and the quantum phase transition

Min-Fong Yang*
Department of Physics, Tunghai University, Taichung, Taiwan
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We show that, for an exactly solvable quantum spin model, a discontinuity in the first derivative of the ground-state concurrence appears in the absence of a quantum phase transition. It is opposed to the popular belief that the nonanalyticity property of ground-state concurrence can be used to determine quantum phase transitions. We further point out that the analyticity property of the ground-state concurrence in general can be more intricate than that of the ground-state energy. Thus there is no one-to-one correspondence between quantum phase transitions and the nonanalyticity property of the concurrence. Moreover, we show that the von Neumann entropy, as another measure of entanglement, cannot reveal quantum phase transitions in the present model. Therefore, in order to link with quantum phase transitions, some other measures of entanglement are needed.

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Quantum entanglement, as one of the most fascinating features of quantum theory, has attracted much attention over the past decade, mostly because its nonlocal connotation [1] is regarded as a valuable resource in quantum communication and information processing [2]. Recently a great deal of effort has been devoted to the understanding of the connection between quantum entanglement and quantum phase transitions (QPTs) [3–17]. Quantum phase transitions [18] are transitions between qualitatively distinct phases of quantum many-body systems, driven by quantum fluctuations. In view of the connection between entanglement and quantum correlations [19], one anticipates that entanglement will furnish a dramatic signature of the quantum critical point. People hope that, by employing quantum entanglement, the global picture of the quantum many-body systems could be diagnosed, and one may obtain fresh insight into the quantum many-body problem. Hence, in addition to its intrinsic relevance with quantum information applications, entanglement may also play an interesting role in the context of statistical mechanics.

The aforementioned studies are based on the analysis of particular many-body models. Recently a general framework of the relation between QPTs and bipartite entanglement was proposed [20]. They show that a discontinuity in or a divergence of the ground-state concurrence [the first derivative of the ground-state concurrence] can be both necessary and sufficient to signal a first-order QPT (1QPT) [second-order QPT (2QPT)]. This conclusion is only justified under conditions where artificial and/or accidental occurrences of nonanalyticity in both the entanglement measure (or its derivatives) and the derivatives of the ground-state energy are excluded. However, one may wonder if their results can be extended further for more general Hamiltonians, and if the correspondence between QPTs and bipartite entanglement can still be valid when the conditions are not satisfied.

In this paper, the entanglement properties (the ground-state concurrence and the von Neumann entropy) are calculated for an exactly solvable quantum spin model [21]. Contrary to conventional wisdom, we find that there exists a discontinuity in the first derivative of the concurrence, *at which there is no quantum critical point*. In fact, similar results had already been reported in Ref. [7] for a quantum spin model on a simplex in a magnetic field. Here we give general arguments to show why the analyticity property of the concurrence is more intricate than that of the ground-state energy. Furthermore, for the one-dimensional *XXZ* model at the critical point of the isotropic ferromagnetic case, it is found that the first derivative of the concurrence is discontinuous [6]. However, it is a 1QPT, instead of a 2QPT. The reason why the nonanalyticity of the ground-state energy of the *XXZ* spin chain does not faithfully reflect that of concurrence is explained. We note that, for our case and those in Refs. [6,7], the anomalous nonanalyticities in the concurrence all come from the operation of finding maximum value required by the definition of concurrence, but not originating from the density operator. Thus these cases seem to indicate that, for generic models, QPTs can not be distinctly characterized through the analysis of the analyticity properties of concurrence when some of the conditions mentioned in Ref. [20] are violated. That is, it is not always possible to infer the existence of QPTs from concurrence. Moreover, we show that, for the model considered in this paper, the von Neumann entropy remains constant even crossing the critical point. That is, the von Neumann entropy cannot always detect QPTs. Therefore, in order to have close connection with QPTs, some other measures of entanglement are needed.

