Extreme fluctuations of entropies in quantum systems

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The intuition that we have about entropy – coming largely from the Boltzmann entropy – is that the maximum entropy state is very close to the equilibrium state, while low entropy is associated with highly non-equilibrium states. It this paper, we investigate two well-developed definitions of entropy relevant for describing the dynamics of isolated quantum systems, and ask if they lead to this same intuition, by studying their extreme fluctuations. We choose entanglement entropy, because it is very often used, and Observational entropy, which is a recently introduced generalization of Boltzmann entropy to quantum systems, for comparison. While entanglement entropy is an important measure that quantifies non-local correlations, we find that Observational entropy, which quantifies localization of particles instead, matches better with our intuition from the Boltzmann entropy. For example, the distribution of particles in the equilibrium state is very different from that of the maximum entanglement entropy state, but very similar to that of the maximum Observational entropy state. Considering these differences, we conclude that Observational entropy could accompany the entanglement entropy to better understand the concept of thermalization in isolated quantum systems.

I. INTRODUCTION

There are a number of distinct notions of entropy throughout physics – including for example definitions by Clausius, Boltzmann, Gibbs, von Neumann, Bekenstein-Hawking, and others. Often these notions qualitatively and quantitatively coincide in the limits of large numbers of particles in equilibrium under some set of constraints. Yet, physical systems in nature are generally in – at best – quasi-equilibrium states and are essentially always very far from equilibrium from the standpoint of fundamental physics. This raises a question of whether the intuition we have about the entropies that we often use are, in fact, valid when taken out of the context of equilibrium systems.

For instance, what are the types of entropies that are relevant even out-of-equilibrium, and still match with our common intuitions of entropy such as a measure of disorder, of an ability to perform work, or of the information content an observer has about the physical system?

In this work, we ask these questions, and study numerically the out-of-equilibrium behavior and the extreme fluctuations of two well-developed notions of entropy that are relevant and interesting in isolated thermodynamic systems.

The first of the two entropies we consider is the entanglement entropy [1–4], which is a well-known entropy measure that quantifies the amount of non-local correlation between a subsystem and its compliment. It has a wide range of use and is important in understanding thermalization in isolated systems [5–7], quantum correlations and phase transitions [8–10], the holographic principle and black hole entropy [11, 12], as well as quantum information theory [13–15]. The second entropy we consider is the Observational entropy [16–18], which is a generalization of Boltzmann entropy to quantum systems.

Originally introduced by von Neumann [19, 20] as a resolution to the fact that the [von Neumann] entropy does not increase in isolated systems, then briefly mentioned by Wehrl [21] as “coarse-grained entropy”, Observational entropy has experienced a significant resurgence recently: it was generalized to multiple coarse-grainings [16, 17], found to dynamically describe thermalization of isolated quantum [17, 22] and classical [18] systems, discussed in relationship with other types of entropies [23], found to increase under Markovian stochastic maps [24], and argued for as a natural candidate for entropy production [25] because its definition does not need an explicit temperature dependence.

Fluctuations in entropy were discussed far before these two types of entropy were introduced. The concept of entropy itself originated from Clausius, who laid the ground work for the second law of thermodynamics in the mid 19th century.

It was Boltzmann who interpreted this concept statistically by inventing the infamous $H$-theorem [26], which then led to a new definition of entropy that makes use of the statistical weight of the macrostate; for a given macrostate, the Boltzmann entropy is defined as $S_B = \ln \Omega$, where $\Omega$ is the number of constituent microstates. It is proportional to Clausius’s entropy for systems in thermal equilibrium but is also meaningful for systems out of equilibrium, unlike the original definition of entropy [27].

Boltzmann postulated that his entropy (the negative of the quantity $H$) always increases, and did not mention anything about possible downward fluctuations. This was criticizes by Zermelo, and Boltzmann explains in a later letter [28] that fluctuations in entropy are indeed unlikely but possible. For example, particles can in prin-
ciple spontaneously contract into a small space (e.g., corner of a room), and thus intuitively decrease the (Boltzmann) entropy. This laid the groundwork for the study of fluctuations in entropy.

Much later, the relations that constrain the probability distribution of entropy fluctuations, i.e. the Fluctuation Theorems (FTs), became one of the most significant discoveries in non-equilibrium statistical physics [29–33]. Fluctuation relations for closed [34–36] and open systems [37–39] pertain when an external force drives the system out of equilibrium.

These studies do not, however, explore how high or low the entropy of a quantum system can get if it has access to long time scales; this is the focus of this work. We do this for an isolated system, meaning that there is no exchange of energy or particles between the system and the surrounding, and the system evolves unitarily in the absence of any external drive.

We also examine what the states with such extreme entropies looks like, how they compare for different types of entropies, and how they depend on system size and inverse temperature.

Interestingly, we find that although entanglement entropy is connected to the thermodynamic entropy when the full system is in thermal equilibrium [7, 40–42], in the extreme cases studied in this paper, the behavior of entanglement entropy does not fit typical intuitions about entropy. For example, there are macrostates with very many microstates that correspond to minimal entanglement entropy, and macrostates with very few microstates that correspond to maximal entanglement entropy. This shows that outside of equilibrium, entanglement entropy is fundamentally different from Boltzmann’s idea of entropy. A type of Observational entropy, $S_{\text{ent}}$, on the other hand, associates larger entropy with larger macrostates, in accordance with Boltzmann.

