Entanglement Heating, Entanglement Cooling & Irreversibility

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(Dated: July 14, 2024)

We show that irreversibility emerges from microscopically reversible dynamics in the entanglement and subsequent disentanglement of quantum states. To this end, we entangle an initial random quantum state using gates chosen randomly from a set of gates, and try to disentangle it with a Metropolis-inspired algorithm. The emergent dynamics do not depend on the particular choice of the set of gates, but only on whether the chosen gate set is universal or not. Furthermore, we show that the spacing of consecutive singular values reveals if the disentanglement procedure succeeds or not: Universal gate sets induce spacings that follow the Gaussian Orthonormal Ensemble spacings, while non-universal gate sets induce Poisson-like distributed spacings. This is an example of Loschmidt's Paradox in quantum systems, revealing the universal tension between microscopically reversible dynamics and macroscopic irreversibility.

I. INTRODUCTION

How can irreversible phenomena in phyiscs occur? This question has been unanswered for a long time [9], and has been treated from different angles [5, 14]. The heart of the problem is that the microscopical laws of nature (Classical Mechanics, Particle Physics) are reversible in nature, yet macroscopic dynamics can be irreversible, as is set in stone most famously by the second law of thermodynamics.

Recently, this question has been approached using Quantum Mechanics and, more specifically, entanglement [1, 12, 14]. The question of irreversibility seems even less tractable in Quantum Mechanics; all dynamics are unitary and thus reversible. Non-unitary dynamics occur only when considering, e.g. quantum channels, which model unitary dynamics from the perspective of a subsystem. Subsystems experience the non-classical phenomenon of entanglement among each other, making this a natural entry point for irreversibility to be introduced into Quantum Mechanics.

In this work, we show how the creation of entanglement is irreversible in the sense that random dynamics cannot, under certain conditions, disentangle the systems under consideration. The paper is structured as follows: We introduce the formalism of entanglement and the algorithm in Section II. Afterwards, we give details on the simulations we carried out in Section III. Our results are discussed in Section IV.

II. ENTANGLEMENT AND UNIVERSALITY

Quantum Mechanics offers many phenomena that are thoroughly non-classical, most notably entanglement. The term "entanglement" refers to a phenomenon where the state of one system cannot be fully described without knowledge of another system; we say that the two systems are "entangled". Consider the Hilbert space $\mathcal{H}$, and states ρ therein. The full Hilbert space may be partitioned into two spaces $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. The state on subsystem A then becomes

$$\rho \mapsto \mathrm{tr}_B \rho \equiv \rho_A. \tag{1}$$

If there exist states $|\psi_A\rangle \in \mathcal{H}_A$ and $|\psi_B\rangle \in \mathcal{H}_B$ s.t. $\rho = |\psi_A\rangle\langle\psi_A| \otimes |\psi_B\rangle\langle\psi_B|$, we say ρ is a product state. If, on the other hand, we can write

$$\rho = \sum p^{(i)} \rho_A^{(i)} \otimes \rho_B^{(i)}, \tag{2}$$

we call ρ a "separable state". In both cases, there is no entanglement present in the system, since we are able to express the state using objects that live in only one of the subsystems. If on the other hand, ρ is not a product state, i.e. there are no $\rho_A^{(i)}$, $\rho_B^{(i)}$ s.t. Equation 2 holds, then we say ρ is "entangled". This means that ρ cannot be fully characterized from the two subsystems; it lives on the bipartite Hilbert space.

Entanglement sits at the core of many non-classical effects of Quantum Mechanics [2] and is used widely in Quantum Computing [7, 15], making it not only a mechanism of high conceptual relevance but also a resource to be used in computation.