The exactly solvable quantum spin model considered here is the isotropic spin-$\frac{1}{2}XY$ (or spin-$\frac{1}{2}XX$) chain with three-spin interactions [21],

$$H = -\sum_{i=1}^{N}\left[\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \frac{\lambda}{2}(\sigma_{i-1}^x\sigma_i^z\sigma_{i+1}^y - \sigma_{i-1}^y\sigma_i^z\sigma_{i+1}^x)\right], \tag{1}$$

where N is the number of sites, σ_i^α ($\alpha=x,y,z$) are the Pauli matrices, and λ is a dimensionless parameter characterizing

*Electronic address: mfyang@mail.thu.edu.tw

the three-spin interaction strength (in unit of the nearest-neighbor exchange coupling). The periodic boundary condition $\sigma_{N+1}=\sigma_1$ is assumed. This model can be solved by using the Jordan-Wigner transformation [22,23], and all physical quantities can in principle be calculated exactly. It is shown that the three-spin interaction can lead to a 2QPT at $\lambda_c=1$ [21].

Here we consider the entanglement between two specific spins in the ground state of a quantum system. The state of two spins i and j in the ground state of a quantum system is described in terms of the two-particle reduced density matrix ρ_{ij} obtained by tracing over other spins.

The structure of ρ_{ij} follows from the symmetry properties of the Hamiltonian. The Hamiltonian in Eq. (1) is real and it has the following two symmetries. One is a global $U(1)$-rotation symmetry about the spin-z axis, another is a Z_2 symmetry of a global π rotation about the spin-x axis [24]. These symmetries guarantee that ρ_{ij} has the form [25]

$$\rho_{ij}=\begin{pmatrix} u_{ij} & 0 & 0 & 0 \\ 0 & w_{ij} & z_{ij} & 0 \\ 0 & z_{ij} & w_{ij} & 0 \\ 0 & 0 & 0 & u_{ij} \end{pmatrix} \qquad (2)$$

in the standard basis $\{|\uparrow\uparrow\rangle,|\uparrow\downarrow\rangle,|\downarrow\uparrow\rangle,|\downarrow\downarrow\rangle\}$. Wang and Zanardi [26] have shown that the matrix elements of ρ_{ij} can be expressed in terms of the various correlation functions $\langle\sigma_i^\alpha\sigma_j^\beta\rangle$ $(\alpha,\beta=x,y,z)$

$$u_{ij}=\frac{1}{4}(1+\langle\sigma_i^z\sigma_j^z\rangle),$$

$$w_{ij}=\frac{1}{4}(1-\langle\sigma_i^z\sigma_j^z\rangle),$$

$$z_{ij}=\frac{1}{4}(\langle\sigma_i^x\sigma_j^x\rangle+\langle\sigma_i^y\sigma_j^y\rangle). \qquad (3)$$

Note that $u_{ij},w_{ij}\geqslant 0$ because of the inequality $|\langle\sigma_i^z\sigma_j^z\rangle|\leqslant 1$, which is a special case of the Schwarz inequality $|\langle A^\dagger B\rangle| \leqslant \sqrt{\langle A^\dagger A\rangle}\sqrt{\langle B^\dagger B\rangle}$ for $A=I$ (I is the identity operator) and $B=\sigma_i^z\sigma_j^z$.

From ρ_{ij}, the ground-state concurrence [27] quantifying the entanglement is readily obtained as [25,26]

$$C_{i,j}=2\max\{0,|z_{ij}|-u_{ij}\}$$
$$=\frac{1}{2}\max\{0,|\langle\sigma_i^x\sigma_j^x\rangle+\langle\sigma_i^y\sigma_j^y\rangle|-\langle\sigma_i^z\sigma_j^z\rangle-1\}. \qquad (4)$$

Because the entanglement between a pair of adjacent spins is expected to be dominant compared with a pair of non-nearest-neighbor spins, we focus on the nearest-neighbor case in the following discussions.