The paper is structured as follows. In section II, we introduce the model at hand as well as the entropies under study. Next III, we examine the probability distribution of entropies over long time unitary evolution of the system and find the minimal and maximal values of entropy, given infinite time. We then compare the states with minimal, maximal and average entropy. In sections IV and V, we investigate the dependence of extreme values of entropy on system size and inverse temperature, respectively. We find that Observational entropy never reaches values significantly below 1/2 of its maximum value, as argued in a previous study [43]; this is in contrast to entanglement entropy of the small subsystem, which can reach very close to zero in the limit of large system and bath size. In section VI, we provide numerical evidence that the result of [43] is correct in the case of a physical system such as a fermionic lattice. Finally, in section VII, we connect the results of IV and VI; we show that for a highly localized state – i.e. a state for which the probability of localization in a small region is maximized – has minimal Observational entropy, but not entanglement entropy.

In this paper we consider a system of $N_p$ spin-less fermions in a 1-dimensional lattice of size $L$. The Hamiltonian describing fermions in $L$ sites is

$$\hat{H} = \sum_{i=1}^{L} [-t(f_i + f_{i+1} + h.c.) + V n_i^f n_{i+1}^f - t'(f_i + f_{i+2} + h.c.) + V' n_i^f n_{i+2}^f].$$

Here $f_i$ and $f_i^\dagger$ are fermionic annihilation and creation operators for site $i$ and $n_i^f = f_i^\dagger f_i$ is the local density operator. The nearest-neighbor (NN) and next-nearest-neighbor (NNN) hopping terms are respectively $t$ and $t'$ and the interaction strengths are $V$ and $V'$ as illustrated in Fig. 1.

In all simulations, we take $t = t' = 1.9, V = V' = 0.5$. In most simulations we take the inverse temperature to be $\beta = 1/T = 0.01$ (the reason for this choice is discussed in detail in section VI) with exceptions in Figures 6 and 7, where we illustrate the dependencies on temperature. We take number of particles $N_p$ to be either 2 or 3, and we use different system sizes $L$. The eigenvalues and eigenvectors of relevant Hamiltonians are computed using exact diagonalization. Using this method however limits us to small size systems due to the exponential rise in computation time and memory requirements with system size, hence the use of only 2 or 3 particle systems.

For entanglement entropy, we consider a bipartite system with Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$, where A and B label the two partitions. Entanglement entropy is then defined as

$$S_{\text{ent}}(\hat{\rho}_{AB}) = -\text{tr}[\hat{\rho}_A \ln \hat{\rho}_A]$$

where $\hat{\rho}_A = \text{tr}_B[\hat{\rho}_{AB}]$ is the reduced density matrix. This entropy measures the amount of correlations, or “entanglement” between $A$, the subsystem of interest, and $B$, the bath. We take sizes of $A$ and $B$ to be $\Delta x = 4$ and $L - \Delta x = L - 4$ sites respectively. The exception to this is in Sec. VI where we consider the subsystem to be of size $\Delta x = 5$ sites in order for the subsystem to be large enough to contain all $N_p = 3$ particles.

![FIG. 1. A lattice of size 5 sites and 3 particles is shown. The right hand side of the figure illustrates the hopping terms $t$ and $t'$, i.e., particles move to the nearest-neighbor (NN) and next-nearest-neighbor (NNN) sites respectively. The left hand side of the figure shows the interactions of strengths $V$ and $V'$ between NN and NNN respectively.](image-url)
It is worth mentioning that there are other definitions of entanglement entropy in which the system has multiple partitions and the entanglement entropy of the system is the sum of the entanglement entropies of each partition, i.e., the entanglement of each partition with the rest of the system [5, 44, 45]. However, entanglement entropy is most commonly used in the context of bipartite systems in the literature, for example, in relation to the Bekenstein-Hawking entropy of a black hole where the existence of a horizon leads to the bipartition of the degrees of freedom on a Cauchy surface [46]. It is also common to use in studying quantum information protocols [47, 48] and understanding phases of matter [49, 50].

Next, we consider Observational entropy with position and energy coarse-graining [16–18]

\[ S_{\text{OE}}(\hat{\rho}) = S_{\text{C}}(\hat{C}_X) C_{\hat{R}}(\hat{\rho}). \]  
(3)

Positional (configuration) coarse-graining \( \hat{C}_X \) \( \equiv \hat{C}_{N_1 \otimes \ldots \otimes N_m} \) defines the partitions of the system (regions), and corresponds to measuring the number of particles in each of the \( m \) regions. Energy coarse-graining \( \hat{C}_{\hat{E}} \) is the coarse-graining by energy eigenstates of the system, corresponding to measuring the total energy. In contrast with the entanglement entropy, there is not a subsystem or a bath; instead the entire system is divided into equally sized partitions. We set the size of each partition to be \( \Delta x = 4 \), so in a system of size \( L \), there will be \( m = \frac{L}{\Delta x} = \frac{L}{4} \) number of partitions.

This entropy can be interpreted as “dynamical” thermodynamic entropy: it approximates the sum of thermodynamic entropies of each partition [17, 18]. As these partitions exchange particles and/or heat, this entropy rises to thermodynamic entropy of the entire system, which corresponds to partitions being in thermal equilibrium with each other. Therefore, \( S_{\text{OE}} \) measures how close to thermal equilibrium these partitions are.

