Universality in entanglement of quasiparticle excitations

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(Dated: February 16, 2012)

PACS numbers: 03.65.Ud, 05.70.Ce, 75.10.Jm

We show that the entanglement entropy of single quasiparticle excitations of one dimensional systems exceeds the ground state entanglement entropy for \( \log(2) \), if the correlation length of the system is finite. For quadratic fermion systems we show that the excess of entanglement is related to the number of quasiparticles in the excited state. This observation is confirmed by numerical examples of one dimensional quantum many-body systems, including nonintegrable. Tensor network methods to describe quasiparticle excitations are discussed.

The entanglement is of central interest in quantum information theory, quantum computation and plays an important role in quantum many-body physics. On one hand, it is a valuable resource in quantum computation and the reason why quantum algorithms can be more powerful than classical ones [1]. On the other hand, it makes classical simulation of quantum many-body systems more difficult in terms of tensor network methods relying on a low degree of entanglement, such as the density matrix renormalization group [2] or matrix product states [3,4] where the number of parameters scales roughly exponentially with the entanglement entropy [5].

The entanglement of quantum many-body systems at zero temperature has been extensively studied and, in particular for one dimensional lattice systems, it was shown that the ground state is much less entangled than generic quantum states, which makes a classical simulation tractable [6], and on the other hand provides a signature of quantum critical behavior [7] where the entanglement entropy violates the area law [8], connected to the central charge of the corresponding quantum field theory [9,11]. Much less, however, is known about the entanglement of excited states. It was shown by Alba, Fagotti and Calabrese [12] that entanglement entropies of excited states of integrable systems appear in a band-like structure and their ratios with the ground state entanglement entropy scale either extensively or logarithmically with the block size. For a critical Ising model, an exact scaling relation was obtained by Berganza, Alcaraz, and Sierra [13] using a field theoretical approach. Still, no indication has been given that the banded structure of the excess of entanglement, as the difference from the ground state entanglement entropy is called in [13], comes from the quasiparticle picture at low temperatures where a quasi particle causes an excess of \( \log(2) \) to the entanglement entropy as compared to the ground state. This is what we show in the present Letter, assuming a translation invariance, a finite correlation length and a validity of a quasiparticle description at low energies. For quadratic models we also show that in the thermodynamic limit, the entanglement entropy of \( k \)-quasiparticle excitation exceeds the entanglement entropy of the ground state for \( k \log(2) \). The observation is supported by numerical simulations of spin chains: the Heisenberg XY model, the Ising model in a transverse field and the Ising model in a mixed field, the last being a nonintegrable model [14]. Finally, we show that the excess of entanglement for the Bloch-like Ansatz for excited states [15] is exactly equal to \( \log(2) \) and is as such well suited to describe single particle excitations.

