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Excited state entanglement in one-dimensional quantum critical systems: Extensivity and the role of microscopic details

T. Pálmai*

Scuola Internazionale Superiore di Studi Avanzati Trieste, Via Bonomea 265, 34136 Trieste, Italy;
Istituto Nazionale di Fisica Nucleare, Sezione Trieste, Italy;
and Budapest University of Technology and Economics, Budafoki ut 8, 1111 Budapest, Hungary

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We study entanglement via the subsystem purity relative to bipartitions of arbitrary excited states in (1+1)-dimensional conformal field theory, equivalent to the scaling limit of one-dimensional quantum critical systems. We compute the exact subpurity as a function of the relative subsystem size for numerous excited states in the Ising and three-state Potts models. We find that it decays exponentially when the system and the subsystem sizes are comparable until a saturation limit is reached near half-partitioning, signaling that excited states are maximally entangled. The exponential behavior translates into extensivity for the second Rényi entropy. Since the coefficient of this linear law depends only on the excitation energy, this result shows an interesting relationship between energy and quantum information and elucidates the role of microscopic details.

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Entanglement is the essence of quantum theory. Beyond quantum informational aspects, the amount of entanglement coded into a quantum many-body system is an increasingly important quantity that provides a universal way to characterize quantum fluctuation. The ground state entanglement in particular can classify quantum phases; e.g., it can inform us about interesting, topological phases [1] and whether a system is close to criticality [2].

On the other hand, entanglement of excited states is also a very interesting quantity. In fact, recently there has been a quickly growing interest in this subject [3]. While ground states characterize system specific quantum fluctuations and they usually follow the area law [4], the entanglement entropy of highly excited states are expected to be more generic, independent of the specific system, and go to an extensive, thermodynamic entropy instead.

This picture gets modified for critical systems. Here the area law for the ground state is enhanced into a logarithmic law [5,6] with a universal coefficient. For low-lying excited states the logarithmic behavior was shown to remain unchanged when the subsystem size is infinitesimal compared to the whole. On the other hand, when the subsystem is comparable to the whole interesting features emerge, in particular hints of a thermodynamic behavior for very small (but not infinitesimal) subsystem sizes, connecting energy with the amount of entanglement in a universal way [7,8]. Despite these advances, there is still very little known about the entanglement of excited states in critical systems, which however are especially interesting because of universality. Interesting questions include the following. What happens for highly excited states? How does entanglement behave for comparable subsystems? What is the relationship between entanglement and excitation energy beyond the small subsystem limit?

In this paper we endeavor to answer these questions by studying excited states in (1+1)-dimensional (unitary) conformal field theories. We set up a systematic framework to compute the Rényi entropies for *arbitrary* excited states relative to connected bipartitions, by generalizing the approach of [8], where the case of primary states was considered. The main motivation is that primary states represent only the lowest-lying excitations and in many important cases (e.g., minimal models) there are only a few of them in the Hilbert space. In order to examine more excited states, and, in particular, to access highly excited ones, it is necessary to generalize the previous approach to descendant states.

We study in particular the scaling of the second Rényi entropy $S_2(d)$ (defined precisely below) with the relative subsystem size $d = L_A/L$ in the critical Ising and three-state Potts models for several individual excited states. We chose the second Rényi entropy in addition to being computationally the simplest case, because it has the interpretation of being the logarithm of the purity of the subsystem (defined as the participation ratio in the Schmidt basis; also see later). We note that the choice of the particular models is arbitrary and one could choose any other minimal model, or in general a (1+1)-dimensional conformal field theory (CFT), where the four-point functions of primary fields are known, and obtain the Rényi entropies by the present approach.