In all cases, we take the initial state to be a random pure thermal state (RPTS) (also known as thermal pure quantum or canonical thermal pure quantum state [51–53]), which we define as

\[ |\psi\rangle = \frac{1}{\sqrt{Z}} \sum_E c_E e^{-\beta E/2} |E\rangle, \]  
(4)

where \( |E\rangle \)'s are the eigenstates of the total Hamiltonian, computed using exact diagonalization. The coefficients \( \{c_E\} \) are random complex or real numbers, \( c_E \equiv (x_E + iy_E)/\sqrt{2} \), and \( c_E \equiv (x_E + y_E)/\sqrt{2} \) respectively, which leads to what will refer to as the complex or the real RPTS, with \( x_E \) and \( y_E \) obeying the standard normal distribution \( \mathcal{N}(0,1) \), and \( Z = \sum_E |c_E|^2 e^{-\beta E} \) is the normalization constant. These states emulate a thermal state, while being pure. They are then evolved as \( |\psi_t\rangle = e^{-iT\hat{H}} |\psi\rangle \).

III. DISTRIBUTION OF FLUCTUATIONS IN ENTROPY

In this section we explore downward and upward fluctuations in entanglement and Observational entropy, and the states achieving extreme values in entropy.

First, we plot histogram of fluctuations in entanglement (Fig. 2) and Observational entropy (Fig. 3), in a system of size \( L = 16 \): starting from a complex RPTS, the system is evolved, and at each small fixed time step we read out the value of entropy. Evolving for a long time, we therefore achieve sufficient statistics that tells us how likely it is to find any given value of entropy.

We can also ask what the minimum and maximum values of entropy are, given infinite time. Due to the exponential suppression of these extreme values, histogram cannot provide this minimum; we therefore use a minimization algorithm, explained below, and add the results to the histogram (orange and blue vertical lines in Figs. 2 and 3).

To find the extreme values of entropy we use the simplex search algorithm [54]. For a given \( L \) and \( \beta \), we initialize the state in the same complex RPTS as the one we used to create the histograms in 2 and 3. We then find the maxima and minima for this initial state by maximizing over phases \( \phi_E = Et \). As long as ratios of \( E \)'s are irrational (or close to being irrational), this method must give the same result as maximizing over all times \( t \).

A. Entanglement entropy

We can see that entanglement entropy achieves a minimal value that is very close to zero. We plot the heat map (below the histogram in Fig. 2) of the particle density of the state that corresponds to this minimum. We can see that in this situation, the particles moved almost entirely into the bath, thus naturally producing a separable state \( |\psi_{\text{min}}\rangle \approx |0\rangle_A \otimes |\psi\rangle_B \), where \( |0\rangle_A \) denotes vacuum in the subsystem. One might think that an alternative state \( |\psi_{\text{min}}\rangle \approx |\psi\rangle_A \otimes |0\rangle_B \), could also lead to zero entanglement entropy. However, as it is explained in the Section VI, one can not cluster all particles in a small region, when starting in a RPTS.

On the other hand, the state with maximum value of entanglement entropy is the one where the subsystem and the bath contain the same average number of particles. The smaller region therefore has a higher density of particles, as illustrated on the heat map. Intuitively, there have to be some particles in the subsystem and some in the bath, for any correlations to exist; and to create the maximum correlation, there should be the same amount of particles on either side. As can be seen from comparing the heat maps in Fig. 2, the state that has the maximum entanglement entropy is quite different from the thermal equilibrium state, where particles are distributed uniformly.
FIG. 2. Semi-log probability histogram of entanglement entropy, $S_{\text{ent}}$. The y-axis represents the probability of finding the state at any given value of the entropy represented on the x-axis. The left tail, representing the downward fluctuations in entropy, can be fitted with a linear function: this shows that fluctuating to small values is exponentially suppressed in this data set. The blue vertical line on the left is the minimum value the entanglement entropy can achieve, and is found using a minimization algorithm. This value is very close to zero. The heat map below shows the particle density on the lattice of the state that corresponds to this minimum. We can see that in this situation, the particles moved almost entirely into the bath, thus naturally producing a separable state.

The minimum in $S_{\text{ent}}$ is achieved by simply localizing the particles in one of the regions to the extent possible (it does not matter significantly which one, as they all give almost equal entropy; however, if one of the regions was smaller than the others, it would localize into this smallest region). The minimal value of $S_{\text{ent}}$ never goes below about half of the maximal entropy; this, again, has to do with the inability to cluster all particles in a small region, when starting in an RPTS (see Sec. VII for a better intuition). The maximum of $S_{\text{ent}}$ is given by a state where particles are uniformly distribution across all regions. $S_{\text{ent}}$ is therefore in accordance with the Boltzmann entropy, in contrast to entanglement entropy.

The orange vertical line on the right is the maximum value of the entanglement entropy, and is also obtained by the minimization algorithm. The heat map above shows the particle density on the lattice of the state that corresponds to this maximum. In this situation, both the subsystem and the bath have the same number of particles, hence we see a higher density of particles in the subsystem. The state that gives the maximal entanglement entropy, is very far from the thermal equilibrium state.