Entanglement can be measured by the von-Neumann entanglement entropy S. Consider again the "reduced state" ρ_A on subsystem A, that results from tracing out subsystem B (Equation 1). Diagonalizing ρ_A gives it's spectrum $\sigma = \{\lambda_i\}$ of eigenvalues. The entanglement entropy of this state is defined as[1]

[1] Note that we have introduced entanglement as a notion that is only explainable by considering bipartite systems, yet we are defining a measure of entanglement using an object that lives on only one of the systems. This is possible because the spectrum σ of the reduced state $\rho_A = \mathrm{tr}_B \rho$ is related to the Schmidt coefficients of the state on the whole system. Let $\sigma = \{\lambda_i\}$ and let $\rho = |\psi\rangle\langle\psi|$ be a pure state. Then it's Schmidt decomposition is $|\psi\rangle = \sum_i \sqrt{\lambda_i}\, |\psi_A^{(i)}\rangle \otimes |\psi_B^{(i)}\rangle$. This explains why it is possible to characterize the entanglement between two subsystems by considering the reduced state on one of the systems.

$$S(\rho_A) = -\mathrm{tr}\left(\rho_A \log_2 \rho_A\right) = -\sum_i \lambda_i \log_2 \lambda_i. \tag{3}$$

Non-entangled states give $S(\rho) = 0$, while $S(\rho) > 0$ signifies the presence of entanglement. In particular, $S(\rho) = 0$ for separable states and product states.

Let us now consider states of N qubits, such that the Hilbert space is $\mathcal{H} = \mathbb{C}^{2^N}$. The state of this system may be changed by applying unitary transformations $U : \mathbb{C}^{2^N} \to \mathbb{C}^{2^N}$. We refer to these as "gates", in analogy to classical computing. Gates may act on an arbitrary number of qubits. Gates that act on more than one qubit can create entanglement, while single-qubit gates do not change the entanglement that is present in the system. The irreversibility-paradox in Quantum Mechanics comes to be since transformations U of quantum states are unitary, and thus reversible. Since entanglement can be created, it can thus also be destroyed.

In this work we investigate the possibility of entanglement being created and then destroyed by random quantum circuits. The first step consists of creating entanglement. Starting from a random product state

$$|\psi\rangle = |\psi\rangle_0 \otimes \ldots \otimes |\psi\rangle_{N-1}\,, \tag{4}$$

we iteratively and randomly choose a gate U from a set $\mathcal{I}$ and apply it to a random subset of qubits. Single-qubit gates further randomize the state, while multi-qubit gates create entanglement. The entanglement creation is measured by the von-Neumann entropy $S(\rho_A)$: For every iteration, we measure the entanglement entropy S_{N_A} for every bipartition

$$\mathbb{C}^{2^N} \mapsto \mathbb{C}^{2^{N-N_A}} \otimes \mathbb{C}^{2^{N_A}} \tag{5}$$

into two systems of N_A and $N - N_A$ (consecutive) qubits, respectively. This iterative procedure creates a random quantum state, which we can expect to be highly entangled with high probability [6, 13]. After entanglement has been created, we try to disentangle the state using a Metropolis-inpired algorithm [1, 12, 14]: In every iteration, we choose again a random gate $U \in \mathcal{I}$ from the same set of gates, and apply it to a random set of qubits. In doing this we obtain the new state $|\psi^{(j+1)}\rangle = U\,|\psi^{(j)}\rangle$. We measure the entanglement and obtain, after the jth iteration, the entanglement entropies $\{S^{(j)}_{N_A}\}$ of every bipartition (recall Equation 5). Some gates will increase S, while others decrease it. The new state $|\psi^{(j+1)}\rangle$ is accepted if the mean entanglement entropy $\langle S^{(j+1)}_{N_A}\rangle \equiv S^{(j+1)}$ has decreased[2]. If entanglement has not decreased, we accept it with a probability

[2] To be more specific, $\langle S^{(j+1)}_{N_A}\rangle = \frac{1}{N-1}\sum_{N_A=1}^{N-1} S^{(j+1)}_{N_A}$, i.e. we are averaging over the bipartitions of Equation 5.

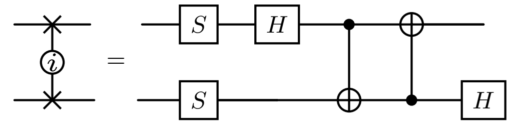

FIG. 1. The iSWAP gate is reducible to H, S and CNOT using the circuit identity above. Recall also that $S = T^2$, so the universality of $\{\mathrm{iSWAP}, H, T\}$ follows from the universality of $\{\mathrm{CNOT}, H, T\}$.

$$P = e^{-\beta(S^{(j+1)} - S^{(j)})}, \tag{6}$$

where β plays the role of an inverse temperature. Emphasizing the similarity to the Metropolis algorithm [11], we call this second step "entanglement cooling". Conversely, the first step is referred to as "entanglement heating".