We find that for almost all the excited states there are three distinct regimes of the second Rényi entropy as a function of the relative subsystem size. The first regime has already been understood in earlier works [7,8] and it corresponds to the small subsystem size limit described by a logarithmic scaling with the first *correction* being linear in the excitation energy

$$S_2^{\Psi}(d \to 0) = \frac{c}{4} \log \sin \pi d + \frac{(\Delta^{\Psi} + \bar{\Delta}^{\Psi})}{2} (\pi d)^2 + \cdots , \tag{1}$$

with c the central charge and Δ_Ψ, $\bar{\Delta}_\Psi$ the chiral and antichiral scaling weights of the operator Ψ. (Here and in the rest of this paper we do not write out additive constants common to all states, e.g., the UV regularization factor.) Although this form was proved rigorously only for primary states it is expected to hold for other excited states as well [7], and we could confirm

*tpalmai@sissa.it

this for the states that we considered. Beyond this regime no general feature was known until now.

The second regime is the most interesting and its identification is the main result of this Rapid Communication. It is characterized by an extensive Rényi entropy, growing linearly with the subsystem size

$$S_2^{\Psi}(d) \approx s(E^{\Psi})d, \quad d_{\log} < d < d_{\text{sat}}. \tag{2}$$

The scaling law only depends on the excitation energy and it is *sublinear* in it. In other words, in the accessible energy range we see a quasithermodynamic entropy. Extensivity translates for the subsystem purity as exponential decay, signaling that the excited states are maximally entangled. We refer to [9] where extensive terms were observed for special states in the entanglement entropy in holographic systems.

There is a third regime, which turns out to be unique to every state and it corresponds to the saturation of the entropy to facilitate the symmetry $S(d) = S(1-d)$. This part of the Rényi entropy can be used to differentiate between degenerate states and allows for instance the identification of excited states of the microscopic theory in terms of CFT states (suggested first in [8]).

In our explicit calculations we determined that these regimes can be found for all (primary and descendant) states in the accessible energy range, except for the lowest-lying excitation in the Ising CFT corresponding to the twisted vacuum in the spin chain model. Therefore, it is reasonable to believe that these features constitute a general property of the second Renyi entropy (subsystem purity) for most of the excited states. In fact, the only states for which Eqs. (1) and (2) are expected to break down are those corresponding to ground states of some local Hamiltonians (see [10] and also [11] for an analysis in the XY spin chain).

In addition to the present results we expect that generalizing the computation of Rényi entropies to arbitrary states in CFT will enable a number of exciting future applications, e.g., the study of ground and excited state entanglement in one-dimensional massive field theories (integrable or not) through the truncated conformal space approach [12] or the study of local quenches [13] in both gapless and gapful systems.

In the rest of this paper we first introduce the measure of entanglement considered here and then outline the computation technique to find the exact Rényi entropies and, in particular, the second one equivalent to the subsystem purity, for arbitrary excited states. We also present representative results for excited states in the Ising and three-state Potts universality classes.

Rényi entropies in CFT. To define a measure of entanglement for a system in a pure state it is enough to look at a spatial bipartition $(A \cup B)$. A family of measures coming from the reduced density matrix on A consists of the Rényi entropies, defined as

$$S_n = \frac{1}{1-n} \log \operatorname{Tr}_A \rho_A^n, \quad \rho_A = \operatorname{Tr}_B |\Psi\rangle\langle\Psi|. \tag{3}$$

Beside the von Neumann entropy $S_1 = \lim_{n\to 1} S_n$, also especially important is the second Rényi entropy that measures the purity of the subsystem. The concept of purity can be introduced considering the Schmidt decomposition,

$$|\Psi\rangle = \sum_m c_m |a_m\rangle |b_m\rangle. \tag{4}$$

In terms of these bases relative to the partitions the reduced density matrix takes the form

$$\rho_A = \sum_m c_m^2 |a_m\rangle\langle a_m|, \tag{5}$$

where we can see that the coherences are zero and in this sense the basis involved in the Schmidt decomposition is a maximally entangled basis. The participation ratio $P = \sum_m c_m^4 = \operatorname{Tr}_A \rho_A^2$ on this basis then describes the purity of the subsystem. If the subsystem can be described by a pure state purity would be one, while for mixed states it would give the inverse of the effective number of maximally entangled states needed to describe it. The more this number goes to zero the less pure the mixed state is, therefore the more the partitions are entangled. Since the dimension of the subsystem Hilbert space scales exponentially with its size, exponential decay (i.e., extensivity of the Rényi entropy) would mean maximally entangled states.