FIG. 3. Similar to entanglement entropy, downward fluctuations of $S_{\text{xE}}$ to small values is exponentially suppressed in this data set. However, in contrast to entanglement entropy, the minimum of $S_{\text{xE}}$ represented by the blue vertical line does not go to zero; it is at about 63% of the maximum value. This is because it is impossible to localize the particles entirely into the small region, and the remaining regions still contribute significantly to the total entropy. As one can see from the heat map of the state corresponding to the minimum, a significant number of particles moved into one of the partitions of size 4 sites, resulting in partitions being far from thermal equilibrium from each other. The right vertical line represents the maximum value that $S_{\text{xE}}$ can achieve. The heat map above shows the uniform distribution of particles for such state. In contrast with entanglement entropy, the states that gives the average and maximal values of $S_{\text{xE}}$ are very similar to each other, as one would naturally expect from the intuition given by Boltzmann entropy.

### B. Observational entropy $S_{\text{xE}}$

The minimum in $S_{\text{xE}}$ is achieved by simply localizing the particles in one of the regions to the extent possible (it does not matter significantly which one, as they all give almost equal entropy; however, if one of the regions was smaller than the others, it would localize into this smallest region). The minimal value of $S_{\text{xE}}$ never goes below about half of the maximal entropy; this, again, has to do with the inability to cluster all particles in a small region, when starting in an RPTS (see Sec. VII for a better intuition). The maximum of $S_{\text{xE}}$ is given by a state where particles are uniformly distribution across all regions. $S_{\text{xE}}$ is therefore in accordance with the Boltzmann entropy, in contrast to entanglement entropy.

### IV. DEPENDENCE OF EXTREME VALUES ON THE SYSTEM SIZE

Next, we study the dependence of the minimum, maximum, and mean values of entropy on the system size. The minimum and maximum values are found using the minimization algorithm as in figures 2 and 3, and the average value is found by evolving the system for a long time.

#### A. Entanglement entropy

These values are shown for entanglement entropy in Fig. 4. The size of the subsystem is kept fixed at $\Delta x = 4$ while the system size (and hence the bath size) is varied.
in Fig. 4 with increasing system size $L$. It is clear that as the bath (of size $L$) gets larger, it becomes easier to cluster all the particles in the larger bath, which makes the subsystem emptier, thus creating a state that resembles very closely a product state, and thus has a very small entanglement entropy.

It is important to emphasize that reduction in entanglement entropy is not achieved through disentangling the particles, but by disentangling the regions through the means of particles hopping and emptying the smaller region. Therefore the following question is raised: how much entropy would be reduced if particles’ hopping between the regions was forbidden? A simulation of this case – where the hopping terms between the two regions are zero – revealed that the reduction of entanglement entropy is much smaller: about 20% reduction.

The upper bound on maximum of entanglement entropy was derived in [55] for closed, fermionic and bosonic systems. Specifically, in Fig. 4, where a (1-dimensional) fermionic lattice is considered, we have

$$S_{\text{ent}}(\text{max}) \leq \ln \sum_{n_A=0}^{N_p} \min \left\{ \frac{\Delta x}{n_A}, \frac{L - \Delta x}{N_p - n_A} \right\}. \quad (5)$$

In the case of $N_p = 2$ and $\Delta x = 4$ explored in Fig. 4, $S_{\text{ent}}(\text{max})$ achieves exactly this upper bound at $\ln 6 = 1.79$. The upper bound (5) is independent of the size of the bath in the limit of large $L$, which explains the constant maximum value in Fig. 4 (the large $L$ in this case is already $L \geq 12$, and $L = 8$ gives coincidentally the same value).

The average entanglement entropy should be approximately equal to the thermodynamic entropy of the sub-
system [5, 56, 57], which is a fraction of the total thermodynamic entropy,

\[ S_{\text{ent}}(\text{ave}) = S_{\text{th}}(A) = \frac{\Delta x}{L} S_{\text{th}}(A + B), \]  

(6)

where \( S_{\text{th}} \) is computed as the von Neumann entropy of a thermal state. This has been confirmed in various numerical simulations [6, 7, 58]. We see that this prediction, plotted as a red dashed line in Fig. 4, fits quite well with the data.

Comparing the maximum value of entanglement entropy with the average, we stress that \( S_{\text{ent}}(\text{max}) \) is constant while \( S_{\text{ent}}(\text{ave}) \) decreases with \( L \), which is reasonable to expect, since the average state spreads the particles uniformly over the entire system, creating less entanglement between the subsystem and the bath, while maximizing entanglement entropy maximizes correlations, by putting about a half of the particles in the subsystem, independently of the total system size. This adds to Fig. 2 in demonstrating the difference between states leading to the average and the maximal entanglement entropy.

B. Observational entropy \( S_{\text{OE}} \)

Using the same procedure, we find the mean values of minima, maxima, and averages of \( S_{\text{OE}} \), and their variances, and plot them as a function of the system size in Fig. 5. Partitions have equal sizes fixed at \( \Delta x = 4 \) and the system size \( L \) (and therefore the number of partitions \( m = \frac{L}{\Delta x} \)) is varied.

