Diagonal Entropy in Many-Body Systems: Volume Effect and Phase Transitions

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We investigate the diagonal entropy of the ground state of quantum many-body systems. Diagonal entropy is concerning about only the diagonal form of the ground state reduced density matrix, which can be obtained more easily in comparison to the whole reduced density matrix. We show that the diagonal entropy can be represented as a volume term plus a logarithm term on the number of spins and a constant term. Remarkably, the diagonal entropy provides signatures of all quantum phase transitions for the studied XY-model. The quantum phase transitions characterized by diagonal entropy agree well with the phase diagram. Besides, by combining the entanglement entropy and diagonal entropy, we naturally find the relative entropy of quantum coherence. Our findings show that the diagonal entropy contains rich physics and is worth exploring in studying various quantum systems.

Introduction.— A quantum phase transition may occur as a parameter in the Hamiltonian of a many-body system varies at zero temperature. Over the past years, many types of quantum properties of ground states, in particular quantum entanglement and other non-classical correlations, have been successful in distinguishing different quantum phases, see, for example, Refs. [1–18]. Intuitively, it is because of that a highly entangled ground state plays a central role for a large variety of collective quantum phenomena. Therefore, it is believed that different quantum phenomena might be identified by the characteristics of the entanglement or other non-classical quantum correlations of the ground state and fields. Additionally, the profoundly entangled ground state can also embrace topological entanglement entropy on occasions, which characterizes the global feature of the topologically ordered for the system [19, 20].

On the other hand, a density matrix in diagonal form is considered as classical from the point of view of quantum information science. For a ground state of a many-body system, the diagonal part of its density matrix, which is obtained by deleting all the off-diagonal elements, has no entanglement or any other non-classical correlations. It is curious, though, whether this diagonal matrix still contains intrinsically any information of quantum properties of the system such as the evidence in identifying quantum phase transitions. The answer is of great importance both theoretically and experimentally. It is interesting in theory that a new signature, which has long been believed as essentially a classical quantity, would be found in relating with quantum phase transition. For experiment of quantum information processing, from the operational point of view, a density matrix for a \( N \)-qubit system can be standardly obtained by state tomography, however, with exponentially growing effort in the number of qubits for covering all necessary measurement bases [18, 21]. It is therefore intractable to obtain a density matrix when \( N \) is large. Moreover, the off-diagonal entries are quite difficult to measure on many experimental platforms [22]. In contrast, the diagonal part of the density matrix can be much more easily obtained by only measurements in the computational basis.

In this Letter, we will investigate the diagonal entropy (DE), defined as the von Neumann entropy of the diagonal matrix of the density matrix, for the ground states of many-body systems. It can be considered as a modification of quantum entanglement [35–37]. Surprisingly, we find that DE contains rich information of quantum properties of the many-body systems including the quantum phase transitions. It is then established that DE would provide us a useful method in studying quantum many-body systems.

Entanglement entropy (EE) has been extensively studied for many-body systems, especially for those where the area law is satisfied [23–27]. It is also well known that the sub-leading term for topologically ordered state can lead to topological entanglement entropy [19, 20]. The motivation to study DE has two folds: First, DE is an independent quantity different from EE. Secondly, quantum coherence, which can also be considered as resource for quantum information processing like entanglement, can be quantified as difference between DE and EE [28]. As a result, DE being the difference between EE and quantum coherence quantifies the remaining quantum re-
source of entanglement after subtracting the contribution from quantum coherence. Quantum coherence itself is worth exploring for many-body systems [29–31]. Now, with the available results for EE, the exploration of DE and then subtraction EE will directly lead to the result of quantum coherence. We emphasize that DE for ground states of quantum many-body systems does not depend on partitions which is generally artificial, but necessary in defining quantum entanglement.

The XY-model and the ground state diagonal reduced density matrix.—We study the XY-model of spin-1/2 chain. The Hamiltonian is written as,

$$H = -\sum_{l=0}^{N-1} \frac{1}{2} [(1 + \gamma) \sigma_x^l \sigma_x^{l+1} + (1 - \gamma) \sigma_y^l \sigma_y^{l+1}] + \lambda \sigma_z^l,$$

(1)

where $\sigma_x^l$, $\sigma_y^l$ and $\sigma_z^l$ are Pauli matrices and the subscript $l$ is the site number. This model describes a variety of XY spin-spin interactions between nearest neighbours as well as the effect of an external magnetic field along the Z direction. It is associated with several one-dimensional quantum systems. For $\gamma = 0$, the Hamiltonian becomes the XX-model. For $\gamma = \pm 1$, it becomes the Ising model with transverse field. The length of the spin chain is infinite $N \to \infty$, and periodic boundary condition is assumed.