Let us consider a one-dimensional quantum lattice system of length \( n \) described by a Hamiltonian \( \hat{H} \) which is invariant to spatial reflections, \([\hat{H},\hat{R}]=0\), and conserves a parity of the system, \([\hat{H},\hat{P}] = 0\). In a symmetric bipartition of the system into two parts of length \( L = n/2 \), any pure state can be parametrized by a matrix \( \psi \) as \( |\psi\rangle = \sum_{i,j} \psi_{i,j} |i\rangle \otimes |j\rangle \) where indices \( i,j \) run over configuration states of the subsystems. The Schmidt decomposition reads \( |\psi\rangle = \sum_k \sigma_k \sum_i \alpha_{i,k} |i\rangle \otimes \sum_j \beta_{j,k} |j\rangle \) where \( \sigma \) is given by the von Neumann entropy of the reduced density matrix of the system, \( \text{tr}_{\text{right}}[\Omega |\Omega\rangle] \), is simply \( \Omega^H \) and the entanglement entropy, defined as the von Neumann entropy of the reduced density matrix, reads \( S[\Omega] = -\text{tr}[\Omega^H \log(\Omega^H)] \). In the following we shall be interested in the entanglement of single particle excitations \( |\Phi\rangle = X^\dagger |\Omega\rangle \) where \( X \) is a quasiparticle annihilation operator fulfilling canonical anticommutation relations (CAR) \( \{\hat{X},\hat{X}^\dagger\} = 1 \) and \( \{\hat{X},\hat{X}\} = 0 \) and flipping the parity, \( \{\hat{X},\hat{P}\} = 0 \). We shall call \( \Delta S \equiv S(|\Phi\rangle) - S(|\Omega\rangle) \) the excess of entanglement, as introduced in [13]. Like the ground state, the excited states must also obey the symmetries of the system, being either symmetric or antisymmetric to reflections, \( \hat{R} |\Phi\rangle = \pm |\Phi\rangle \), and of an odd parity. Because of these symmetry constraints, there exist maps \( \hat{X}_l \) and \( \hat{X}_r \), acting only on the left/right part of the system, such that \( |\Phi\rangle = \frac{1}{\sqrt{2}} (X_l^\dagger + X_r^\dagger) |\Omega\rangle \), and \( \{\hat{X}_{l,r},\hat{P}\} = 0 \). They anticommute \( \{\hat{X}_l,\hat{X}_r\} = \{\hat{X}_l,\hat{X}_r^\dagger\} = 0 \) and thus \( \{\hat{X}_{l,r},\hat{X}_{l,r}^\dagger\} = \frac{1}{2} I \) and \( \{\hat{X}_l,\hat{X}_r\} = -\{\hat{X}_r,\hat{X}_l\} \).
Let us now assume a finite correlation length \( \xi \), such that \(|\langle \hat{x}_i \hat{x}_j \rangle - \langle \hat{x}_i \rangle \langle \hat{x}_j \rangle| < Ce^{-|i-j|/\xi}\) for any two local operators \( \hat{x}_i, \hat{x}_j \) at sites \( i, j \). Although the quasiparticles are not localized, simultaneous presence in both halves of the systems gets unlikely for \( n \to \infty \),

\[
||\langle \Omega| \hat{X}_l \hat{X}_r^\dagger |\Omega \rangle|| < \frac{\text{const}}{n \sinh \left( \frac{\xi}{2} \right)} = O(n^{-1}) \quad (1)
\]

which results from \( \hat{X} = \frac{1}{N} \sum_{i=1}^{N} (f_i \hat{c}_i^\dagger + g_i \hat{c}_i) \) where \( \{ \hat{c}_i \} \) are real particle annihilation operators at sites \( \{ j \} \) and \( f_j \) and \( g_j \) are bounded. The actual quasiparticles might be of a different form but they still behave like real particles and this is a valid assumption. This bound also results in \( |||\langle \Omega \rangle \hat{X}_l \hat{X}_r^\dagger |\Omega \rangle = -\langle \Omega | \hat{X}_l^\dagger \hat{X}_r |\Omega \rangle = O(n^{-1}) \).

The reduced density matrix \( \rho \) for the excited state \( \hat{X}_l^\dagger \hat{X}_r \) vanishes, whereas the mixed terms \( \hat{X}_l^\dagger \hat{X}_r \) are distinguishable whereas the mixed terms vanish in the thermodynamic limit. Let us first fix the states where either of the terms \( \hat{X}_l^\dagger \hat{X}_r \) and \( \hat{X}_l \hat{X}_r^\dagger \) are orthonormal which allows us to write \( \Gamma_{\{a\}} \) in a way that we obtain a free fermion model \( \hat{H} = \sum_k \varepsilon_k \hat{b}_k^\dagger \hat{b}_k \). As shown in [9,12], a \( 4 \times 4 \) correlation matrix \( \langle \psi | \hat{w}_i \hat{w}_j | \psi \rangle = \delta_{i,j} + i \Gamma_{ij} \) where \( \Gamma_{ij} \) is a real skew symmetric matrix with eigenvalues \( \pm i \nu_l \), determines the eigenvalues of the reduced density matrix \( \rho_{ij} \equiv \langle \psi_{\{a\}} | \psi_{\{a\}} \rangle \) as \( \nu_{m_{\{a\}}} m_{\{a\}} = \prod_{j=1}^{1+m_{\{a\}}} \frac{i + \mu_j \nu_j}{2} \) with \( m_j = \pm 1 \). The entanglement entropy of \( \psi \) reads \( S(\psi) = -\sum \frac{\langle \psi_{\{a\}} | \psi_{\{a\}} \rangle}{i + \mu_j \nu_j} \log \left( \frac{1 + i \Gamma_{ij}}{2} \right) \). Let us denote the upper part of \( V \), referring to sites \( \{ 1, \ldots, L \} \), as \( u \in \mathbb{C}^{2L \times n} \), where we also reshuffle the columns \( u_k \) in a way that \( w_{2k-1} - w_{2k} = 0 \). For the ground state, it is easy to check that \( \langle u^T | w \rangle = 0 \), and \( \Gamma_{ij} = \langle i | u^T u - u^T u \rangle \). Bases \( \{ \sqrt{\nu_{2k-1}} \} \) and \( \{ \sqrt{2 \nu_{2k}} \} \) are orthonormal which allows us to write \( \Gamma_{ij} \) as a sum of \( L \) rank-2 terms