III. HEATING AND COOLING SIMULATIONS

In this section, we give details on the numerical simulation of the heating and cooling steps. In both steps, we simulate quantum states $|\psi\rangle$ as full statevectors $|\psi\rangle \in \mathbb{C}^{2^N}$.

A. Entanglement heating

As per convention in Quantum Computing, the initial state is $|0\rangle^{\otimes N}$. A random product state is created by applying the rotation gate

$$R_Y(\theta) = e^{-i\theta Y/2} \doteq \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix} \tag{7}$$

on every qubit, with angles θ randomly selected from $[0, \pi]$. Afterwards, we choose randomly a gate U from a gate set $\mathcal{I}$ and choose randomly the qubits it is applied to. The gate sets we investigate are

$$\begin{array}{ll} \{\mathrm{CNOT}, H, Z\}, & \{\mathrm{iSWAP}, H, T\}, \\ \{\mathrm{CNOT}, H, X\}, & \{\mathrm{iSWAP}, H, S\}, \\ \{\mathrm{CNOT}, H, S\}, & \{\mathrm{iSWAP}, H, X\}, \\ \{\mathrm{CNOT}, H, T\}, & \{\mathrm{iSWAP}, H, Z\}. \end{array} \tag{8}$$

Note that among these, only $\{\mathrm{CNOT}, H, T\}$ and $\{\mathrm{iSWAP}, H, T\}$ are universal gate sets [4] (see also Figure 1). A universal gate set is a gate set such that every unitary operation can be approximated with arbitrary precision using gates from the set.

We apply $R_{\mathrm{heat}} = 250$ gates during the heating procedure. This gives a highly entangled state $|\psi_{\mathrm{heat}}\rangle$.

B. Entanglement cooling

The entanglement cooling step starts with the state $|\psi_{\text{heat}}\rangle$ that the heating step terminated in. On this state, we again apply a random gate $U \in \mathcal{I}$ from the gate set that was used in the heating step, again on a random set of qubits. The new state is only accepted if the mean entanglement decreases, or with the probability given in Equation 6. This is repeated for $R_{\text{cool}} = 6000$ iterations, with β fixed.

We repeat heating and cooling 100 times and average over the results. The number N of qubits was chosen as $N \in [4, 11]$ and the (inverse) temperature is $\beta = 5$, if not stated otherwise.

IV. RESULTS

The heating rate is consistent across different realizations, with negligible deviations. The entanglement of states with different sizes N grows with the same rate, before individual system sizes converge to their maximum entanglement. An explanation for the comparable rates of entanglement creation is rooted in the fact that we are using two-qubit gates to create entanglement. A two-qubit gate can only create entanglement between the two qubits it is applied to, and the entanglement in such a system is limited to $S \leq \log_2 d = 2$. Thus, no matter the system size, the gates we use create entanglement at the same rate.

The maximum entanglement we reach during the heating step is proportional to N:

$$\max_{N_A} \langle S_{N_A} \rangle \propto N. \tag{9}$$

This is in line with the known scaling $S \propto \log_2 d$ [13] of the entropy of a random quantum state, where d is the dimension of the local Hilbert space (recall that here, $d = 2^{N_A}$). The rate of entanglement creation is slightly smaller for gate sets that contain the iSWAP gate, but maximum entanglement values are equal. See also Figure 5.

The entanglement cooling rate does not depend on the value of β; for $\beta \in [1, 10]$, cooling occurs at the same rate. See Figure 2.

We move on to the central result of this work, which concerns irreversibility: The entanglement cooling step does not always succeed. If the creation of entanglement were reversible, cooling would always be able to lower the entanglement back (or close to) zero[3]; this is not the case, however. Specifically, entanglement cooling fails, whenever the gate set that is used is universal. Disentangling occurs at the same rate regardless of system size N and whether it succeeds or fails, for the same reason that entanglement heating occurs at the same rate[4]. Disentangling begins later during the cooling process for larger systems. See also Figure 3.

