Entanglement in quantum phase transition

Huihuo Zheng*

Department of Physics, University of Illinois at
Urbana-Champaign Urbana, IL 61801-3080, USA

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Abstract

A quantum phase transition (QPT) happens when the zero-temperature quantum fluctuations in a quantum many-particle system cause a transition from one type of ground state to another. Such transitions are induced by the change of a physical parameter. Long-range correlations in the ground state also develop at quantum critical regime. It turns out the property responsible for the long-range correlations is entanglement. The system state is strongly entangled at the critical point. Therefore we expect that systems near quantum critical points can be characterized in terms of entanglement. In this paper, we studied the use of entanglement measures for identifying and characterizing quantum phase transitions, and examined the scaling behavior of entanglement near quantum critical point, and finally studied the renormalization of entanglement under real space renormalization.

^{*} hzheng8@illinois.edu

I. INTRODUCTION

The crucial difference between a quantum mechanical many body system with a classical one is the entanglement between different parts of the system. "...the fact that the best possible knowledge of a whole does not necessarily include the same for its parts..., The whole is in a definite state, the parts taken individually are not...This is not one, but the essential trait of the new theory, the one which forces a complete departure from all classical concepts." [1] In fact, a highly entangled ground state is at the heart of a large variety of collective quantum phenomena. Entanglement plays a central role in the study of quantum state of matter, especially the zero temperature quantum phase transition (QPT).

QPT happens when the zero-temperature quantum fluctuations in a quantum many-particle system cause a transition from one type of ground state to another. [2] Such transitions are induced by the change of a physical parameter magnetic field, chemical potential, pressure,... that enhances the quantum fluctuations. Similar to the conventional finite temperature phase transition, at critical point, there are long-range correlations in the system. Given that the entanglement itself has the property of "effective" non-locality, we may intuitively expect to see certain relations between the long-range correlations occurs at criticality and the quantum entanglement of the system. It is found that the system state is strongly entangled at the critical point. The entanglement shows divergence behaviors at quantum critical point. It is believes that the property responsible for the long-range correlations is entanglement. [3] We therefore expect further that systems near quantum critical points can be characterized in terms of entanglement.

This paper is aimed at revealing the roles of entanglement in quantum phase transition. We will study the use of entanglement measures for identifying and characterizing quantum phase transitions. The outline of the paper is as follows. in Section II, we explicitly study the behavior of entanglement at quantum criticality; we will first introduce the measure of entanglement, and then show that entanglement can help to identify different universality class; the scaling behavior of entanglement is examined by using a exactly solvable spin model. In Section III, we will study the behavior of entanglement under renormalization group transformation, specifically, we are focus on the real space renormalization of the state. We hope this paper would provide a comprehensive picture about entanglement in QPT.

II. ENTANGLEMENT IN QUANTUM CRITICALITY

In this section, we will focus on the entanglement near quantum critical points. But before delving into this subject, let us briefly introduce how to quantify the amount of entanglement – entanglement entropy.

A. Quantify of entanglement in many body system

The problem of measuring and quantifying quantum correlations, or entanglement, in many body quantum systems is a field of research in its own. But here, we will not delve too deep into this subject; instead, we shall only discuss the Von Neumann entropy as a figure of merit for entanglement. [4] Remember in quantum mechanics text book, the entanglement

is first introduced in system of two electrons. They lie in the following state,

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle). \tag{1}$$

We say such a state is an entangled state since when we spatially separate the two electron far away from each other, and measure the spin of one electron, the other electron collapses to the state different from the one being measured, no matter how far they are separated. In contrast to the singlet state, the electrons are less entangled in $|\uparrow,\uparrow\rangle$. The latter is usually called a product state. Generically speaking, if a state cannot be written in a product state no matter what basis we choose, we say it is an entangle state. The Van Neumann entropy is one of the simplest one to quantify the entanglement between to bodies. In a quantum system, we are interested at how part of the system get entangled with the rest of the system (environment). To formulate this, we first bipartition the system into subsystem A and B, and then trace out the B degree of freedom in the density matrix of the system,

