Entanglement entropy from nonequilibrium work

Jonathan D’Emidio
Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

The Rényi entanglement entropy in quantum many-body systems can be viewed as the difference in free energy between partition functions with different trace topologies. We introduce an external field $\lambda$ that controls the partition function topology, allowing us to define a notion of nonequilibrium work as $\lambda$ is varied smoothly. Nonequilibrium fluctuation theorems of the work provide us with statistically exact estimates of the Rényi entanglement entropy. This framework also naturally leads to the idea of using quench functions with spatially smooth profiles, providing us a way to average over lattice scale features of the entanglement entropy while preserving long distance universal information. We put these ideas to use in the context of quantum Monte Carlo simulations of SU(N) symmetric spin models in one and two dimensions. In both cases we detect logarithmic violations to the area law with high precision, allowing us to extract the central charge for the critical 1D models and the number of Goldstone modes for the magnetically ordered 2D models.

Entanglement entropy is a quantity of basic importance in the characterization of quantum many-body wavefunctions. It signals the departure from a simple tensor product of subsystem wavefunctions for a spatial bipartition. Though in general the entanglement entropy depends only on the boundary size of the bipartition—the “area law”—and captures local correlations, violations to the area law can contain long distance universal information [1–3]. For instance, one dimensional critical systems show a logarithmic growth of the entanglement entropy with subsystem size where the prefactor depends on the central charge of the underlying conformal field theory [4–6]. Examples of universal features in higher dimensions include logarithmic contributions in symmetry broken phases with gapless Goldstone modes [7–16] and a universal negative constant in topological phases [17–19].

Remarkable progress has been made in the ability to compute entanglement entropy in strongly correlated lattice models, especially in the realm of quantum Monte Carlo (QMC) simulations where a priori one lacks direct access to the eigenvalues of the reduced density matrix. The interpretation of the Rényi entanglement entropies in terms of replica partition functions with different trace topologies has enabled the introduction of various QMC estimators [20–23]. While this has allowed for the investigation of many physical systems, the calculations remain costly due to the need to perform independent simulations either as a function of temperature or to incrementally compute the entanglement entropy for the region of interest. These inefficiencies are compounded in dimensions $d > 1$ where the area law dominates and universal features are subtle. Though improved estimators have been introduced [24,15], these represent either incremental advancements or are restricted to specific models.

At the same time, the ability to view the Rényi entanglement entropy as a difference of free energies begs the question of whether one can apply nonequilibrium work relations [25, 26] that have been widely used in the molecular dynamics community [27]. Indeed, this idea was recently explored in the context of classical path integral Monte Carlo [28], paving the way for the extension to QMC that we present here. To accomplish this we introduce an external field that couples directly to the trace topology of the degrees of freedom and does not appear in the Hamiltonian of the model. This not only allows for the efficient computation of the Rényi entanglement entropy of large regions in a single nonequilibrium simulation, but also naturally leads to the idea of smooth space-dependent quench functions. We show that this allows us to suppress lattice scale features of the entanglement entropy at the boundary between subsystems while preserving the long wavelength universal properties, and conveniently allows for the computation of the Rényi entanglement entropy as a function of subsystem size in a single nonequilibrium simulation.

General method: The Rényi entanglement entropy is given by

$$S_A^{(n)} = \frac{1}{1-n} \log(\text{Tr} \rho_A^n),$$

Figure 1. Nonequilibrium quench of the replica trace topology. Here the partition function $Z = \text{Tr} e^{-\beta H}$ of a 1D system is depicted as a cylinder due to the periodicity of the trace. $Z^{(2)}_\alpha$ is then represented as two independent cylinders, while $Z^{(2)}_A$ has a modified trace topology in the spatial region $A$ resembling a pair of pants. The nonequilibrium process takes place in the space of configurations contained in $Z^{(n)}_A$ (Eq. (3)), starting from equilibrium $Z^{(2)}_\phi$ configurations and driving them toward $Z^{(2)}_A$ configurations. The exponential average of the work done in this process gives the Rényi entanglement entropy $S^{(2)}_A$. 
where $n$ is the Rényi index (taken to be an integer larger than one in this work) and $\rho_A = \text{Tr}_B \rho$ is the reduced density matrix of a subsystem $A$. We express the density matrix as $\rho = e^{-\beta H}/Z$ with the partition function $Z = \text{Tr} e^{-\beta H}$. In what follows $\beta$ will be made sufficiently large so that only the ground state contributes.