Using the method adopted by Lieb, Schultz, and Mattis [28], one can calculate the spin-spin correlation functions exactly [21],

$$\langle\sigma_i^x\sigma_{i+1}^x\rangle=\langle\sigma_i^y\sigma_{i+1}^y\rangle=G,$$

$$\langle\sigma_i^z\sigma_{i+1}^z\rangle=-G^2, \qquad (5)$$

with

$$G=\begin{cases}\dfrac{2}{\pi}, & \lambda<1,\\ \dfrac{2}{\pi\lambda}, & \lambda\geqslant 1.\end{cases} \qquad (6)$$

We find that, for the nearest-neighbor cases, two correlation functions $\langle\sigma_i^x\sigma_{i+1}^x\rangle$ and $\langle\sigma_i^z\sigma_{i+1}^z\rangle$ are dependent, and the latter can be written in terms of the former. Thus the nearest-neighbor concurrence is only determined by a single correlation function G. By substituting the results of the correlation functions into Eq. (4), the exact expression of the concurrence between a pair of adjacent spins becomes

$$C_{i,i+1}=\frac{1}{2}\max\{0,(G+1)^2-2\}. \qquad (7)$$

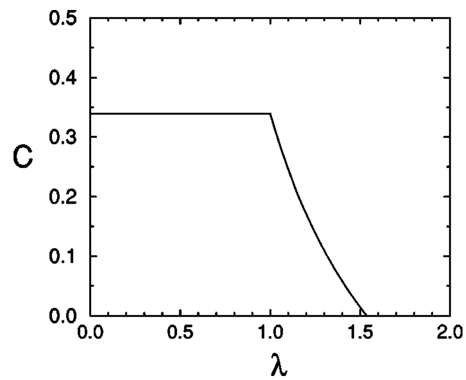

FIG. 1. The ground-state concurrence of the nearest-neighbor spins $C_{i,i+1}$ as a function of λ for the XX chain with three-spin interactions in Eq. (1).

The dependence of $C_{i,i+1}$ on λ is plotted in Fig. 1. We see that, both at $\lambda=\lambda_c=1$ and $\lambda=\lambda_0=2/(\sqrt{2}-1)\pi\approx 1.5369$, the first derivative of the concurrence $\partial C_{i,i+1}/\partial\lambda$ shows discontinuities, while $C_{i,i+1}$ is continuous. The discontinuity in $\partial C_{i,i+1}/\partial\lambda$ at $\lambda=\lambda_c=1$ do indicate the 2QPT of the present model, consistent with the proposal in Ref. [20]. However, an unexpected discontinuity in $\partial C_{i,i+1}/\partial\lambda$ occurs at $\lambda=\lambda_0$, which is *not* a critical point. The origin of nonanalyticity in the concurrence at $\lambda=\lambda_0$ comes from the requirement that the concurrence should be non-negative, but not from the nonanalyticity of ρ_{ij}. Therefore, the discontinuity in $\partial C_{i,i+1}/\partial\lambda$ needs not always indicate the existence of nonanalyticity in the ground state energy and show any QPT.

In a recent work studying the one-dimensional extended Hubbard model [15], the authors show that QPTs can be identified at places where the von Neumann entropy is extremum or its derivative is singular. The von Neumann entropy, another measure of entanglement, is defined as $S\equiv-\mathrm{tr}(\rho_j\log_2\rho_j)$, where ρ_j is the one-particle reduced density matrix obtained by tracing over all sites except the jth site, and therefore $\rho_j=\mathrm{tr}_i(\rho_{ij})$ (tr_i stands for tracing over the ith site). One may wonder if this measure of entanglement will still work for the present model. By using Eqs. (2) and (3) and after tracing over the ith site for ρ_{ij}, one obtains $\rho_j = \frac{1}{2}I$, and the von Neumann entropy $S=1$ for all λ. The von Neumann entropy thus fails to detect the QPT of the present model. It is because the nonanalyticity in the matrix elements of ρ_{ij} cancel each other by taking trace over the ith site. Hence the von Neumann entropy is not always useful to detect QPT.