The minimum values of Observational entropy \( S_{\text{OE}} \) reduces to about a half of its maximum value independent of the system size, as long as it is large. These values could be indirectly estimated by simply assuming that the spatial localization is key in minimizing the entropy (see Fig. 9 and Eqs. (7) and (8)).

The maximum value of \( S_{\text{OE}} \) is almost exactly the same as the thermodynamic entropy of the full system, and very close to the average value of \( S_{\text{OE}} \). This is expected from the theory [17], that shows \( S_{\text{OE}}(\text{ave}) \leq S_{\text{OE}}(\text{max}) \leq S_{\text{th}} \), and \( S_{\text{OE}}(\text{ave}) \) differs from thermodynamic entropy \( S_{\text{th}} \) by order-1 corrections (that depend on the energy distribution of the initial state), by \( \ln N \) corrections (that depend on how close the initial state is to the thermal state), both of which become irrelevant in the thermodynamic limit, and by finite-size corrections (coming from interaction energy between partitions), which become irrelevant when partitions are large enough.

V. DEPENDENCE OF EXTREME VALUES ON TEMPERATURE

In this section, we look at the dependencies of the average and both extremes of \( S_{\text{ent}} \) and \( S_{\text{OE}} \) on inverse temperature \( \beta \). Each data point in Figures 6 and 7 are computed by taking the mean of the min, max, and average entropies over 6 different complex RPTSSs. We also included the thermodynamic entropy of the subsystem, \( S_{\text{th}}(A) \), and of the total system, \( S_{\text{th}}(A + B) \), in Figures 6 and 7 respectively.

A. Entanglement entropy

Fig. 6 plots the entanglement entropy versus \( \beta \). As one would expect, there are high fluctuations in the low \( \beta \) (high temperature) limit. In this limit, the average entanglement entropy coincides with the thermodynamic entropy of the subsystem, which is known as the Volume law [53]. Both maximal and minimal entanglement entropy diverge from the average at low \( \beta \), and are almost constant in this limit: \( S_{\text{ent}}(\text{max}) \approx 1.79 \) (which is the high-temperature limit obtained previously in Fig. 4), and \( S_{\text{ent}}(\text{min}) \approx 0.05 \). There are almost no fluctuations in the opposite high \( \beta \) (low temperature) limit, where the thermal state is almost identical to the ground state, and therefore it does not evolve. The entanglement entropy approaches a constant value given by the Area law [15, 59, 60].

B. Observational entropy \( S_{\text{OE}} \)

Fig. 7 plots the Observational entropy \( S_{\text{OE}} \) versus \( \beta \), and we took the same settings as with entanglement entropy. One can notice two interesting features in this graph.

First, values of \( S_{\text{OE}} \) at high \( \beta \) (low temperature) limit are quite large, and do not seem to follow the \( S_{\text{th}}(A + B) \) anymore. The fact that the \( S_{\text{OE}} \) is not zero in this low temperature limit is because measuring position does not commute with measuring energy. By measuring the position of the ground state, which is highly non-local, one would add a lot of energy to it, as well as uncertainty in energy. Therefore, since \( S_{\text{OE}} \) measures the total uncertainty when measuring the position first and then energy, this total uncertainty will be large. \( S_{\text{OE}} \) can be also interpreted as a thermodynamic entropy of the system, as if the numbers of particles in each bin were fixed, but the energy between the bins was still allowed to exchange [16–18]. It therefore makes sense that the value of this entropy is relatively large, since by measuring the position we fix the number of particles in each bin, and this state has a relatively large thermodynamic entropy. This effect gets to be smaller (\( S_{\text{OE}} \) for high \( \beta \) is smaller), when size of the partition \( \Delta x \) becomes large compared to the size of the full system, since position measurement does not affect energy as much in that case. We note that this is a purely quantum effect, however, switching the order of coarse-grainings (while taking some small coarse-graining of width \( \Delta \) in energy as well), \( S_{\text{OE}} \) leads to an entropy that is bounded above by \( S_{\text{th}}(A + B) \) even at such low temperatures. This is because measuring en-
energy of a ground state does not affect this state at all, and additional measurement in position does not add any new information (see Theorem 8 in [17]). This effect was not noted in the original paper [17], mainly because defining microcanonical entropy at such low temperatures is problematic, as the energy density of states is not well defined.\footnote{Fig. 7 in [17] does not show $S_{\text{th}}$ nor microcanonical entropy for really low, or really high energies $E$.}

The second interesting feature of this graph is the dip in $S_{\text{th}}(\min)$ at $\beta \approx 0.5$. This dip is a result of two competing factors: first, by increasing the temperature, we increase the ability of the system to localize. Generally, localizing the system in one of the partitions leads to a decrease in $S_{\text{th}}$ (see Section VII). Thus, with high enough temperature the system is able to localize in one of the partitions of size $\Delta x = 4$ and decrease the entropy. However, further increasing temperature does not help in decreasing $S_{\text{th}}(\min)$ anymore, as the further ability to localize is already below the resolution of the positional coarse-graining in $S_{\text{th}}$, and its only effect is then an increase in the total thermodynamic entropy, and hence also an increase $S_{\text{th}}(\min)$.

That is also why we see the increase in $S_{\text{th}}(\min)$ for really high temperature (low $\beta$), in a shape that approximately follows Eqs. (7) and (8).