$S_A^{(n)}$ can be conveniently re-expressed as [6]

$$S_A^{(n)} = \frac{1}{1-n} \log \left( \frac{Z_A^{(n)}}{\rho_A^{(n)}} \right), \quad (2)$$

where the replica partition functions are defined as $Z_A^{(n)} = \text{Tr} \left( (\text{Tr}_A e^{-\beta H})^n \right)$ and $\rho_A^{(n)} = (\text{Tr} e^{-\beta H})^n = Z^n$ (see Fig. 1). Notice that $Z_A^{(n)}$ and $\rho_A^{(n)}$ are defined in exactly the same way, where $\emptyset$ means that there are no sites in the $A$ subsystem. We now wish to define a function $Z_A^{(n)}(\lambda)$ such that $Z_A^{(n)}(0) = \rho_A^{(n)}$ and $Z_A^{(n)}(1) = Z_A^{(n)}$. This can be written explicitly as

$$Z_A^{(n)}(\lambda) = \sum_{B \subseteq A} \lambda^{N_B} (1-\lambda)^{N_A-N_B} Z_B^{(n)}, \quad (3)$$

where here $B$ denotes all possible subsets of $A$ including the empty set $\emptyset$ and $A$ itself. $N_A$ and $N_B$ denote the number of sites contained in the sets $A$ and $B$, respectively. Here $\lambda$ controls the probability for an individual site in the $A$ subsystem to be traced out once. To ease the notation in what follows we define

$$g_{BA}(\lambda, N_B) = \lambda^{N_B} (1-\lambda)^{N_A-N_B}.$$

The entanglement entropy can then be computed as:

$$S_A^{(n)} = \frac{1}{1-n} \int_0^1 d\lambda \frac{\partial \ln Z_A^{(n)}(\lambda)}{\partial \lambda}. \quad (4)$$

If one wanted to numerically compute this quantity using quantum Monte Carlo techniques, independent equilibrium simulations on a fine grid of points between $\lambda = 0$ and $\lambda = 1$ would need to be performed. Each simulation would measure the equilibrium average $\partial \ln Z_A^{(n)}(\lambda)/\partial \lambda = \langle N_B + N_A^{-1} - N_B \rangle \lambda$ and the resulting curve from all the simulations would need to be numerically integrated.

This approach has obvious practical limitations. It is much more desirable to estimate the entanglement entropy directly from a single simulation. Fortunately, this can be done by defining a nonequilibrium process in which $\lambda$ is varied smoothly from 0 to 1:

$$W_A^{(n)} = -\frac{1}{\beta} \int_{t_i}^{t_f} dt \frac{d}{dt} \ln g_A(\lambda(t), N_B(t)) \frac{\partial}{\partial \lambda}. \quad (5)$$

Here $\lambda(t_i) = 0$, $\lambda(t_f) = 1$ and $W_A^{(n)}$ is the total work done throughout the process. We emphasize here that the work is a random variable that will follow a distribution. One instance of the work is given by the sum of the increments $\partial \ln g_A(\lambda(t), N_B(t))$ along a nonequilibrium path in the configuration space of $Z_A^{(n)}(\lambda)$ as $\lambda$ is varied from 0 to 1. The average $\beta\langle W_A^{(n)} \rangle/(n-1)$ then approaches $S_A^{(n)}$ as $t_f - t_i \to \infty$. If the quench time is finite then the average will overestimate $S_A^{(n)}$ due to the nonequilibrium entropy production associated with irreversibility.

Again the situation is undesirable, since we would like to accurately estimate the entanglement entropy even when the quench time is finite. Here we can greatly prosper from a well known nonequilibrium fluctuation theorem of work, Jarzynski’s equality [25], which in this context reads:

$$S_A^{(n)} = \frac{1}{1-n} \log \left( \langle e^{-\beta W_A^{(n)}} \rangle \right), \quad (6)$$

Remarkably this equality holds true regardless of the quench time, though convergence of the exponential average over independent work realizations is best in the slow quench limit.