Turning now to the computation of this subpurity in our field theoretical setting we expand the traces in (3): the relevant expression can be written in terms of sums on two bases relative to A and B (e.g., but not necessarily the Schmidt bases). Since we are in finite volume the energy levels are quantized and we can write

$$P = \operatorname{Tr}_A \rho_A^2 = \sum_a \langle a| \left(\sum_b \langle b||\Psi\rangle\langle\Psi||b\rangle \right)^2 |a\rangle \tag{6}$$

$$= \sum_{aa'bb'} \langle ab|\Psi\rangle\langle\Psi|a'b\rangle\langle a'b'|\Psi\rangle\langle\Psi|ab'\rangle, \tag{7}$$

where states labeled by a, a' live on the partition A, while b, b' live on B. The main problem is that *a priori* it is not clear how to obtain the sets of states living on restrictions in terms of those living on the full domain. However, one can reinterpret the sum by noticing that it is equivalent to a four-point function (first noticed in [8]) on a nontrivial geometry, that consists of two sheets (with periodic boundary conditions on each) sewed together along A in a circular manner (for a pictorial representation, see e.g. [6] where this surface is denoted by $\mathcal{R}_2$).

It is useful to go from interconnected cylinders ($\mathcal{R}_2$) to interconnected planes ($\bar{\mathcal{R}}_2$) by the exponential mapping $\xi = e^{-\frac{2\pi i}{L}(x+it)}$, where the physical energy eigenstates are generated by the insertion of the usual primary and descendant fields. The purity is then just the unusually normalized four-point function

$$P = \mathcal{N}_\Psi F_\Psi = \mathcal{N}_\Psi \langle \Psi(0_1)\Psi(0_1)^\dagger \Psi(0_2)\Psi(0_2)^\dagger \rangle_{\bar{\mathcal{R}}_2}, \tag{8}$$

where the operator Ψ implements the state $|\Psi\rangle$ on the complex plane as

$$\Psi(0)|0\rangle = |\Psi\rangle \tag{9}$$

and the normalization $\mathcal{N}_\Psi$ is such that $\operatorname{Tr}\rho = 1$.

To evaluate P we map $\bar{\mathcal{R}}_2$ to a single complex plane by the transformation

$$\zeta = f_d(\xi) = \left(\frac{e^{i\pi d}\xi - e^{-i\pi d}}{1-\xi}\right)^{1/2}. \tag{10}$$

The above mapping consists of the composition of a global conformal mapping (Moebius transformation) and taking the square root. The first component maps to a surface topologically identical to the Riemann surface of the square root, being two sheeted with the connecting branch cut on the positive real line. Taking the square root then maps to the complex plane, and the two sheets are prescribed to be mapped to the two branches of the complex square root, e.g., $\xi = 0_{1,2}$ maps to $e^{\frac{i\pi}{2}(2m-1-d)}$, $m = 1,2$. It is important to perform UV and IR regularizations by excluding the neighborhoods of the common points of A and B and going to finite volume, making the entropies finite. The UV regulator will only appear in the normalization.

In case of the vacuum $\Psi \equiv 1$ the nontrivial part is given by only the normalization

$$\mathcal{N}_\Psi = \mathcal{N}_1 = \frac{Z_{\bar{\mathcal{R}}_2}}{Z^2_{\bar{\mathcal{R}}_1}} = \left(\frac{L}{\pi\varepsilon}\sin\pi d\right)^{-\frac{c}{4}}, \tag{11}$$

with c being the central charge, L the IR, and ε the UV regulators. $\mathcal{N}_1$ gives rise to the ubiquitous logarithm law [5,6] for the ground state. This formula can be seen simply by noticing that the transformed geometry is equivalent to a finite cylinder where the partition function is well known. It is also easy to see that the leading logarithmic law for small subsystem sizes is universal and it is independent of which state is examined by considering that $\bar{\mathcal{R}}_2$ goes to two independent planes when the subsystem size goes to zero. Then, the four-point function gives 1 because the states are normalized on the plane and only $\mathcal{N}_\Psi$ remains.