We note that the present example will not be the only exception for the anticipation that the nonanalyticity property of concurrence can be used to determine QPT. In general, the concurrence [27] is defined by $C_{ij}=\max\{0,\widetilde{C}_{ij}\}$ with $\widetilde{C}_{ij} \equiv \gamma_1 - \gamma_2 - \gamma_3 - \gamma_4$. Here γ_α are the four eigenvalues, in descending order, of the matrix $R_{ij} \equiv \sqrt{\sqrt{\rho_{ij}}(\sigma_i^y \otimes \sigma_j^y \rho_{ij}^* \sigma_i^y \otimes \sigma_j^y)\sqrt{\rho_{ij}}}$ with ρ_{ij}^* being the complex conjugate of the reduced density matrix ρ_{ij} in the standard basis. We emphasize that, even for the models such that $\widetilde{C}_{ij}$ is always non-negative and *the matrix elements of* ρ_{ij} *change smoothly* as the physical parameter, say λ, is varied, the concurrence (in this case $C_{ij}=\widetilde{C}_{ij}$) can still show a cusplike singularity at some $\lambda=\lambda_0$. For example, this will happen (cf. Eq. (7) of Ref. [19]) if at least one of the γ_α takes the form of $|A-B|$ (where A and B denote two functions of λ), and $A-B$ changes sign at $\lambda=\lambda_0$. Therefore, the concurrence can be nonanalytic, but it again does not correspond to a QPT. That is, although the eigenvalues γ_α are algebraically related to the matrix elements of ρ_{ij}, $\widetilde{C}_{ij}$ may still have *different* analyticity properties from ρ_{ij}. Remembering that $\max\{0,\widetilde{C}_{ij}\}=|\widetilde{C}_{ij}|/2+\widetilde{C}_{ij}/2$, it is clear that the two possibilities of the unexpected discontinuities in $\partial C_{i,i+1}/\partial\lambda$ discussed above all originate from the nonanalyticity of the absolute-value function. As mentioned before, an unexpected discontinuity in $\partial C_{i,i+1}/\partial\lambda$, which does not indicate a QPT, had already been reported in Ref. [7]. We believe that the nonanalyticity in the concurrence in that case may be due to the reason explained above.

Even though the discontinuity in the first derivative of the concurrence does indicate a QPT, it may not be 2QPT. An example is the one-dimensional *XXZ* model,

$$H_{XXZ} = \sum_{i=1}^{N} [\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \Delta\sigma_i^z\sigma_{i+1}^z]. \qquad (8)$$

It is shown that, at the critical point $\Delta=-1$ (corresponding to the ferromagnetic Heisenberg model), $\partial C_{i,i+1}/\partial\Delta$ is discontinuous, while $C_{i,i+1}$ is continuous and $C_{i,i+1}|_{\Delta=-1}=0$ [6]. However, it is a 1QPT (see below), instead of 2QPT. The reason why the nonanalyticity of the concurrence of the *XXZ* spin chain does not faithfully correspond to that of the ground-state energy is explained below.

We first show the relations among the ground state energy (and its first derivative), the matrix elements of the reduced density matrix, and the concurrence for the *XXZ* spin chain. The concurrence of the *XXZ* spin chain has the same expression as Eq. (4) [5,19,26,29]. Due to the translational invariance, the ground-state energy per site for the *XXZ* spin chain can be written as $\mathcal{E}=\langle\sigma_i^x\sigma_{i+1}^x\rangle+\langle\sigma_i^y\sigma_{i+1}^y\rangle+\Delta\langle\sigma_i^z\sigma_{i+1}^z\rangle$. Employing the Hellmann-Feynman theorem [30], one has $\partial\mathcal{E}/\partial\Delta = \langle\sigma_i^z\sigma_{i+1}^z\rangle$. Thus, for the nearest-neighbor spins, two matrix elements $u_{i,i+1}$ and $z_{i,i+1}$ of the reduced density matrix can be written as

$$u_{i,i+1} = \frac{1}{4}\left(1 + \frac{\partial\mathcal{E}}{\partial\Delta}\right),$$

$$z_{i,i+1} = \frac{1}{4}\left(\epsilon - \Delta\frac{\partial\mathcal{E}}{\partial\Delta}\right), \qquad (9)$$

and the nearest-neighbor concurrence becomes $C_{i,i+1}=\max\{0,\widetilde{C}_{i,i+1}\}$ with

$$\widetilde{C}_{i,i+1} = -\frac{1}{2}\left[(\mathcal{E}+1) + (1-\Delta)\frac{\partial\mathcal{E}}{\partial\Delta}\right]. \qquad (10)$$

Here we use the fact that $\langle\sigma_i^x\sigma_{i+1}^x\rangle+\langle\sigma_i^y\sigma_{i+1}^y\rangle \leqslant 0$. This inequality is satisfied for the *XXZ* spin chain in Eq. (8), because the ground-state wave function obeys the Marshall-Peierls sign rule [31].