**Quench protocols:** In the previous section we outlined the general method in its simplest form, taking the quench parameter $\lambda$ to be constant in space over the $A$ subsystem and varying in time between 0 and 1. This is depicted in panel (a) of Fig. 2. While this provides us with a very efficient way of computing the entanglement entropy of large regions (see supplemental material), this work will focus on another quench protocol that com-
The second Rényi entanglement entropy using the quench protocol in Eq. (7) for an SU(2) $L = 64$ periodic chain. Here we quench the chain with three different values of $\delta$ which represents the smoothing of the subsystem boundary. For $\delta = 0.3$, individual sites of the chain can be resolved and one observes oscillations as a function of subsystem size. For larger $\delta$ the contribution from the boundary is averaged over several sites and oscillations disappear. By performing fits to the universal scaling form in Eq. (9) as a function of data dropped from the edges ($l_{drop}$), we see that the estimation of the central charge is insensitive to the presence of $\delta$ which only affects the area law constant $b$.

Figure 3. The second Rényi entanglement entropy as a function of subsystem size in a single nonequilibrium simulation.

Computes the entanglement entropy as a function of subsystem size in a single nonequilibrium simulation.

This can be achieved by making $\lambda$ a function of both time and space in such a way that the subsystem partition “slides” across the lattice, in which case Eq. (3) and Eq. (5) can be easily adapted (see supplemental material). This naturally leads us to the idea that $\lambda$ should be a smooth function of space so that individual sites are quenched gradually while the partition moves. A particularly convenient choice that we will use in the rest of this work is given by

$$\lambda(x, l(t), \delta) = \frac{1}{1 + e^{-(x-l(t))^{2}/\delta}}.$$  \hspace{1cm} (7)

Here $x$ is the spatial coordinate (from 0 to $L - 1$) along a periodic chain and $\lambda$ depends on time through the parameter $l(t)$ which represents the center of one boundary between the $A$ subsystem and the rest of the chain (see panel (b) and (c) of Fig. 2). A shift of $1/2$ is introduced so that $l(t)$ is centered between sites of the chain. We have also introduced a parameter $\delta$ that controls the width of the boundary. As we will discuss momentarily, $\delta$ allows us to suppress lattice scale features of the entanglement entropy while preserving the universal features.

The quench protocol as defined by Eq (7) involves varying $l(t)$ linearly in time from $l(t_i) = -p\delta$ to $l(t_f) = L - 1 + p\delta$, where the constant $p$ is used to ensure that $\lambda(x, l(t_i), \delta)$ and $\lambda(x, l(t_f), \delta)$ are approximately 0 and 1 everywhere, respectively. As $l(t)$ is varied along the length of the chain, the total work is computed as a function of time. Since $l(t)$ represents the current location of the subsystem boundary, this allows us to compute the entanglement entropy as a function of subsystem size in a single nonequilibrium simulation. Furthermore, since $l(t)$ is real valued, the entanglement entropy is computed as a continuous curve that can be sampled up to the number of time steps used in the nonequilibrium process.

We now wish to discuss the role of the parameter $\delta$, which is a central idea that emerges from our new method. When $\delta$ is small enough so that the width of the subsystem boundary is much less than the lattice spacing, our protocol allows for the exact computation of $S^{(2)}_\delta$ as a function of subsystem size. The entanglement entropy thus defined contains strong lattice-scale features that can often obscure universal properties that one wants to extract. By increasing $\delta$ so that the subsystem partition is spread over a few lattice sites we effectively average over features below a certain scale. As we intuitively expect, the presence of $\delta$ will only affect nonuniversal features of the entanglement entropy, namely the area law contribution. We will demonstrate in the following sections that this allows for the efficient extraction of universal features of the Rényi entanglement entropy in one and two dimensions.