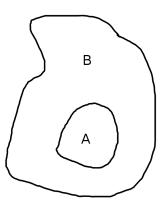


FIG. 1. Bipartition of the system

$$\rho_A = \text{Tr}_B |\Psi\rangle\langle\Psi|\,,\tag{2}$$

and then define the entanglement entropy as

$$S_A = -\text{Tr}\rho_A \log_2 \rho_A. \tag{3}$$

To be more explicitly, we know that and in general the state of the whole system can be written as a superposition of direct product states (this can be done by using Smith decomposition),

$$|\psi_{AB}\rangle = \sum_{i}^{\chi} \alpha_{i} |\varphi_{i}\rangle_{A} |\phi_{i}\rangle_{B}, \quad S_{A} = S_{B} \equiv -\sum_{i} \alpha_{i}^{2} \log \alpha_{i}^{2}.$$
 (4)

One can get that the entanglement entropy for singlet state is 1, and for $|\uparrow,\downarrow\rangle$ is 0.

From the above discussion, we already see that highly entangled states are usually those superposed by many product states rather than one. This is the key that highly entangled states have long range correlations. For a purely product state, it is easy to verify that

$${}_{c}\langle\Psi|O_{i}O_{j}|\Psi\rangle_{c} \equiv \langle\Psi|O_{i}O_{j}|\Psi\rangle - \langle\Psi|O_{i}|\Psi\rangle\langle\Psi|O_{j}|\Psi\rangle = 0 , \qquad (5)$$

Quantum systems are ultimately characterized by correlations of various observables. Far from quantum criticality, the correlation of an observable decays exponentially as a function of the distance separating them; whereas in the case the system undergoes a phase transition, it decays algebraically. The correct assessment of these quantum correlations is tantamount to understanding how entanglement is distributed in the state of the system. This is easily understood as follows. Let us consider a connected correlation.

There are some intuitive properties of the Von Neumann entropy;

- 1. For a pure state, $S_A = S_B$ (all the pure states can be smith decomposed into a superposition of direct product states)
- 2. The entanglement entropy characterized the number of "communication" channels between two parts systems. In system with finite correlation length, it is proportional to the area of the boundary, $S = \gamma A + \dots$ This is called area law. While the proportional constants are usually depends on the geometry of the boundary [5].
- 3. For critical system, the correlation length is infinity, we expect that the entanglement "saturates through the whole system". If we calculate the entanglement entropy between a subsystem A with the rest of the system B, it depends on the size of A, rather than the boundary between A and B. This is seen in (1+1D) critical system, where $S_A \propto \log L$. And the proportional constants is different for different universality classes.

Another interesting fact about the entanglement entropy is that, there might be a constant term which do not depend on the size of the system. This term call topological entanglement entropy, which only exist in some topological nontrivial system, for example Toric code model, Kitaev model, fractional quantum hall system, etc. [6] In fact, this size independent term tell us that the topological entanglement entropy is a global long-range correlation/entanglement.

B. Entanglement entropy in identifying universality classes in (1+1) quantum system critical system

From renormalization group theory, we know that critical systems are classified into different universality classes based on symmetry and dimension of the system. Mathematically, the symmetry are described by conformal group, which includes the rotation, translation, scaling and spatial transformation (the last one might be unfamiliar). And the different universality class are simply different representations of the conformal symmetry. In two dimension, it is special, the conformal group is infinitely dimensional. All the conformal transformations are described by homogeneous function in complex analysis, or mathematically, the representation of Virasoro algebra, which are generators of global and local conformal symmetry. [7, 8]. We will not going to details of the conformal field theory, one can refer the book "Conformal field theory" [9].