VI. MAXIMAL PROBABILITY OF LOCALIZATION

In this section we show numerically that the result of Deutsch et al. [43] – shown analytically for a toy model with random energy eigenvectors as well as for a non-degenerate weakly interacting gas – holds true for a physical system of a fermionic lattice. We do this because in Sec. VII we would like to use this result to explain the connection, already hinted in the previous sections, between the spatial localization and the minimization of entropies.

In particular, Deutsch et al. showed that starting from a RPTS, under certain conditions, the maximum probability $P_{\text{max}} \equiv P_{(N,0)}$ that all particles are localized into the subsystem of interest is $1/2$ in the case of initial real RPTS and $\pi^2/16$ in the case of complex RPTS. This, as shown in section VII, is key in minimizing $S_{\text{th}}$.

We are going to require that the same conditions as in [43] to be satisfied: The first condition is that the dimension $M$ of the subspace $X$ (the subspace of Hilbert space associated with “all particles being in the subsystem of interest”) is much smaller than the dimension $N$.  

FIG. 6. The minimum (blue), maximum (orange), and average (green) values of entanglement entropy is computed for 6 different initial random states (complex RPTSs); the means of these 6 values are illustrated in this figure for various inverse temperatures, $\beta$. We take $L = 16$, $\Delta x = 4$, and $N_x = 2$. In low $\beta$ limit, $S_{\text{ent}}(\text{ave})$ follows the volume law, and is approximately equal the thermodynamic entropy of the subsystem $S_{\text{th}}(A)$. In high $\beta$ limit, the initial state is practically the energy ground state, and therefore it does not evolve, so all values coincide, at a value given by the area law.

FIG. 7. The minimum (blue), maximum (orange), and average (green) values of Observational entropy $S_{\text{th}}$ is computed for 6 different initial random states (complex RPTSs); the means of these 6 values are illustrated in this figure for various system sizes. We take $L = 16$, $\Delta x = 4$, and $N_x = 2$. In low $\beta$ limit, $S_{\text{th}}(\text{ave}) \approx S_{\text{th}}(\text{max}) \approx S_{\text{th}}(A + B)$, and $S_{\text{th}}(\min)$ has the same shape, and about a half of the maximum value, as expected from Eqs. (7) and (8). All values coincide in the high $\beta$ limit where the initial state is practically the energy ground state. Its higher value compared to $S_{\text{th}}(A + B)$ is expected from the fact that measuring position of this highly non-local state first, creates a large uncertainty in energy, and therefore also large $S_{\text{th}}$. The dip in $S_{\text{th}}(\min)$ is the result of two competing factors: higher temperature results in higher entropy on average, but also higher ability of the system to localize, and therefore possibly lower values of $S_{\text{th}}$. $\beta \approx 0.5$ is the lowest possible temperature such that the state can localize in one of the bins of size $\Delta x = 4$.\n
That is also why we see the increase in $S_{\text{th}}(\min)$ for really high temperature (low $\beta$), in a shape that approximately follows Eqs. (7) and (8).
FIG. 8. (a) Maximum probability \( P_{\text{max}} \) of localizing all particles in the middle 5 sites for real (crosses) and complex (stars) initial RPTSs, in a lattice of size \( L=10 \) (blue), \( 20 \) (green), and \( 30 \) (red), with 3 particles as a function of \( \sqrt{\beta} \). This plot illustrates that at low \( \beta \), \( P_{\text{max}} \) approaches different constant values for real (0.5 red line) and complex (\( \pi^2/16 \) black line) RPTSs when the system size is large enough. In the same limit, \( P_{\text{max}} \) approaches unity for smaller systems. For higher values of \( \beta \), \( P_{\text{max}} \) approaches zero independent of system size. (b) The maximal probability \( P_{\text{max}} \) is computed for a range of dimensions of Hilbert space \( N \), while \( M \) — dimension of the subspace of the Hilbert space associated with “all particles in the localized region” — is kept fixed. Hence the size of the physical region in which particles are localized is kept fixed as well, at \( \Delta x = 5 \) sites. For each \( N \), we start in 100 different real and complex RPTSs with the same temperature, and plot the mean and standard deviation of \( P_{\text{max}} \) (real as red bars, complex as black bars). This plot indicates that in the limit of large system sizes, the maximum probability of localization of all particles into a small region approaches \( \sim 0.5 \) (red line) in the case of real initial states and \( \sim \pi^2/16 \) (black line) in the case of complex initial states.

of the full system, \( N \gg M^2 \), which can be for example satisfied in the case of dilute gas (small number of particles) when the size of the subsystem of interest \( \Delta x \) into which we localize the particles is much smaller than the size \( L \) of the full system, \( L \gg \Delta x \). At the same time, the second condition is that the size of the subsystem is much larger than a thermal wavelength (specified below), \( \Delta x \gg \lambda_T \). The third condition is that the size of the subsystem of interest, \( \Delta x \), is also much greater than the scattering length, i.e., we consider the Hamiltonian with only local interactions, leading to a weakly correlated system. However unlike what is used in [43] – in which the energy eigenstates of the toy model are randomly distributed or are that of a non-degenerate weakly interacting gas – in our case the energy eigenstates are that of a Hamiltonian modeling a fermionic lattice.