**SU(N) chain:** As a first test case for our new method, we start with the SU(N) Heisenberg antiferromagnet on a periodic one dimensional chain [29, 30]. The Hamiltonian can be written simply as a nearest neighbor permutation:

$$H = \frac{J}{N} \sum_i \sum_{\alpha,\beta=1}^N |\alpha_i\beta_{i+1}\rangle\langle\beta_i\alpha_{i+1}|.$$  \hspace{1cm} (8)

The ground state of this model is critical, and belongs to the family of conformally invariant Wess-Zumino-Witten
nonlinear sigma models with central charge \( c = N - 1 \) [30]. This system gives rise to the celebrated log violation of the area law which is described by the following form:

\[
S^{(n)}(l) = \frac{c}{6} \left( 1 + \frac{1}{n} \right) \log \left( \frac{L}{\pi \sin \left( \frac{\pi l}{L} \right)} \right) + b. \tag{9}
\]

The Rényi entanglement entropies of this system also show oscillations as a function of subsystem size [31]. In Fig. 3 we use our newly developed nonequilibrium method in the framework of the stochastic series expansion QMC algorithm [32], combined with quench protocol in Eqn. (7) to show that lattice scale oscillations of the entanglement entropy can be suppressed by smoothing out the subsystem boundary using the parameter \( \delta \). Crucially the central charge is insensitive to the presence of \( \delta \), which only affects the nonuniversal constant (area law) contribution.

Since lattice scale features are averaged over, the resulting data is remarkably precise as demonstrated by Fig. 4 where we compute the second Rényi entropy for \( l = 120 \) chain for SU(2), SU(3) and SU(4), finding the expected central charges \( c = N - 1 \). To explore the full capability of this technique, we next turn to two dimensional systems.

2D staggered SU(N) Model: Recently, the entanglement entropy has been used to detect Goldstone modes in magnetically ordered systems [7, 15]. To this end, we select a family of two dimensional SU(N) symmetric models that support gapless spin wave excitations. The Hamiltonian is given by [33]

\[
H = -\frac{J_1}{N} \sum_{\langle ij \rangle} \sum_{\alpha, \beta = 1}^{N} |\alpha_i \alpha_j \rangle \langle \beta_i \beta_j | - \frac{J_2}{N} \sum_{\langle \langle ij \rangle \rangle} \sum_{\alpha, \beta = 1}^{N} |\alpha_i \beta_j \rangle \langle \beta_i \alpha_j |. \tag{10}
\]

Here we consider periodic square lattices, using the fundamental representation of SU(N) on one sublattice and the conjugate to the fundamental on the other sublattice. \( J_1 > 0 \) and \( J_2 > 0 \) are the nearest and next-nearest neighbor couplings, respectively.

This model is an SU(N) generalization of the spin 1/2 Heisenberg antiferromagnet with ferromagnetic next-nearest neighbor interaction. When \( J_2 = 0 \) the ground state is magnetically ordered with gapless Goldstone modes for \( 2 \leq N \leq 4 \) and forms a valence bond solid for \( N \geq 5 \) [34]. When \( J_2 > 0 \) magnetic order is enhanced which greatly facilitates the ability to accurately extract the number of Goldstone modes by fitting to our entanglement entropy data.

The presence of Goldstone modes produces a log contribution to the entanglement entropy [7]. In the simplest case, we can take an \( L \times L \) cylinder and cut it in half. The resulting entanglement entropy as a function of the linear system size \( L \) is given by

\[
S^{(n)}(L/2) = aL + N_g \frac{N}{2} \log(L) + b. \tag{11}
\]

Here \( N_g \) is the number of Goldstone modes and \( b \) contains a geometrical constant.

We again apply our nonequilibrium method in combination with the quench protocol in Eq. (7), where now the quench function is taken to be spatially constant in the \( y \)-direction and the partition is swept along the \( x \)-direction. Fig. (5) shows the resulting curves for system sizes \( L = 6, 8, \ldots, 20 \) for SU(2). We take the midpoint of our data and perform a fit to Eq. (11). This procedure is performed for SU(2), SU(3) and SU(4) with \( J_2/J_1 = 1, 2, 3, 5 \), respectively. The inset of Fig. (5) shows the entanglement entropy at the center cut with the area law piece subtracted. On semi-log axes, the log contribution manifests itself as a straight line. Within one percent accuracy we find the number of Goldstone modes to be \( N_g = 2, 4, 6 \) for \( N = 2, 3, 4 \) respectively.