An important fact which we already mentioned in last section is that the entanglement entropy in critical ground states of one dimension (1+1) diverges with the size of the subsystem, [4]

$$S_{A,PBC} \sim \frac{c}{3} \log \left(\frac{L}{a}\right) + c_1' + \dots$$
 periodic boundary condition, (6)

$$S_{A,OBC} \sim \frac{c}{6} \log \left(\frac{L}{a}\right) + \tilde{c}'_1 + \dots$$
 open boundary conditions. (7)

Here L is the size of the subsystem, and a is certain microscopic length scale of the system. Surprisingly, the proportion coefficient determined can be used to characterize universality classes of critical systems. Hence, c is called central charges. Note that we have different coefficients 1/6 and 1/3 for OBC and PBC is simply due to that we have two boundaries in PBC. Central charge is different in different universality classes. For free fermion, it is 1/2, and free bosons, it is 1. And based on conformal field theory, we know, in most of the case, c uniquely determines the representation of the field theory in Virasoro algebra (an exception is c = 1, in which case we need Luttinger parameters to uniquely determines the universality class). Well it is hard to intuitively describe the physical meaning of the central charges. Two important facts may help us to understand this (1) c is related to the degree of freedom of the system. If we put two c = 1 free bosons field together, we get c = 2 field theory. (2) c is related to vacuum energy of the system (Casimir energy), if we change the geometry of the space (for example from a 2D plane to a cylinder), the energy shift will be proportional to the central charge (in fact, c emerges whenever we do local transformation). In a sense, central charge can sense the geometry of the system.

Therefore, by studying the finite size scaling behavior of the system at critical regime, we can extrapolate the central charge of the system and hence identify the universality class of the system. We will study the quantum Ising model with transverse magnetic field to show this results.

C. Non-analyticity and scaling behavior of entanglement entropy near quantum critical point

As we know, quantum phase transitions happen when the ground state energy level cross or touch the first excited state energy level. It directly leads to non-analyticity of the energy of the system. However, we also know that the system sits in the ground state. We should be able to probe similar non-analyticity behavior of the state near quantum phase transition by measuring the entanglement entropy near quantum critical point. A non-analyticity in the ground state automatically propagates into the elements of the density matrix and hence the entanglement entropy of the system. And indeed, this conjecture has been confirmed in many one dimensional exactly solved spin chain model. For example, Fig. 2 shows the entanglement entropy between one block of spins with the rest of the system in paramagnetic quantum Ising model with transverse magnetic fields,

$$H = -\lambda \sum_{\langle s_1, s_2 \rangle} \sigma_{s_1}^x \sigma_{s_2}^x - \sum_s \sigma_s^z, \tag{8}$$

which is exactly solvable by mapping this system to a free fermion using a standard trick: Jordan-Wigner transformation. The exact results for entanglement entropy are, [4]

• $\lambda < 1$ (Paramagnetic phase)

$$S = \epsilon \sum_{j=0}^{\infty} \frac{2j+1}{1 + e^{(2j+1)\epsilon}} + \sum_{j=0}^{\infty} \log(1 + e^{-(2j+1)\epsilon}).$$
 (9)

(2) $\lambda > 1$ (Ferrermagnetic phase)

$$S = \epsilon \sum_{j=0}^{\infty} \frac{2j}{1 + e^{2j\epsilon}} + \sum_{j=0}^{\infty} \log(1 + e^{-2j\epsilon}).$$
 (10)

Here, ϵ is defined as

$$\epsilon = \pi \frac{K(\sqrt{1 - k^2})}{K(k)}, \quad k = \min[\lambda, \lambda^{-1}], \tag{11}$$

Using this formula, one can easily deduce that the entanglement has logarithm diverges at $\lambda = 1$.

$$S \propto \ln|1 - \lambda| \,. \tag{12}$$

The plot of the entanglement entropy is in Fig. 2. From the data, we also see that, for $\lambda \to 0$, the system goes to a product state $\uparrow, \uparrow, \cdots \uparrow$ so that the entanglement entropy vanishes. And for $\lambda \to \infty$, the system goes to $\frac{1}{\sqrt{2}}(|\leftarrow \leftarrow \cdots \leftarrow \rangle + |\rightarrow \rightarrow \cdots \rightarrow \rangle$, the entanglement entropy is log 2.