When moving on to excited states one needs to evaluate a nontrivial F_Ψ. This transforms under the same mapping f_d into the equal-time ($|\zeta| = 1$ in radial quantization) four-point function

$$F_\Psi = \langle \mathcal{T}\{\Psi(0_1)\}\mathcal{T}\{\Psi(0_1)^\dagger\}\mathcal{T}\{\Psi(0_2)\}\mathcal{T}\{\Psi(0_2)^\dagger\}\rangle_{\mathbb{C}} \tag{12}$$

on the complex plane. $\mathcal{T}$ represents the transformation of the fields under $f_d(\xi)$. For primary states the transformation of the fields is simple,

$$\mathcal{T}\{\Psi(0)\} = f_d'(0)^{2h+2\bar{h}}\Psi(f_d(0)), \tag{13}$$

with h ($\bar{h}$) being the (anti)chiral primary weights. In this case F_Ψ is given by a four-point function of the same operators Ψ that generate the physical state [8,14],

$$F_\Psi \propto f_d'^{8h+8\bar{h}}\langle\Psi(\zeta_1)\Psi(\zeta_2)\Psi(\zeta_3)\Psi(\zeta_4)\rangle_{\mathbb{C}}, \tag{14}$$

with $\zeta_{1,2} = e^{\frac{i\pi\mp i\pi d}{2}}$, $\zeta_{3,4} = e^{\frac{3i\pi\mp i\pi d}{2}}$, and the only ambiguity is a phase factor that is set by F_Ψ being positive real.

Descendant states. For descendants Eq. (12) must be evaluated much more carefully. In fact, in this case because of the generation of lower descendants when performing the transformation for every descendant state there is a different formula in terms of four-point functions on the plane, which can in turn be evaluated by standard methods.

To make progress we need to transform descendant operators under f_d. (Note that the images of the adjoints can be obtained from fields living in $\xi = 0$ by f_{-d}.) The first term of the transformation law of a (chiral) descendant operator (with the nonchiral case being a product of the chiral and antichiral contributions) is easily obtained in general as

$$\mathcal{T}\{\phi(\zeta)\} = \left(\frac{\partial f}{\partial\zeta}\right)^{\Delta}\phi(f(\zeta)) + \cdots \tag{15}$$

for a field ϕ with scaling weight Δ; however, for a descendant field all the lower descendants in the given tower are also generated (represented above by "$\cdots$") and they can by no means be disregarded in the four-point functions. To perform this transformation for general fields we propose to use the construction of [15] prescribing the form

$$\mathcal{T}\{\phi(\zeta)\} = \left[\prod_{n=0}^{\infty} e^{R_n[f,\zeta)L_n}\phi\right](f(\zeta)). \tag{16}$$

After expanding the exponentials the infinite product of operators can be rewritten as

$$\prod_{n=0}^{\infty} e^{R_n[f,\zeta)L_n}\phi = e^{R_0L_0}\left(1 + R_1L_1 + \frac{1}{2}R_1^2L_1^2 + R_2L_2 + \cdots\right)\phi. \tag{17}$$

There is a finite number of terms since any string of generators with a combined descendance level larger than the descendance level m of ϕ (of scaling dimension $\Delta = h + m$) gives zero. The appearing $R_n[f,\zeta)$ coefficients are also known [15], the first few being

$$R_0[f,0_{1,2}) = \log f' = \log(\pm e^{i\pi d/2}\sin\pi d), \tag{18}$$

$$R_1[f,0_{1,2}) = f''/2f' = \frac{3+e^{2i\pi d}}{4}, \tag{19}$$

$$R_2[f,0_{1,2}) = Sf/6 = \left(\frac{e^{2i\pi d}-1}{4}\right)^2, \tag{20}$$

with the Schwarzian Sf. The sign in the first line is crucial and comes form mapping the first and second planes to the different branches of the square root. By evaluating (17) it is a matter of algebraic manipulations to find the transformation law for any specific field ϕ.