Conclusion: We have introduced a new highly efficient nonequilibrium method for computing the Rényi entanglement entropy in the context of QMC simulations. This method offers as well a different perspective, where the entangling region becomes a dynamic variable that is coupled to an external field \( \lambda \). We expect that this will allow for improved methods of extracting universal features from the entanglement entropy, for instance by considering smooth disk-shaped subsystems and studying in detail the dependence on \( \delta \).

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SUPPLEMENTAL MATERIAL

QMC sampling and measurement

Our task is to perform nonequilibrium simulations in the space of configurations contained in $Z_A^{(n)}(\lambda)$ and add up all of the increments $\partial \ln g_A(\lambda(t), N_B(t))$ along a path between $\lambda = 0$ and $\lambda = 1$. We must first describe how to stochastically sample the $Z_A^{(n)}(\lambda)$ configurations in equilibrium. We employ the stochastic series expansion QMC algorithm [32] using the replica trick [21], where one samples $n$ independent copies of the partition function in one simulation. These are the configurations of $Z_A^{(n)}$ which are one subset of $Z_A^{(n)}(\lambda)$. In order to transition to other subsets, spins in different (independent) traces need to be joined into a single trace. This can be done if the spin states in the different traces match each other. The weight of the configuration will also change upon joining spins, since this changes the fraction probability of joining or splitting spins (with the requirement that the spin states must match) to be the ratio of the weights of the new and old configurations. This gives the acceptance probabilities

$$P_{\text{join}} = \min \left\{ \frac{\lambda}{1-\lambda}, 1 \right\}, \quad P_{\text{split}} = \min \left\{ \frac{1-\lambda}{\lambda}, 1 \right\}. \quad (12)$$

Each site in the $A$ subsystem is given the opportunity to join or split (depending on its current trace topology). Once this rewiring is done, the connectivity of the configuration is fixed and one may perform a standard QMC update.

We now need to know how to measure the work increments as we move along a nonequilibrium trajectory in the space of configurations contained in $Z_A^{(n)}(\lambda)$. The increment between time $t_m$ and $t_{m+1}$ is given by

$$\Delta \ln g_A(\lambda, N_B) = (N_A - N_B(t_m)) \ln \left( \frac{1-\lambda(t_{m+1})}{1-\lambda(t_m)} \right) + N_B(t_m) \ln \left( \frac{\lambda(t_{m+1})}{\lambda(t_m)} \right). \quad (13)$$

In other words, the increment is calculated by fixing the configuration and computing the change in $\ln g_A$ as $\lambda$ is incremented. This is in direct analogy to the way in which nonequilibrium work increments are computed in classical systems, except there one computes the change in energy of a configuration.

At this point two comments are in order. Firstly, one can avoid numerical rounding errors incurred by summing the log increments by instead taking a product of the arguments. Secondly, the factor of $-1/\beta$ in the definition of the work (Eq. (5)) completely drops out of the formulation when one uses Jarzynski’s equality (Eq. (6)). It is only included to give $W_A^{(n)}$ the proper units of work. With these ideas in mind, we can succinctly write the Jarzynski estimator for the Rényi entanglement entropy as follows:

$$S_A^{(n)} = \frac{1}{2n} \log \left( \prod_n \left[ \frac{\lambda(t_{m+1})}{\lambda(t_m)} \right]^{N_A(t_m)} \left[ \frac{1-\lambda(t_{m+1})}{1-\lambda(t_m)} \right]^{N_A(t_m)} \right). \quad (14)$$

Now that we have the ingredients necessary to update and perform work measurements on our configurations, we will briefly outline the main steps of the algorithm. First we equilibrate the system in the $Z_\delta^{(n)}$ ensemble of configurations (i.e. $\lambda = 0$). The equilibrated configuration is then saved to a file, and the nonequilibrium process begins. First we measure the work increment by Eq. (13) (or better to multiply the $\lambda$ factors from the first time step in Eq. (14)), then the current value of $\lambda$ is incremented and each spin in the $A$ subsystem is given the opportunity to change its trace topology according the the probabilities in Eq. (12). The trace topology is then held fixed and a regular QMC update is performed. Then the cycle begins again by computing the next increment and so on. Throughout the entire nonequilibrium process all of the work increments are accumulated and saved, in practice sampling them at regular intervals.