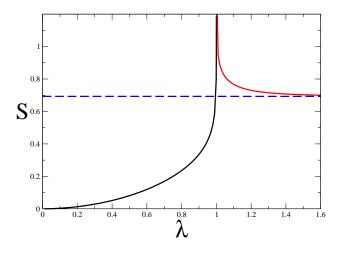


FIG. 2. Scaling of entanglement entropy near quantum critical point. $\lambda_c = 1$, quoted from [4]

III. RENORMALIZATION OF ENTANGLEMENT ENTROPY

Renormalization group (RG) achieve great success in the study of quantum phase transition in the last decades. In this section, we will study the effect of renormalization to entanglement entropy. But here, we focus the real space numerical renormalization, called density matrix renormalization method. We will have two benefits in studying this subject. From one hand, we can better understand the properties of entanglement entropy, especially their relations to the system's microscopic degree of freedom; from the other hand, by comparing the traditional renormalization group method with the DMRG, we will see how entanglement play a crucial role in quantum state of matter, which in turns can help us build up new effective numerical methods.

Let us briefly introduce the traditional numerical renormalization group method based on Wilson's RG[10], and DMRG method.

A. Real space renormalization group transformation

The key idea of the renormalization group is to successively discard degrees of freedom in a system until the dominant terms may be identified. In each renormalization step, we make a decision about what degrees of freedom in a system are important. Normally, if we are interested in the low energy (long range) physics of the system, we simply integrate out high momentum (microscopic degree of freedom), and successfully coarse grain the system and finally keep only the macroscopic degree of freedom. In fact, this is the traditional RG procedures when it was first developed. Based on the traditional RG, a numerical implementation for quantum systems was developed and was first successfully applied to Kondo problem. [10] Following the computational physicist community, we will call this method numerical renormalization group (NRG). The basics NRG procedure is as follows,

- 1. Start at a finite size of block with Hilbert space N;
- 2. Double the size, now the Hilbert space increases to $N \times N$;
- 3. Solve the double-sized system exactly, but project to the lowest energy N states.
- 4. treat the new projected Hamiltonian (with Hilbert space dimension N) as new starting point, and redo [1], [2], [3] & [4] until everything converges.

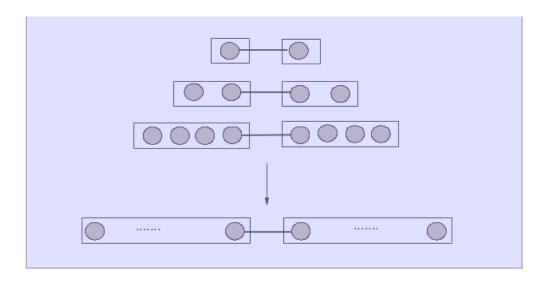


FIG. 3. Schematic procedures of NRG

By such we start from a finite size and if we are lucky enough, we will successfully approach the thermodynamic limit. This method works very well for Kondo problem, but the convergence behavior is not good for other systems. In fact, examine the heart of the RG method, it is safe to say that the decision we have made to discard those what we thought is important restrict the validity of our specific RG method. White [11, 12] is the first to found and resolve the key issue of NRG. He then developed a new renormalization group scheme, DMRG.

Basically, the only change of the DMRG with respect to NRG is that it keep those basis which strongly entangled with other parts of the system. We start at L and R blocks, and increase the size of both L and R blocks. Solve them exactly and take the ground state of

new enlarged system, build up the reduced density matrix of the L' and R'; project L' and N' to those states corresponding to larger eigenvalue of the reduced density matrix. And based on the renormalized \tilde{L} and \tilde{R} , we repeat the procedures. The key here is that for most quantum state of matter, different part of the system are closely entangled. And those degree of freedom greatly entangled with other parts of the system are most relevant to the system. So based on the failure of RNG and and success of DMRG, we see what a important role entangle has played in quantum phase of matter.