After the transformation one is left with a sum of four-point functions of descendant fields in the form

$$F_\Psi = \sum_{abcd} c_{abcd}\langle\phi_a(\zeta_1)\phi_b(\zeta_2)\phi_c(\zeta_3)\phi_d(\zeta_4)\rangle_{\mathbb{C}}. \tag{21}$$

The exact evaluation of such n-point functions is in principle known and it can be obtained from the four-point function of the associated primary fields by acting on it with an appropriate differential operator. The simplest example is the four-point function of three primaries and one descendant, e.g.,

$$\langle L_{-n}\Phi_1(x_1)\Phi_2(x_2)\Phi_3(x_3)\Phi_4(x_4)\rangle = \sum_{i=2}^{4}\left\{\frac{(n-1)h_i}{(x_i-x_1)^n} - \frac{1}{(x_i-x_1)^{n-1}}\frac{\partial}{\partial x_i}\right\} \times \langle\Phi_1(x_1)\Phi_2(x_2)\Phi_3(x_3)\Phi_4(x_4)\rangle, \tag{22}$$

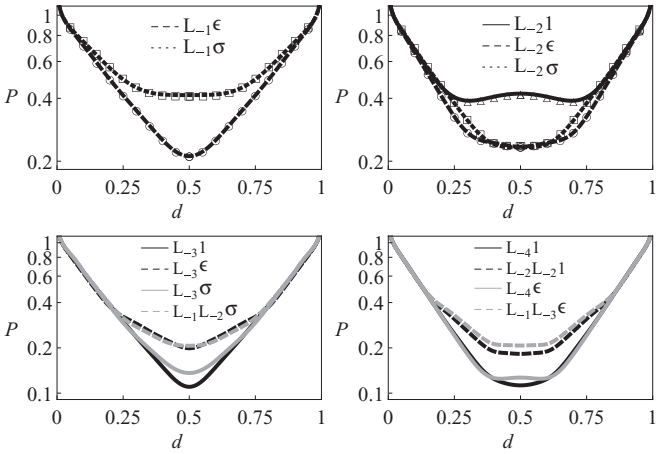

FIG. 1. (Logarithmic) plots of the subsystem purities of the first few spin-zero excited states in the Ising universality class ($\Psi = \psi\bar{\psi}$; the legend shows only the chiral generators ψ). We organized the plots according to the descendance level of the excited states (and the primaries are not shown). The exponents of the purity in the (first) exponential domain depend on the excitation energy in a nonlinear way. The Rényi entropy $S_2 = -\log P$ can also be read off these plots. For the level one and two states we also show data from the critical Ising spin chain marked on the plots by points. The agreement is very convincing and serves as a check of the present framework. Note that the scale is arbitrary depending on the regularization (e.g., system size) and was set so that the exponential decay would begin around $P = 1$.

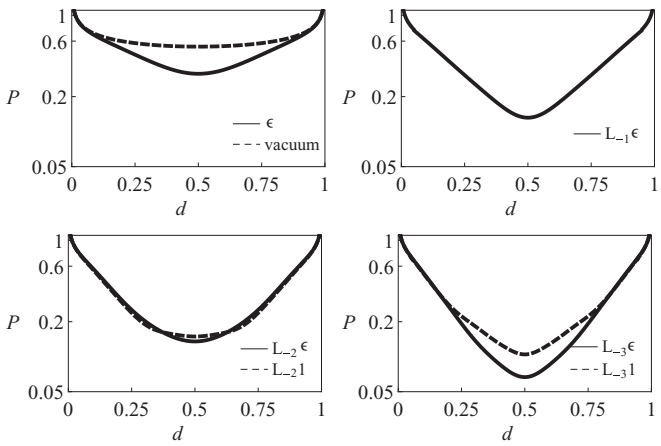

FIG. 2. (Logarithmic) plots of the subsystem purities of the first few spin-zero excited states from the identity and energy towers in the Potts universality class.