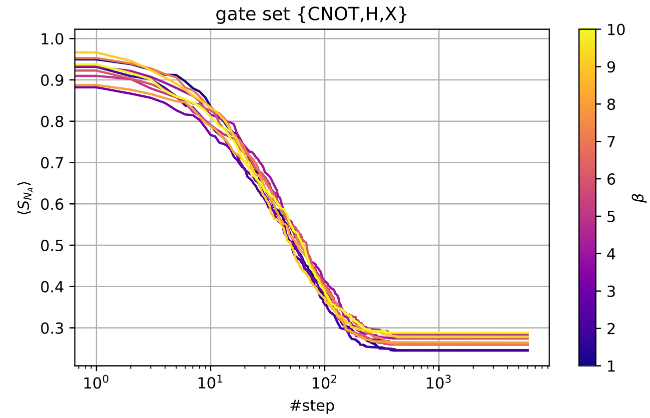

FIG. 2. We simulated entanglement cooling for $\beta \in [1, 10]$ in a system of four qubits ($N = 4$). The temperature β has no influence on the cooling rate, as is shown above for one particular gate set.

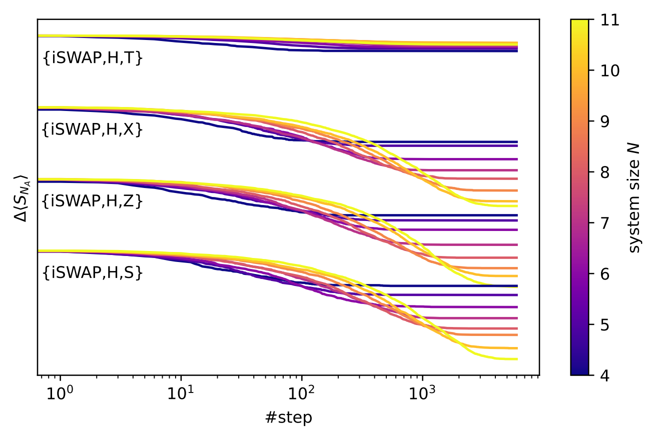

FIG. 3. The entanglement cooling process for gate sets that contain an iSWAP gate. This plot only shows differences in mean entanglement. The rate of disentangling is similar for different gate sets.

[3] Where disentangling succeeds, there remain differences in how much entanglement the cooling step is able to remove from the state. The gate sets that contain CNOT are able to fully disentangle the state in question. The sets containing iSWAP are able to remove a significant amount of entanglement, however, they cannot reduce S back to zero. See Figure 6.

[4] Stated more precisely, the shapes of the curves of $\langle S_{N_A}\rangle$ match. The process of disentangling starts later for larger systems, however. Why this is remains an intriguing direction for future work.

At this point we may ask ourselves how we can characterize the scenarios where disentangling succeeds, versus the ones where it does not. The answer can be found in the spectrum of consecutive spacings of Schmidt values. Consider the equal bipartition of a system of size N in two parts of size $N_A = \lfloor N/2 \rfloor$ and $N_B = N - N_A$. The spectrum of the associated density matrices ρ_A and ρ_B is $\sigma_{N/2} = \{\lambda_i\}$, and it coincides with the Schmidt values of the complete state $|\psi\rangle$. Assume the Schmidt coefficients λ_i to be sorted in descending order, then the consecutive spacings are $\Delta_i = \lambda_i - \lambda_{i+1}$. Their expected distribution

$$P(\Delta\lambda) = \sum_{i=0}^{N-2} \langle \delta(\Delta - \Delta_i) \rangle \tag{10}$$

differs for states that were generated using different gate sets. States that stem from universal gate sets show spacing statistics that closely follow the Gaussian Orthogonal Ensemble (GOE) [1]. This refers to the distribution of eigenvalue spacings of random orthogonal matrices [10]; the "Wigner surmise" states that their distribution can be described by [3]

$$P(\Delta) \approx C\Delta^{\beta} e^{-A\Delta^2}, \tag{11}$$

for appropriately chosen C, β, A. The spacing statistics of states from non-universal gate sets exhibit a different distribution, more closely related to a Poisson-distribution. This holds true for gate sets containing either iSWAP or CNOT. See Figure 4.