We consider a block of $L$ contiguous spins in the chain, which should be translational invariant. For convenience, we choose the block to contain qubits $l = 1, \ldots, L$. The corresponding reduced density matrix, $\rho_L$, for the ground state of the Hamiltonian can be expanded in terms of Pauli matrices and the identity $\sigma^0_l$ as,

$$\rho_L = 2^{-L} \sum_{\mu_1, \ldots, \mu_L} \rho_{\mu_1, \ldots, \mu_L} \sigma_{\mu_1}^{l_1} \cdots \sigma_{\mu_L}^{l_L},$$

(2)

where the coefficients $\rho_{\mu_1, \ldots, \mu_L}$ are given by the ground state as, $\rho_{\mu_1, \ldots, \mu_L} = \langle \sigma_{\mu_1}^{l_1} \cdots \sigma_{\mu_L}^{l_L} \rangle$. To calculate DE only the diagonal elements are necessary, and we just need to consider the terms, $\mu_l = \{0, z\}$. Hereafter, we will focus on the diagonal matrix $\rho_{\mu_1, \ldots, \mu_L}^{\text{diag.}}$ with the corresponding coefficients $\rho_{\mu_1, \ldots, \mu_L}^{\text{diag.}}$, which means that condition $\mu_l = \{0, z\}$ is taken. Explicitly, we have,

$$\rho_{\mu_1, \ldots, \mu_L}^{\text{diag.}} = \langle \sigma_{\mu_1}^{l_1} \cdots \sigma_{\mu_L}^{l_L} \rangle, \quad \mu_l = \{0, z\}.$$  

(3)

We follow the method in Ref.[4], and introduce the Majorana operators defined as,

$$c_{2l} = \left( \sum_{m=0}^{l-1} \sigma_m^x \right) \sigma_l^x, \quad c_{2l+1} = \left( \sum_{m=0}^{l-1} \sigma_m^z \right) \sigma_l^y.$$  

(4)

Then the operator $\sigma_l^z$ can be written by Majorana operators as,

$$\sigma_l^z = -i c_{2l+1} \sigma_l^y = -i c_{2l} c_{2l+1}.$$  

(5)

Substituting this representation into Eq.(3), the coefficients $\rho_{\mu_1, \ldots, \mu_L}^{\text{diag.}}$ can be calculated. The procedure is to calculate the terms classified by the number of zs. For example, for the case $\mu_m, \mu_n = z$ and $\mu_{l \neq m, n} = 0$, the coefficient is rewritten as

$$\rho_{0\ldots0\ldots0\ldots0} = \langle \sigma_{1}^{0} \cdots \sigma_{m}^{z} \cdots \sigma_{n}^{z} \cdots \sigma_{L}^{0} \rangle = (\delta_{m+n} - \sin \phi \cos \phi) / 2 \sin \phi,$$

(6)

In the last equation, the Wick theorem is applied. Each expectation value in Eq.(6) can be obtained by using the correlation matrix which is given as follows, see [4, 32],

$$\langle c_{m} c_{n} \rangle = \delta_{m+n} + i(\Gamma_L)_{mn}$$

(7)

where

$$\Gamma_L = \begin{bmatrix} \Pi_0 & \Pi_1 & \cdots & \Pi_{L-1} \\ \Pi_{-1} & \Pi_0 & \cdots & \vdots \\ \vdots & \ddots & \ddots & \ddots \\ \Pi_{1-L} & \cdots & \Pi_0 \end{bmatrix},$$

(8)

For an infinite spin chain, $\gamma$ takes the form,

$$g_l = \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-il\phi} \cos \phi \lambda - i\gamma \sin \phi.$$  

(9)

We notice that the diagonal elements of the matrix $\Pi_l$ are zeroes, so the expectation values of two odd or even operators, for example, $\langle c_{2m} c_{2n} \rangle$ or $\langle c_{2m+1} c_{2n+1} \rangle$, are vanishing. Now, Eq.(6) can be written as,

$$\rho_{0\ldots0\ldots0\ldots0} = g_0^2 - g_{n-m} g_{m-n}.$$  

(10)

Summarizing the above calculations, we can derive the diagonal reduced density matrix as,
\[
\rho_{L}^{\text{diag.}} = 2^{-L}[(\sigma_1^0 \cdots \sigma_1^0) + \sum_{n=1}^{L} g_0(\sigma_1^0 \cdots \sigma_n^0 \cdots \sigma_L^0) + \frac{1}{2!} \sum_{m+n=L}^{L} (g_{m-n}^2 - g_{m-n} g_{m+n}) (\sigma_1^0 \cdots \sigma_m^0 \cdots \sigma_n^0 \cdots \sigma_L^0) \\
+ \frac{1}{3!} \sum_{l+m+n=L}^{L} (g_{l-m}^3 - g_{l-m} g_{l-m} g_{l+n} + g_{l-n} g_{l-n} - g_{l+n} g_{l+n} g_{l+n}) \\
(\sigma_1^0 \cdots \sigma_l^0 \cdots \sigma_m^0 \cdots \sigma_n^0 \cdots \sigma_L^0) + \cdots + \frac{1}{L!} g_{l+m+n}(\sigma_1^0 \cdots \sigma_L^0)].
\]

where the intermediate terms and the explicit form of \(g\) in the last term are omitted. However, all of them can be obtained explicitly based on the rules presented above and will be computed in our numerical calculations.