In order to initiate a new nonequilibrium process, we first read in the saved configuration that was equilibrated at the beginning, then we re-equilibrate for some smaller number of QMC steps (always staying in the $Z_\delta^{(n)}$ ensemble) and again save the configuration to a file. This new starting configuration is used for the next nonequilibrium process.

Space dependent quench functions

In order to clearly see how to treat space dependent quench functions, we write the formula for $Z^{(n)}(\lambda)$ as:

$$Z^{(n)}(\lambda) = \sum_{B \in \mathcal{L}} \left( \prod_{x \in B} \chi(\lambda(x)) \prod_{x \notin B} [1-\lambda(x)] \right) Z_B^{(n)}. \quad (15)$$

Here $B$ is now summed over all proper subsets of the entire lattice. One can now interpolate between $Z_\delta^{(n)}$ and $Z_A^{(n)}$ by using the space dependent quench function $\chi(x,t) = \chi(t)\chi_A(x)$, where the indicator function $\chi_A(x) = 1$ if $x \in A$ (zero otherwise), and $\chi(t) = (t-t_i)/(t_f-t_i)$. This is the same function appearing in panel (a) of Fig. 2.

Computing the work increments in this case is no more complicated. First we define the $g$ function as

$$g(\lambda(x), B) = \prod_{x \in B} \chi(\lambda(x)) \prod_{x \notin B} [1-\lambda(x)], \quad (16)$$

$$\Delta \ln g_A(\lambda, N_B) = (N_A - N_B(t_m)) \ln \left( \frac{1-\lambda(t_{m+1})}{1-\lambda(t_m)} \right) + N_B(t_m) \ln \left( \frac{\lambda(t_{m+1})}{\lambda(t_m)} \right). \quad (13)$$

In other words, the increment is calculated by fixing the configuration and computing the change in $\ln g_A$ as $\lambda$ is incremented. This is in direct analogy to the way in which nonequilibrium work increments are computed in classical systems, except there one computes the change in energy of a configuration.

At this point two comments are in order. Firstly, one can avoid numerical rounding errors incurred by summing the log increments by instead taking a product of the arguments. Secondly, the factor of $-1/\beta$ in the definition of the work (Eq. (5)) completely drops out of the formulation when one uses Jarzynski’s equality (Eq. (6)). It is only included to give $W_A^{(n)}$ the proper units of work. With these ideas in mind, we can succinctly write the Jarzynski estimator for the Rényi entanglement entropy as follows:

$$S_A^{(n)} = \frac{1}{2n} \log \left( \prod_n \left[ \frac{\lambda(t_{m+1})}{\lambda(t_m)} \right]^{N_A(t_m)} \left[ \frac{1-\lambda(t_{m+1})}{1-\lambda(t_m)} \right]^{N_A(t_m)} \right). \quad (14)$$

Now that we have the ingredients necessary to update and perform work measurements on our configurations, we will briefly outline the main steps of the algorithm. First we equilibrate the system in the $Z_\delta^{(n)}$ ensemble of configurations (i.e. $\lambda = 0$). The equilibrated configuration is then saved to a file, and the nonequilibrium process begins. First we measure the work increment by Eq. (13) (or better to multiply the $\lambda$ factors from the first time step in Eq. (14)), then the current value of $\lambda$ is incremented and each spin in the $A$ subsystem is given the opportunity to change its trace topology according the the probabilities in Eq. (12). The trace topology is then held fixed and a regular QMC update is performed. Then the cycle begins again by computing the next increment and so on. Throughout the entire nonequilibrium process all of the work increments are accumulated and saved, in practice sampling them at regular intervals.