The *XXZ* spin chain is an exactly solvable model, and the expression of $\mathcal{E}$ can be found in Ref. [32]. For the critical point $\Delta=-1$, one has $\mathcal{E}|_{\Delta=-1}=-1$, $\partial\mathcal{E}/\partial\Delta \to 0$ as $\Delta \to -1^+$ and $\partial\mathcal{E}/\partial\Delta=1$ for $\Delta < -1$. Thus $\partial\mathcal{E}/\partial\Delta$ is discontinuous at $\Delta=-1$, which is a manifestation of a 1QPT. Based on these results, we find that $\widetilde{C}_{i,i+1}$ is indeed not continuous at $\Delta=-1$, where it has a finite jump from -1 to 0. However, because $C_{i,i+1}=\max\{0,\widetilde{C}_{i,i+1}\}$, $C_{i,i+1}$ becomes continuous and equal to zero at $\Delta=-1$. That is, the discontinuity in $\widetilde{C}_{i,i+1}$ is hidden under the operation $\max\{0,\ldots\}$. That is the reason why the nonanalyticity of the concurrence is not faithfully induced by that of the ground-state energy. In short, the discontinuity in the first derivative of $\mathcal{E}$ (and therefore the matrix elements of the reduced density matrix) may not always lead to discontinuity in $C_{i,i+1}$. Therefore, a 1QPT may be misunderstood as a 2QPT through analyzing the nonanalyticity property of concurrence.

There is another critical point of the *XXZ* spin chain at $\Delta=1$ (corresponding to the antiferromagnetic Heisenberg model). It is found that $C_{i,i+1}$ and $\partial C_{i,i+1}/\partial\Delta$ are both continuous at $\Delta=1$, and $\partial C_{i,i+1}/\partial\Delta|_{\Delta=1}=0$ (or $C_{i,i+1}$ reaches its maximum value at $\Delta=1$) [5,6]. It is interesting to see how these results can be realized in the present framework. At the critical point $\Delta=1$, it is shown in Ref. [32] that $\mathcal{E}$ and all of its derivatives with respect to Δ are continuous. Therefore, $C_{i,i+1}$ ($=\widetilde{C}_{i,i+1}$, because $\widetilde{C}_{i,i+1} \geqslant 0$ in this case) and $\partial C_{i,i+1}/\partial\Delta$ will not show discontinuity at $\Delta=1$. Moreover, since

$$\frac{\partial C_{i,i+1}}{\partial\Delta} = -\frac{1}{2}(1-\Delta)\frac{\partial^2\mathcal{E}}{\partial\Delta^2}, \qquad (11)$$

we find that $\partial C_{i,i+1}/\partial\Delta \to 0$ as $\Delta \to 1$. Thus the results in Refs. [5,6] are reproduced.

In summary, although many examples indicate that QPTs can be distinctly characterized through the analyticity properties of concurrence, we stress in this paper that this viewpoint is not true in general. Except those cases of 2QPTs indicated by the discontinuity in $\partial C_{i,i+1}/\partial\Delta$, it is also possible that (i) $\partial C_{i,i+1}/\partial\Delta$ is discontinuous, but there is no QPT

(Ref. [7] and the present case) or (ii) $\partial C_{i,i+1}/\partial\Delta$ is discontinuous, while it is a 1QPT rather than 2QPT (*XXZ* spin chain at $\Delta=-1$ [6]). We further point out that QPTs can not always be diagnosed even by using the von Neumann entropy. As far as we know, there are some other measures of entanglement, say localizable entanglement [10] and global measure of entanglement [11]. Therefore, while the analyticity properties of concurrence and von Neumann entropy are not necessarily related to the existence of critical points, other measures of entanglement may work. Thus more effort is necessary to clarify the relationship between QPTs and entanglement.

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