First, we investigate the second condition, \( \Delta x \gg \lambda_T \) in more detail. At any value of \( \beta \), there exists a spatial scale known as the thermal wavelength such that \( \lambda_T \propto \sqrt{\beta} \) (for example, in the case of an ideal gas, \( \lambda_T = 2h\sqrt{\frac{T}{\beta}} \)). Intuitively, \( \lambda_T \) is the minimum size of quantum wavepackets that describe the particles in a given system at a given temperature. Because of this relation between \( \lambda_T \) and \( \sqrt{\beta} \), we can focus on the dependence of \( P_{\text{max}} \) on \( \sqrt{\beta} \).

Therefore, in Fig. 8(a) we study the maximum probability \( P_{\text{max}} \) of localization for different values of \( \sqrt{\beta} \) while fixing the size of the box \( \Delta x \). We localize in the region of size \( \Delta x = 5 \), and use the lattice sizes \( L = 10, 20, \) and \( 30 \), with \( N_p = 3 \) particles inside. We do this for both real and complex initial RPTSs.

We see that for cold systems (high \( \beta \)), the probability of localization is very small, in fact, \( P_{\text{max}} \) approaches zero. This is in accordance with the result of [43] which asserts that, in the limit of large \( \sqrt{\beta} \) such that \( \Delta x \ll \lambda_T \), \( P_{\text{max}} \propto (\frac{\Delta x}{\lambda_T})^{N_p d/2} \) where \( d \) is the dimension of the lattice (in our case \( d = 1 \)). Intuitively, since \( \lambda_T \) is the minimum size of quantum wavepackets, it makes sense that one can not localize the wavefunction in a subspace smaller than this length scale.

For hot systems (low \( \beta \)), the probability of localization \( P_{\text{max}} \) achieves high values. One notices that for small systems for e.g. \( L = 10 \), the gap between \( P_{\text{max}} \) for the real and complex wave functions disappears. This is trivial, since in this case, the size of the subsystem of interest is becoming comparable to that of the full system, and therefore it is very easy to localize all particles in it. For larger system sizes for e.g. \( L = 20, 30 \) all three conditions stated above are satisfied, and \( P_{\text{max}} \) approaches constant values of \( \sim 1/2 \) in the case of real RPTSs and \( \sim \pi^2/16 \) in the case of complex RPTSs. The low \( \beta \) regime is further explored in Fig. 8(b).

To generate this graph, we used the same algorithm to maximize probability as the one used in [43], and \( \beta = 0.01 \). We start in 100 different real and complex RPTSs, and for each one of them we perform the maximization procedure. We use three fermions and choose the small region to be \( \Delta x = 5 \) sites. \( P_{\text{max}} \) is plotted as a function
in the larger and smaller regions respectively. In this section, we investigate what happens to entanglement entropy when one localizes particles into the small region as opposed to the bath, and the extent to which the spatial localization plays a role in minimizing the $S_{\text{SE}}$.

We compute entropies of localized states, for $\Delta x = 4$ and varying system sizes $L$. We consider $N_p = 2$ particles in the system, and temperature is fixed at $\beta = 0.01$, so that the three conditions from the previous section are satisfied. For each $L$, we start in 6 initial complex RPTSs, and localize them into a physical region of fixed size $\Delta x = 4$, by maximizing probability $P_{\text{max}}$ for each initial state. We then compute the mean values and standard deviations of $S_{\text{ent}}$ and $S_{\text{SE}}$ of such localized states, and plot them in Fig. 9. The mean values of $P_{\text{max}}$ (averaged over 6 initial RPTSs) for system sizes of $L = [8, 12, 16, 20, 24, 28]$ are $P_{\text{max}} = [0.90, 0.73, 0.67, 0.67, 0.65, 0.63]$.

$S_{\text{SE}}(\text{loc})$ is very close to the minimum $S_{\text{SE}}(\text{min})$ (discussed in detail in Fig. 9), showing that spatial localization is key in minimizing $S_{\text{SE}}$. The theory predicts \cite{43} that

$$S_{\text{SE}}(\text{loc}) = S_{\text{th}}(L, N_p, \beta) - P_{\text{max}} \ln \frac{L}{\Delta x} - (1 - P_{\text{max}})N_p \ln \frac{L}{L - \Delta x}$$

for large $L$ (where $S_{\text{th}}(L, N_p, \beta) ≡ S_{\text{th}}(A + B)$), which is bounded below by

$$S_{\text{SE}}(\text{loc}) ≥ (1 - P_{\text{max}})S_{\text{th}}(L, N_p, \beta)$$

which shows that $S_{\text{SE}}(\text{loc})$ cannot fall below a certain fraction of the total thermodynamic entropy of the system. Eq. (7) is plotted as a dashed line in Fig. 9 and as expected from Eq. (8), the ratio $R = S_{\text{SE}}(\text{loc})/S_{\text{th}}(A + B)$ remains approximately constant for large $L$.

The fact that $S_{\text{SE}}(\text{loc})$ and $S_{\text{SE}}(\text{min})$ are almost the same and that $S_{\text{SE}}(\text{min})$ is bounded by a fraction of thermodynamic entropy also explains why the minimum of $S_{\text{SE}}$ in Fig. 3 does not go to zero, and why $S_{\text{SE}}(\text{min})$ in Fig. 7 goes upwards for small $\beta$ (in the case of low $\beta$ $P_{\text{max}} = \pi^2/16$).