Based on the above results, we can calculate the DE, i.e., the von Neumann entropy of the diagonal reduced density matrix, 

\[ S(\rho_{L}^{\text{diag.}}) = -\text{Tr}\rho_{L}^{\text{diag.}} \log_2 \rho_{L}^{\text{diag.}}. \]

For comparison, we remark that EE takes the form 

\[ S(\rho_{L}) = -\text{Tr}\rho_{L} \log_2 \rho_{L}. \]

The quantum coherence can be quantified as DE subtracting EE, corresponding to relative entropy of coherence [28],

\[ C(\rho_{L}) = S(\rho_{L}^{\text{diag.}}) - S(\rho_{L}). \]

We emphasize that we consider, in this Letter, DE is an independent quantity.

**Formulation of DE and quantum phase transitions.**—

For one-dimensional spin chains, EE for a block of contiguous \(L\) spins demonstrates two different behaviors for gapped model and gapless model [1, 4, 6]. For gapped model, EE approaches a constant, while for gapless model, EE grows logarithmically on the number of spins \(L\) in the block, and the factor of the logarithm term is a constant related with the central charges of the corresponding conformal field theory of the model [4].

In the following, based on the results in (11), we will perform numerical calculations to study the DE. In principle, the diagonal density matrix \(\rho_{L}^{\text{diag.}}\) is classical. Intuitively, the leading term of DE will demonstrate at most volume effect depending on \(L\). If volume effect occurs, the factor of this leading term will be important since it might be a constant depending on the model or a variable related to parameters of the Hamiltonian. Similar to EE, the sub-leading term of DE we consider here is of the logarithmic form. Based on those considerations, we expect that the DE will take the following form on the number of spins \(L\) in the block,

\[ S(\rho_{L}^{\text{diag.}}) = aL + b \log_2 L + c. \]

Our aim is to validate this relation and find the coefficients. More importantly, we would like to know whether any signatures of quantum phase transition can be extracted from the coefficients. Here, in principle, we remark that the parameters \(a, b\) and \(c\) should depend on \(\gamma\) and \(\lambda\) in the Hamiltonian.

The phase diagram of XY-model is determined by both parameters \(\gamma\) and \(\lambda\), see Refs.[32–34]. The region \(\lambda > 1\) is the paramagnetic phase, and the region \(\lambda < 1\) is the ferromagnetic phase which is further divided by relation...
\[ \gamma^2 + \lambda^2 = 1 \] into two different phases, ferromagnetic phase \( A \) and ferromagnetic phase \( B \), see FIG. 1.

In order to determine the phase diagram by parameters in DE of Eq. (13), our method is to calculate DE for both parameters \( \gamma \) and \( \lambda \) in the range \( \gamma \in [0, 1] \) and \( \lambda \in [0, 1.5] \). Explicitly, we first fix \( 0 \leq \gamma \leq 1 \), then let \( \lambda \) run through the region \( \lambda \in [0, 1.5] \), to calculate DE according to Eq. (11). The result from Eq. (11) is exact. Fitting the result by Eq. (13), we then can find numerically the parameters \( a, b \) and \( c \) for given \( \gamma \) and \( \lambda \).

Figure 2 shows, for two special cases \( \gamma = 0, \lambda = 0 \) and \( \gamma = 1, \lambda = 1 \), the results of DE for diagonal reduced density matrices with a block of contiguous spins \( L = 1, \ldots, 18 \) for infinite chain \( N \to \infty \) with periodic boundary condition, and the fitting of Eq. (13). We find that Eq. (13) can be perfectly satisfied such that \( a, b \) and \( c \) can be obtained with high precision for the case \( \lambda = 0 \) or \( \lambda = 1 \). We then let \( \lambda \) run in the region \( \lambda \in [0, 1.5] \) by repeating the same calculations to find the whole results of \( a, b \) and \( c \), which are presented in Figure 3.