\[
\Gamma_{ij} = \sum_{k=1}^{L} \chi_{2k-1} \quad \chi_k \equiv 2i (\nu_{2k-1}^+ \nu_{2k-1}^T - \nu_{2k-1} \nu_{2k}^T).
\]

For an excited state \( \psi_{\{a\}} \equiv \hat{b}_i^\dagger | \Omega \rangle \), it is easy to see that \( \Gamma_{ij} - \chi_k = \sum_{k \neq k'} \chi_{2k'} \), assuming \( \kappa = 2n' - 1 \), which is obviously rank deficient with \( \dim \ker \Gamma_{ij} = 2 \). This makes the spectrum of the reduced density matrix double degenerate. The same reasoning is applied to \( \hat{b}_i^\dagger \hat{b}_{2k-1}^\dagger | \Omega \rangle \) (or \( \hat{b}_i^\dagger \hat{b}_{2k}^\dagger | \Omega \rangle \)), resulting in a four times degenerate spectrum of the reduced density operator. Let us now show how \( \Delta S \) approaches \( \log(2) \). Using the Taylor expansion, we write

\[
\Delta S = \sum_{j=1}^{\infty} [2j(2j-1)^{-1/2} \mathrm{tr} \left( (i \Gamma_{ij})^j \right) - (i \Gamma_{ij} - i \chi_k)^{2j}] 2^{-1}
\]
where \( tr[(i\chi_k)^2] \leq 2 \). If \( (\forall k,l) \ u_k \cdot u_l = 0 \), then the trace in above expression equals 2, since \( \chi_k \chi_l = 0 \), and thus \( \Delta S = \log(2) \). Using \( b_{k,L} = \frac{1}{\sqrt{L}} \sum_{i=1}^{2L} u_{i,k} \hat{w}_i \) we see that this is indeed the case for \( n \rightarrow \infty \) where \( \sum |u_k \cdot u_l|^2 = \langle \Omega | b_{k,L} b_{k,L}^\dagger | \Omega \rangle = O(n^{-1}) \) due to \(| \langle 1 \rangle \). Hence, the excess of entanglement for a single quasiparticle excitation equals \( \Delta S = \log(2) \) and for \( k \)-quasiparticle excitation it equals \( k \log(2) \) (if all excited quasiparticles belong to the same reflection symmetry class).

**Results.** From a very generic setting we have seen that the entanglement entropy of excited states is connected with the number of quasiparticles which we shall now confirm by numerical simulations. First we consider an antiferromagnetic Ising chain in a mixed transverse and longitudinal magnetic field, the so-called tilted Ising chain, described by a Hamiltonian \( H = \sum_j (\sigma_j^x \sigma_{j+1}^x + \frac{1}{2} \sigma_j^y \sigma_{j+1}^y + \sum_j J \sigma_j^z) \) where we choose a particular point in the parameter space \((\gamma, h) = (0.5, 0.9)\); any point with \( h \neq 1 \) and \( \gamma \neq 0 \) gives similar results. In Fig. 2 we show the excess of entanglement of all single particle excitations \( b_i^\dagger | \Omega \rangle \) for chain lengths \( n = 128, 256, 512 \) and again observe that it approaches \( \Delta S \rightarrow \log(2) \). The scaling analysis confirms that \( \log(2) - \Delta S \) scales as \( n^{-1} \) as shown in the inset.