What is more, later on, people find that DMRG works well for gapped system, but fails again for gap less systems (critical system). The reason is also due to entanglement. It is find that near the critical points, almost all degree of freedom are strongly entangled. If one examine the eigenenergy of the reduced density matrix, large amount of them are in the same order. They are almost equally important in characterizing the physics of the system. It is hard for DMRG to do a finite truncation of the Hilbert space. This fate of DMRG can be described by a traditional Chinese saying: "Success owes to Xiao He; failure is also due to Xiao He" (Xiao He is a famous soldier leader in history)

B. Entanglement entropy flow under RG

In this subsection, let us discuss the flow of entanglement entropy under renormalization flow. Intuitively, we know that the renormalization group procedures successfully throw away some degrees of freedom. This flow Entanglement entropy is closely related to the system's degree of freedom. Hence, we should expect a monotonically decrease of the renormalized entanglement entropy. We can also understand this from the relations between entanglement and correlations. In each RG step, systems go further and further away from critical point and flow into some "attractive" fix point which characterize some particular phase of the system and at which the correlation length vanishes. Therefore, following this argument, we should expect that

- (a) under the RG flow, the renormalized entanglement decreases and the system eventually flows into a non-entangled product state.
- (b) If the system is exactly sitting at the critical region. The correlation exists in all length scales. Therefore, the entanglement entropy should be invariant under this renormalization transformation.

Our above simple argument have already been studied by Ref. [13]. In Ref. [13], the authors demonstrate the effect of renormalization to entanglement entropy of a anti-ferro magnetic, quantum Ising model with transverse magnetic field,

$$H = \sum_{\langle s_1, s_2 \rangle} \sigma_{s_1}^x \sigma_{s_2}^x + h \sum_s \sigma_s^z,$$
 (13)

This model is exactly solvable. There is a phase transition at h=1.0 Here, in Fig. 4, the unnormalized entanglement entropy are for those system of the same size but without doing any renormalization transformation. The renormalized entanglement are for the renormalized system.

First, the unnormalized entanglement entropy in upper panel (thick blue) scales like log L, which is already mentioned in Section II of this paper. Instead, renormalized entanglement remains constant along successive RG transformations, as a clear manifestation of scale

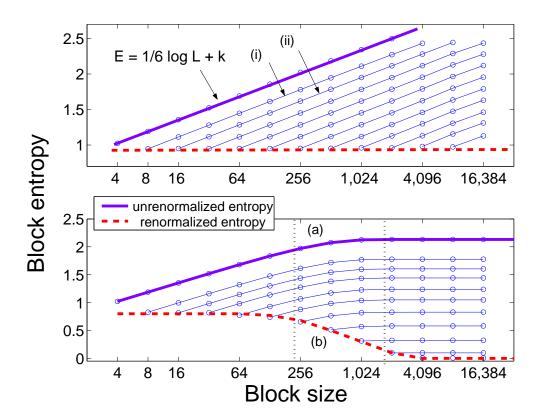


FIG. 4. Scaling of the entropy of entanglement in 1D quantum Ising model with transverse magnetic field. quoted from Ref. [14]

invariance. The proportional coefficient tells us that the central charge of the system is 1/2, belonging to the free fermion universality class. In fact, we already know that by using the Jordan-Wigner transformation, we are able to map this model into a free fermion one.

Second, the renormalized entanglement entropy in the critical point, (red line in upper panel) remains constant under renormalization procedures as we expected.

Third, in the non critical regime (h=1.000, which is still very close to the critical point), the unnormalized entanglement scales roughly as in the critical case until it saturates (a) for block sizes comparable to the correlation length. Beyond that length scale, the renormalized entanglement vanishes (b) and the system becomes effectively untangled.

IV. CONCLUSION

Entanglement play a very important role in quantum state of matter: it is responsible for long-range correlations near the quantum critical regime; It reflects the non analyticity of the ground state during quantum phase transition; it is scale invariant in critical point where as monotonically decreases away from critical point. Therefore, entanglement entropy is a good measure for identifying and characterizing quantum phase transitions.

V. ACKNOWLEDGEMENT

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