Here, we observe that Eq. (13) is satisfied for all regions of \( \gamma \) and \( \lambda \). Thus, we conclude that the leading term of the DE satisfies the volume law, while the factor of the volume term is a function depending on \( \gamma \) and \( \lambda \). The sub-leading term takes the form of logarithm on the number of spins in the block. In short, Eq. (13) demonstrates precisely the behaviors of DE for ground state of XY-model. According to our numerical results, we find that there is no strong evidence that those factors, \( a, b \) and \( c \), can be represented as a constant depending on the model. We remark that some cases of those parameters were numerically studied in Refs. [35–37].

Figure 3 shows the results of \( a, b \) and \( c \) for \( \lambda \in [0, 1.5] \), while \( \gamma \) take values \( \gamma = 0, 0.2, 0.5, 0.7, 1.0 \). In order to observe explicitly the quantum phase transition at critical point \( \lambda = 1 \), we calculate the derivatives of those parameters, \( \partial_\lambda a, \partial_\lambda b \) and \( \partial_\lambda c \). Remarkably, the quantum phase transition at \( \lambda = 1 \) can be explicitly identified by all three parameters. Their derivatives tend to infinity at the critical point, as shown in the FIG. 3. In this sense, DE indeed contains intrinsically the signatures of quantum phase transition for ferromagnetic phase and paramagnetic phase at \( \lambda = 1 \).

In addition, in ferromagnetic phase \( \lambda < 1 \), except for a small region near \( \gamma = 0 \), we notice that parameter \( b \) always tends to be zero, as shown in left panel of FIG. 3 (b). It means that DE may obey the volume law with vanishing logarithm term, while this phenomenon for \( \gamma \) in the limit of 0 seems not so clear. This problem is worth exploring further in the future.

Figure 4 shows that the partition between ferromagnetic phase A and ferromagnetic phase B can be located by the condition \( c = 0 \). This result can also be observed in Figure 3 (c). In FIG. 4, we present more numerical data.
for both parameters $\gamma$ and $\lambda$. One can find that the curve determined by $c = 0$ from the results of DE agree well with the known condition $\gamma^2 + \lambda^2 = 1$, implying that different phases can be identified by parameters in Eq. (13). Here the reason is that in case $\gamma^2 + \lambda^2 = 1$, the ground state is a product state, resulting in both $b = 0, c = 0$ for DE. Therefore, numerically by forcing $c(\lambda) = 0$ in DE, we can distinguish the two different ferromagnetic phases A and B to obtain the partition in the phase diagram.

The Ising model with transverse field is well known. We present the results of Ising model in the supplementary material [38].

**Conclusion.**—We find that DE can be represented faithfully as summation of a volume term, a logarithmic term, and a constant term. The involved parameters provide signatures of quantum phase transitions for the studied XY-model, despite the fact that diagonal form of the reduced density matrix in principle corresponds to a classical state. The combination of EE and DE will result in the quantum coherence, however, we propose that DE itself is an independent quantity applicable in exploring phase transitions of quantum many-body systems. At least for the case of XY model quantum phase transition, we show that the quantum resource embedded in EE is different from that in quantum coherence. Our results provide a new method to the successful toolbox of quantum information science in studying quantum systems.

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[38] The results of Ising model with transverse field are presented in the supplementary material.
Supplementary material: Diagonal Entropy in Many-Body Systems: Volume Effect and Phase Transitions

The Ising model with transverse field is well known. In the following, we will present the results of DE for Ising model. Let $\gamma = 1$, the XY-model will reduce to Ising model with transverse field, its Hamiltonian takes the form,

$$H = - \sum_{l=0}^{N-1} \sigma_i^x \sigma_{i+1}^x + \lambda \sigma_i^z.$$  

(14)

For case of Ising model, the parameters of DE in Eq. (13) presented in the main text can be obtained, as shown in FIG. 5. The derivatives on parameter $\lambda$ are presented in FIG. 6. We can find that the critical point of quantum phase transition $\lambda = 1$ can be clearly identified. Besides, we remark that more evidences are necessary to find whether DE may actually satisfy the volume law, $b(\lambda) = 0$.

![Graph](a)

![Graph](b)

![Graph](c)

FIG. 5. (Color online) Coefficients of Ising model. Here, (a,b,c) give respectively the parameters $a(\lambda), b(\lambda), c(\lambda)$. The Ising model corresponds to $\gamma = 1$ of the XY-model.

![Graph](a)

![Graph](b)

![Graph](c)

FIG. 6. (Color online) The derivatives of coefficients. Here the derivatives of parameter $\lambda$ are presented, respectively, $\frac{\partial a(\lambda)}{\partial \lambda}, \frac{\partial b(\lambda)}{\partial \lambda}, \frac{\partial c(\lambda)}{\partial \lambda}$. It is clear that the critical point $\lambda = 0$ can be identified. The Ising model corresponds to $\gamma = 1$ of the XY-model.