Three-particle excitations are studied on the case of an Ising chain in a transverse field (i.e. the XY model with \((\gamma, h) = (1, 2))\). We choose excitations of a form \( | \Phi \rangle = b_i^\dagger b_k^\dagger b_l^\dagger | \Omega \rangle \) where \( k_1 \) and \( k_2 \) are fixed and correspond to reflection antisymmetric excitations at quasimomenta \( \pi/4 \) and \( 3\pi/4 \). We observe in Fig. 3 that \( \Delta S \rightarrow 3 \log(2) \) for \( n \rightarrow \infty \) except for two peaks at \( i \sim k_1 \) and \( i \sim k_2 \) where two quasiparticles can form a bound state and the excited state looks like a two-particle excitation with the excess of roughly, but more than \( 2 \log(2) \), as the numerical results suggest.

**Discussion.** The main message of this Letter, that the entanglement entropy of single particle excitations exceeds the ground state for \( \log(2) \), can be used to justify the Ansatz for single particle excitations [17]. They are based on a homogeneous matrix product state for the ground state described by a tensor \( A^s \in \mathbb{C}^{D \times D} \) as \(| \Omega \rangle = \sum \psi_l (\cdots A^{s-1} A^0 A^{s+1} \cdots) \psi_l | \rangle \), see [18], and are
which means that whereas isometries with orthogonal support, ˜D is used, together with a phase factor \(\phi\) and so is the reduced density matrix which reads \(\rho = \frac{1}{\sqrt{2}}(\phi \beta^T + \alpha \theta^T)\) where the first/second part contains all excitations on the left/right part of the chain. It is easy to show that also \(\phi^T \theta = \alpha \beta\) whereas \(\theta^T \alpha = \phi^T \beta = 0\) (and \(\phi^T \alpha = 0\) by construction) which means that \(\phi\) is orthogonalized by the same transformation as \(\alpha\), that is \(\phi = \hat{\phi} \hat{L}^{-H}\). The reduced density operator reads \(\rho = \frac{1}{2}(\phi \phi^H + \alpha \alpha^H)\) and we immediately obtain \(\rho = \frac{1}{2}(\phi \widehat{\Xi} \phi^H + \alpha \widehat{\Xi} \alpha^H)\) where \(\phi\) and \(\alpha\) are isometries with orthogonal support, \(\hat{\alpha}^H \hat{\phi} = 0\), and thus \(\rho = \frac{1}{2}(\Xi \oplus \Xi)\). The entanglement entropy of the Ansatz is equal to \(S[\hat{\theta}] = S[\hat{\Xi}] + \log(2)\), irrespectively of the bond dimension \(D\), which we have shown to agree with single quasiparticle excitations in the thermodynamic limit. By this we provide additional support that the Ansatz in [15] is a good Ansatz for describing single particle excitations. Unfortunately, however, the entanglement entropy of almost all other excited states (except e.g. some bound states) goes beyond this limit; in this case a generalized Ansatz should be used where not one but two or more tensors in \(A^s\) the ground state are replaced by some \(B^s\).

Conclusion. We have studied the entanglement entropy of single quasiparticle excitations and shown that it is related to the ground state entanglement entropy with a contribution of \(\log(2)\) for each quasiparticle in the thermodynamic limit, assuming a finite correlation length and a valid quasiparticle description at low energies. We have provided numerical evidence for this universal behavior which suggests a possibility to classify excited states on the basis of the entanglement.

Acknowledgments. Discussions with F. Verstraete and T. Prosen are gratefully acknowledged, as well as financial support by the EU project QUEVADIS. The computational results were in part achieved using Vienna Scientific Cluster.