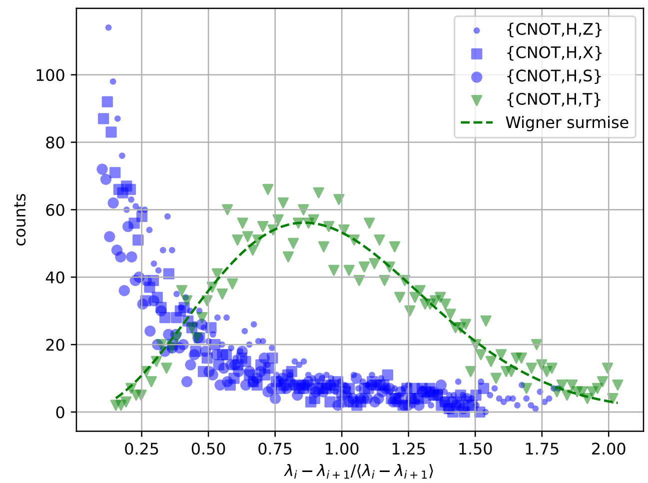

FIG. 4. The level spacing statistics of states with $N = 11$, that were generated with gate sets that contain the CNOT gate. While the universal set $\{\text{CNOT}, H, T\}$ procuces states whose spacings follow the GOE very closely (Equation 11), the non-universal sets follows a Poisson-like distribution. The same holds true for gate sets that contain the iSWAP gate. This plot only shows values $\Delta / \langle\Delta\rangle$ below a value of 2, since the distributions have a long tail. The interested reader is referred to Ref. [8], where all distributions are shown.

V. CONCLUSION & OUTLOOK

Our results demonstrate that the conflict between microscopically reversible dynamics and macroscop irreversibility can be modelled with and found in Quantum Mechanics, specifically in the entanglement of chains of qubits. We demonstrated that randomly generated circuits of single- and two-qubits gates consistently generate highly entangled states at the same rate. Disentangling these states with a Metropolis-inspired algorithm only succeeds when the gate set used to generate the state in question is not universal. The ability of a state to be disentangled is encoded in the distribution of consecutive Schmidt coefficient spacings. For states that can be disentangled, these follow a Poisson-like distribution. The spacings of states that cannot be disentangled follow the GOE distribution. This enables us to treat Loschmidt's Paradox with the tools of Quantum Mechanics and Quantum Computing, thereby opening up avenues for further investigation of the topic.

The value in the method we presented lies in the fact that we are not limited to using statistical methods, as is the case in thermodynamics and statistical physics. Our system of N qubits has a comparably small amount of degrees of freedom, and it's interaction with the environment we subject it to (i.e. the gates we apply) are very well understood and can be easily and exactly simulable. Yet, even in such a controlled environment, we find irreversibility emerging from reversible dynamics.

There remain open questions. Consider for example the aforementioned result that iSWAP-sets create entanglement at a rate slighly slower than CNOT-sets, and the fact that non-universal iSWAP-sets are unable to remove all entanglement from the system. A more exact characterization of the rates at which entanglement is created remains a topic for future work; specifically, if entanglement heating and cooling rates can be increased or decreased depending on the set of gates that is used. A further open question concerns the observation that the disentangling process starts later for larger systems, but progresses at the same rate once it has begun.

A further question that deserves more attention stems from wondering whether a CNOT-set can disentangle a state that was created using an iSWAP-set, and vice-versa. Since the spacing statistics of CNOT-states and iSWAP-states agree, one could expect the answer to be yes; then again, iSWAP-containing sets cannot completely disentangle a state, but only partially. Put more broadly: In what capacity is the ability to be disentangled a property of a quantum state, or of the gate set that is used?

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Appendix A: Code Availability

The code to carry out the simulations as well as the data can be found in the corresponding GitHub Repository [8].