where the particular differential operator is easily inferred from the conformal Ward identities. To find the differential operator in the general case, i.e., for arbitrary strings of Virasoro generators, we rewrote the generators as contour integrals

$$L_n\phi(x) = \frac{1}{2\pi i}\oint_x d\zeta(\zeta - x)^{n+1}T(\zeta)\phi(x) \qquad (23)$$

and we deformed the contours successively from one operator insertion point to the others, back and forth. When doing the deformations the generators $\{L_n\}_{n\geqslant -1}$ are generated which can be seen by expanding $(\zeta_1 - x)^{n+1}$ in powers of $(\zeta_2 - x)$. Using this technique it is possible to reduce any n-point function into a sum of ones that involve only the generator L_{-1}, which is equivalent to partial differentiation. The residual four-point functions of primaries can be obtained exactly, for instance, by means of the Coulomb gas construction [16] as a sum of chiral×antichiral products of hypergeometric functions (conformal blocks) [17]. All these computations become extremely cumbersome, producing a large number of terms for already the simplest descendant states. Therefore, we algorithmized the transformation and the computation of the differential operator and did them still analytically but assisted by computer. Further details of this approach will be discussed in a later publication [18], where we shall present a different application of excited state Rényi entropies.

Results and discussion. In Figs. 1 and 2 we show results for the subsystem purity for excited states in the Ising ($c = 1/2$) and the three-state Potts ($c = 4/5$) models. For the former case we also checked the results for energetically nondegenerate states in the zero momentum sector (where the identification with the corresponding excited states in the CFT is straightforward by comparing excitation energies) by performing calculations on the critical Ising spin chain (of 200 spins) and found perfect agreement (see Fig. 1) [19]. In Table I we show some of the exact F_Ψ functions in the Ising model.

In addition to the general characteristics already discussed we see that for certain states one can identify multiple decay exponents important in different domains of the subpurity. While the first exponent depends only on the excitation energy (2) the further exponents are different for degenerate

TABLE I. Square roots of the scaling functions F_Ψ for some spin zero states in the Ising CFT given as sums of cosines, $\sqrt{F_\Psi(d)} = \sum_{n=0}^{n_{\max}} c_n \cos(2\pi n d)$.

ψ	1	$\cos 2\pi d$	$\cos 4\pi d$	$\cos 6\pi d$	$\cos 8\pi d$	$\cos 10\pi d$	$\cos 12\pi d$
1	1						
ε	$\frac{7}{8}$	$\frac{1}{8}$					
$L_{-1}\varepsilon$	$\frac{1558}{2048}$	$\frac{439}{2048}$	$\frac{26}{2048}$	$\frac{25}{2048}$			
$L_{-2}1$	$\frac{426347}{524288}$	$\frac{53640}{524288}$	$\frac{38076}{524288}$	$\frac{6200}{524288}$	$\frac{25}{524288}$		
$L_{-2}\varepsilon$	$\frac{6085442}{8388608}$	$\frac{1693410}{8388608}$	$\frac{514952}{8388608}$	$\frac{49813}{8388608}$	$\frac{9270}{8388608}$	$\frac{35721}{8388608}$	
$L_{-3}1$	$\frac{5569438}{8388608}$	$\frac{2319464}{8388608}$	$\frac{250807}{8388608}$	$\frac{187108}{8388608}$	$\frac{29426}{8388608}$	$\frac{31924}{8388608}$	$\frac{441}{8388608}$

states. Based on this observation we can also define a purity spectrum $\{p_1, p_2, \ldots, p_n\}$ consisting of all the exponents relative to the specific state. Indeed, it would be very interesting to better understand this form of the purity through an explicit calculation of the exponents in terms of the conformal data and to understand their physical meaning. In fact, a similar structure was found in [11] for the massive XY spin chain and it was suggested that (at least some) excited states can be reinterpreted as ground states of systems of coupled spin chains, where applying the area law leads to an extensive behavior for the entanglement entropy with slope changes depending on the specific state.

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