In order to initiate a new nonequilibrium process, we first read in the saved configuration that was equilibrated at the beginning, then we re-equilibrate for some smaller number of QMC steps (always staying in the $Z_\delta^{(n)}$ ensemble) and again save the configuration to a file. This new starting configuration is used for the next nonequilibrium process.
and the dynamical work is

$$W^{(n)} = -\frac{1}{\beta} \int_{t_i}^{t_f} dt \frac{d\lambda}{dt} \frac{\partial}{\partial \lambda} \ln g(\lambda(x, t), B(t)) .$$

(17)

The work increment accumulated between two adjacent time steps $t_m$ and $t_{m+1}$ is given by

$$\Delta \ln g = \ln \left( \frac{g(\lambda(x, t_{m+1}), B(t_m))}{g(\lambda(x, t_m), B(t_m))} \right) ,$$

(18)
or

$$\Delta \ln g = \ln \left( \prod_{x \in B(t_m)} \frac{\lambda(x, t_{m+1})}{\lambda(x, t_m)} \prod_{x \in B(t_m)} \frac{1 - \lambda(x, t_{m+1})}{1 - \lambda(x, t_m)} \right) .$$

(19)

The total work and Jarzynski estimator for the Rényi entanglement entropy follow naturally, and the space dependent $\lambda$ is used in the joining and splitting probabilities.

QMC versus ED

When using any numerical method, it is always important to compare with exact results. We have gone to great lengths to check the accuracy of our method for small systems that can be exactly diagonalized. Fig. 6 shows a comparison of our QMC method with exact diagonalization of an SU(2) $L = 16$ chain. We have used the quench function in Eq. (7) for different values of $\delta$. The QMC data is the colored curves with shading as the error bar (this can be seen in the zoomed inset), and the black curves are exact results obtained by diagonalizing the reduced density matrices for all possible bipartitions and weighting them with the appropriate factors of $\lambda(x, l, \delta)$. We find perfect agreement between the QMC and ED. We also see that when $\delta$ is made small enough the exact Rényi entanglement entropy of a block subsystem (the black dots) is produced.

We also provide the same type of comparison in Fig. 7 for our two dimensional model on an SU(2) $L = 4$ square lattice with $J_2/J_1 = 2$ using the same quench function as in the main text. Again we find perfect agreement within the error bars.

Efficiency of Method

It is clear from the results presented in the main text that this method is very efficient. But here we would like to give a direct comparison of our nonequilibrium quenches with the extended ensemble method [22] combined with the increment trick [21]. In Fig. 8 we show the statistical error (QMC error bar) as a function of subsystem size $L_A = L/2$ for SU(N) chains. Here we compute the second Rényi entanglement entropy of half of the chain in two ways: (1) by directly quenching the entire

<Figure 6. Here we compare our QMC method (colored curves) with results obtained from exact diagonalization (black curves and black dots) of a periodic $L = 16$ site chain for SU(2). We have used the quench function in Eq. (7) for different values of $\delta$ in our nonequilibrium QMC simulations and compared that with exact results with the same quench function obtained by diagonalizing the reduced density matrices for all possible bipartitions and weighting them with the appropriate factors of $\lambda(x, l, \delta)$. We find perfect agreement between QMC and exact diagonalization, and we see that our quench function reproduces the exact second Rényi entanglement entropy of a block subsystem (the black dots) when $\delta$ is small.

<Figure 7. Here we show the same type of QMC vs ED comparison as in Fig. 6 except applied to the two dimensional model in Eq. (10) for an SU(2) $L = 4$ system with $J_2/J_1 = 2$. Here as in the main text, the same quench function is used, except in the two dimensional case it is taken to be constant in space along the y-direction. Again when $\delta$ is small the exact second Rényi entanglement entropy of ribbon subsystem (black dots) is reproduced.>
Figure 8. Here we compare our new nonequilibrium method (Non-Eql) against the extended ensemble method using the increment trick (Eql Inc). We consider SU(N) Heisenberg chains and plot the QMC error bar (statistical error) versus the subsystem size, where we cut the chains in half fixing $L_A = L/2$. For the extended ensemble method we build up the half chain entanglement entropy by computing the increment ratio for each site individually. This consists of $L_A$ independent simulations. Each simulation produced $28 \times 10$ binned measurements, with each measurement consisting of 10,000 sweeps. In our nonequilibrium method, we quench the entire half chain at once using the spatially constant quench function in panel (a) of Fig. 2. For this we compute $28 \times 10,000$ sweeps. In our nonequilibrium method we quench the entire half chain at once with $28 \times 10,000$ nonequilibrium time steps. The total number of measurement sweeps is then identical between the two methods and we see that the nonequilibrium method is far superior.