VIII. DISCUSSION AND CONCLUSION

In this paper, we have demonstrated the significantly different behavior of extreme values of entanglement and Observational entropy. Studying these extreme values, we found that bipartite entanglement entropy, while being very useful tool for quantifying quantum correlations, does not match in general with the intuition one has from the definition of Boltzmann entropy. Observational entropy however, matches with this intuition.

With regards to extreme values, we found that starting from a random pure thermal state, $S_{\text{ent}}$ can reach values very close to zero during the course of a unitary evolution, whereas there exists a non-zero lower bound for $S_{\text{SE}}$. We showed how these minimal values of the two entropies are achieved through localization in the larger and smaller region for $S_{\text{ent}}$ and $S_{\text{SE}}$, respectively.

We found that in the high temperature limit, the maximum entanglement entropy is independent of the total

VII. ROLE OF LOCALIZATION IN EXTREME VALUES OF ENTROPIES

In figures 2 and 3 we showed that minimizing entanglement and Observational entropy leads to heavy localization in the larger and smaller regions respectively. In this section, we investigate what happens to entanglement entropy when one localizes particles into the small region as opposed to the bath, and the extent to which the spatial localization plays a role in minimizing the $S_{\text{SE}}$.

As one can see, when the system is hot enough, it is possible to localize all the particles into the small region, and the probability that we find them there is at most $1/2$ and $\pi^2/16$ for real and complex RPTSs respectively. The presence of some fluctuations is expected since our model is a real system with non-random energy eigenvectors. This numerically confirms that the results of Deutsch et al. \cite{43} also holds for a realistic quantum thermodynamic system such as ours, and we can apply this result in the next section.
The particle distribution given a state with maximum entanglement or Observational entropy is also markedly different; in the former case, the particles distribute themselves throughout the lattice such that the average number of particles in the subsystem is equal to that of the bath, in pursuit of maximizing correlations between the two subsystems. Whereas in the latter case, particles tend to distribute themselves uniformly, similar to what happens at thermal equilibrium.

These findings are illustrated in Fig. 10. In particular, Fig. 10 (a) and (b) show entropies for various types of macrostates, described by their particle density, in order of smaller to higher entanglement and Observational entropy, respectively. From the Boltzmann point of view, the size of the macrostate is determined by the number of microstates corresponding to the same macroscopic appearance: in this figure, size of the macrostate \( \Omega \) is the number of orthogonal quantum states that give the same distribution of particle density.

One notices that higher entanglement entropy does not necessarily mean that the macrostate is larger – the size of the macrostate appears to be rather unrelated to the amount of entanglement entropy. Specifically, it would be more likely to observe a state with minimal entanglement entropy as compared to the maximal entanglement entropy (as the former has a larger macrostate). The size of the macrostate and the entropy of the state match for the case of Observational entropy, showing that Observational entropy matches well with our intuition from the Boltzmann entropy.

We stress that in this paper we focused on bipartite entanglement entropy, since it is very often used in literature. One could argue that multipartite entanglement entropy, defined as the sum of local von Neumann entropies, could behave similarly to \( S_{\text{E}} \) and be more Boltzmann-like, meaning that the larger macrostates have associated higher values of entropy. This property would be however dependent upon having identically-sized regions, and the equivalence would break even when the size of a single region is different from others. The details of such study will be left for future work. We should emphasize that this does not diminish the central role that entanglement entropy plays in quantifying quantum correlations, not to mention the wide range of applications in the fields of condensed matter, quantum information, and quantum gravity.

Because of its close relation to Boltzmann entropy, Observational entropy could accompany the entanglement entropy to better understand the concept of thermalization in isolated quantum systems, and to illuminate the behavior of out-of-equilibrium states which lie at the heart of statistical mechanics. This entropy is also rather new in the field of quantum thermodynamics and hence further work on this particular entropy is of interest.
Experimentally, for example, Observational entropy could be measured without the need to access the density matrix, and be useful in quantifying how thermalized a given state is. The extreme values of this entropy could possibly be probed as well, for extremely small systems such that the time it takes to reach these values is reasonably small and within reach in laboratories. On the theoretical side, we could make estimations of how long it would take to reach the (near) global minimum or maximum entropy, starting from a random pure thermal state. It would be interesting to compare this time scale to that of the Poincaré recurrence time, in which the state was initialized, for example, as a state of the minimal Observational entropy.

Finally, on a cosmological level, discussions of entropy and the arrow of time (e.g. [61–66]) require a definition that applies to a truly closed system (like the Universe), out of equilibrium, and potentially for indefinitely long timescales over which large entropy fluctuations might occur. These discussions often employ an “informal” definition of entropy that in practice mixes different notions. Observational entropy applies in this context and is rigorously defined, and therefore may be very useful in these discussions. (The primarily remaining obstacle being a lack of understanding of the state-space of gravity and spacetime.) Could this definition of entropy, for example, tell us something new about the arrow of time in isolated quantum systems, and about how to understand extreme entropy fluctuations in the context of the arrow of time?

Extending this work to other types of Observational entropies that are in accordance with thermodynamic entropy (such as FOE [17]) would be of interest as well. This could give us a broader understanding of this new definition of entropy and shed some light on non-equilibrium many-body quantum systems.

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