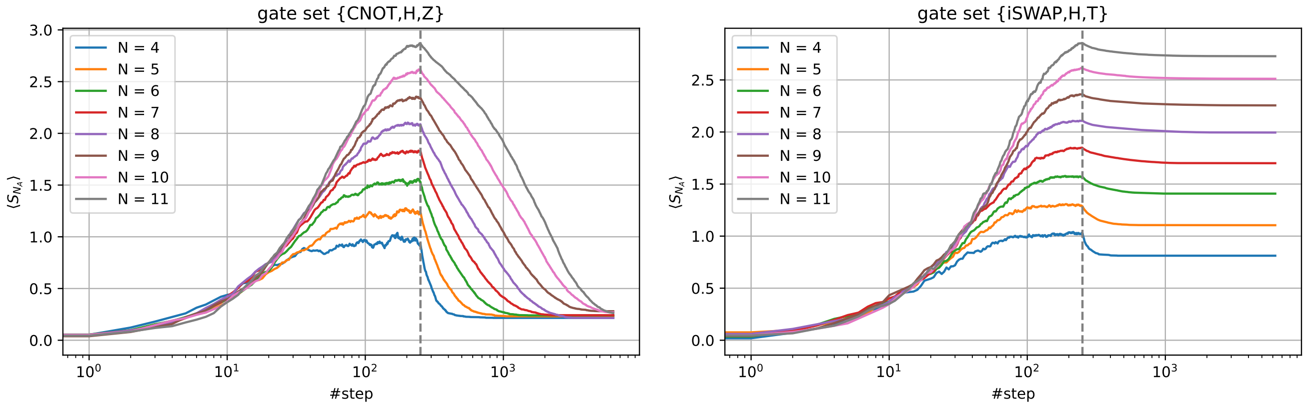

FIG. 5. Two examples of the thermalization of entanglement, i.e. the heating and cooling steps, for two different gate sets. The rates of entanglement heating are very similar, with the iSWAP gate creating entanglement slighly slower than the CNOT. The maximum entanglement that is reached scales linearly with system size N. Cooling succeeds for the non-universal gate set $\{\mathrm{CNOT}, H, Z\}$, it fails however for the universal $\{\mathrm{iSWAP}, H, T\}$.

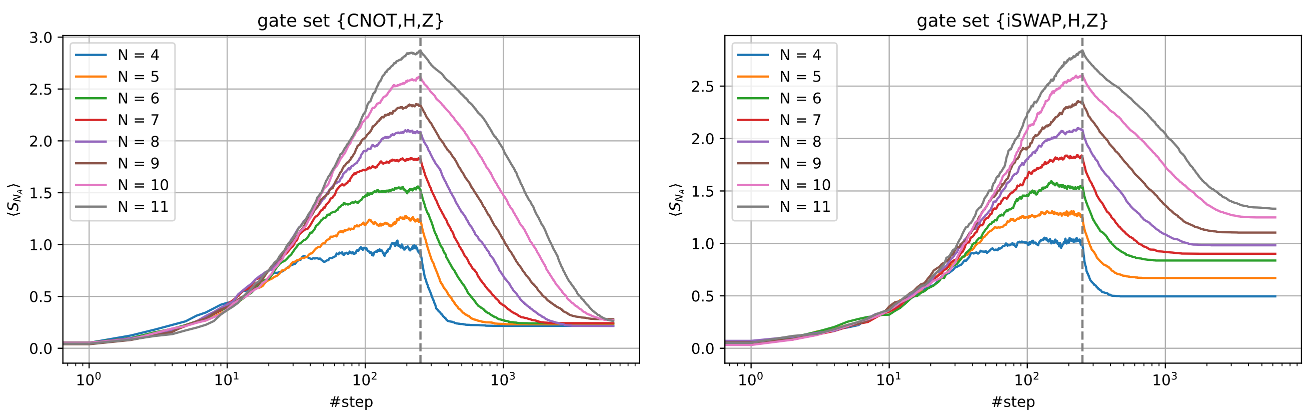

FIG. 6. Two examples of the thermalization of entanglement, i.e. the heating and cooling steps, for two gate sets that only differ in which two-qubit gate they contain. The CNOT-containing set is able to remove almost entanglement from the state, regardless of the system size. Disentangling converges at a value $S \neq 0$ for iSWAP-containing gate sets. Notice that the reamining entanglement scales linearly with the system size, just as the maximum entanglement does.