For the extended ensemble method, we compute each increment in a separate (equilibrium) simulation with $28 \times 10$ binned measurements each consisting of 10,000 measurement sweeps. For our nonequilibrium method we quench the entire half chain at once with $28 \times 10$ work realizations each consisting of $L_A \times 10,000$ nonequilibrium time steps. As such, the total number of measurement sweeps used for each method is identical. Very remarkably, in the nonequilibrium case the error bar stays flat as long as the number of nonequilibrium time steps is increased in proportion to the number of sites quenched. Significant computational resources are also saved on equilibration, since the independent equilibrium increments need to be separately equilibrated.

$T = 0$ converged data for 2D model

Here we would like to provide a more detailed view of the data presented in the main paper for the two dimensional model. In order to obtain $T = 0$ converged data, we have had to set $\beta = L^2$ with $J_1 = 1$. These extremely low temperatures prohibit us from simulating systems much larger than $L = 20$. In Fig. 9 we again show the raw data for SU(2) appearing in the main text, this time with subfigures that show (from left to right) the log contribution on linear axes, the QMC data with the fit subtracted, and the fitted value of $N_g$ as a function of the smallest system size used in the fit ($L_{min}$).

Figure 9. Here we show our zero temperature converged data for the two dimensional model for SU(2) at $J_2/J_1 = 1$. The main plot shows the raw data obtained from our quench function with $\delta = 0.7$, and the upper subplots (from left to right), show the center cut data with the area law piece subtracted, the center cut data minus the fit performed to Eq. (11), and the extracted number of Goldstone modes ($N_{g}$) versus the smallest system size used in the fit ($L_{min}$).

Figure 10. This figure is similar to Fig. 9 except for SU(3) at $J_2/J_1 = 2$.
markably, the finite temperature effects do not influence finite temperature, taking $\beta = 4L$ with $J_1 = 1$ and $J_2/J_1 = 2$ for SU(3). Here finite temperature affects are clearly visible since the density matrix is no longer pure. We are able to reach slightly larger system sizes in this case, and our numerical fits look to be even higher quality than in the $T = 0$ case. We conclude from this that $N_g$ can be reliably extracted even from finite temperature data.

We have also collected data at finite temperatures, this time only scaling $\beta$ proportional to $L$ and not $L^2$. Remarkably, the finite temperature effects do not influence extraction of $N_g$ as we show in Fig. 12 for SU(3) and Fig. 13 for SU(4). These results at finite temperature arguably produce even more high quality fits than the data converged at $T = 0$.

Finally we include data for SU(4) at a lower value of $J_2/J_1$ to illustrate the finite size effects in this case. Fig. 13 except we now set $J_2/J_1 = 2$ to illustrate the presence of finite size effects when $J_2$ is too small. We can see a systematic drift toward $N_g = 6$ as smaller system sizes are excluded from the fit.

Figure 12. This figure is similar to Fig. 9 except computed at finite temperature, taking $\beta = 4L$ with $J_1 = 1$ and $J_2/J_1 = 2$ for SU(3). Here finite temperature affects are clearly visible since the density matrix is no longer pure. We are able to reach slightly larger system sizes in this case, and our numerical fits look to be even higher quality than in the $T = 0$ case. We conclude from this that $N_g$ can be reliably extracted even from finite temperature data.

Figure 13. This figure is the same as Fig. 12 except for SU(4) with $\beta = 3L$ and $J_2/J_1 = 3$. Again we find a very high quality fit even at finite temperature.

Figure 14. This figure is the same as Fig. 13 except we now set $J_2/J_1 = 2$ to illustrate the presence of finite size effects when $J_2$ is too small. We can see a systematic drift toward $N_g = 6$ as smaller system sizes are excluded from the fit.