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Aspects of Quantum Computing and Quantum Field Theory: a Tale of
Magic States, Noise Learning, and Entanglement Entropy

By

LUCAS DAGUERRE

DISSERTATION

Submitted in partial satisfaction of the requirements for the degree of

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of the

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DAVIS

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2026

Dedicated to my parents, Silvina and Lisandro

Abstract

In this Ph.D. thesis, we delve into various aspects of Quantum Computing and Quantum Field Theory.

In the first part, we study one of the most resource-intensive components of a fault-tolerant quantum computer (FTQC): the creation of a logical magic state. We propose a novel low-overhead logical magic state preparation (MSP) protocol via code-switching between color codes and provide the first experimental demonstration of such technique for color codes using a trapped-ion quantum processor. We also introduce the first scalable method for simulating a large class of logical MSP protocols under the influence of circuit-level Pauli noise on a classical computer. Finally, we also develop a noise learning technique for adapting in real-time prior estimates of noise channels associated with quantum gates on a quantum computer, to avoid the repetitive use of costly off-line characterization techniques.

In the second part, we analyze Quantum Field Theories (QFTs) through the lens of quantum information using the entanglement entropy (EE) of the vacuum in spherical regions. Concretely, we compute from first principles the universal logarithmic coefficient of the EE of free massless fermionic field theories in a four dimensional Minkowski space-time, with the aid of a geometric regularization induced by the mutual information. We also study a large class of field theories that admit gravitational dual, and compute the EE in a large radius limit. As a result, we establish entropic irreversibility inequalities that go beyond what has been proven in QFT based on strong subadditivity.

List of Publications

The content of this Ph.D. thesis is based on the following publications:

- **Daguerre L.**, Kim I. “Code switching revisited: low-overhead magic state preparation using color codes”. *Physical Review Research* **7**, 023080 (2025). ArXiv: [2410.07327]. [1]
- **Daguerre L.**, Blume-Kohout R., Brown N., Hayes D., Kim I. “Experimental demonstration of high-fidelity logical magic states from code switching”. *Physical Review X* **15**, 041008 (2025). ArXiv: [2506.14169]. [2]
- Surti S., **Daguerre L.**, Kim I. “Efficient simulation of logical magic state preparation protocols”. *PRX Quantum* (In press) (2026). ArXiv: [2512.23799]. [3]
- **Daguerre L.**, Sarovar M. “Real-time adaptation of quantum noise channel estimates”. *Physical Review A* **111**, 062609 (2025). ArXiv: [2501.18685]. [4]
- Benedetti V., **Daguerre L.**, “Entanglement entropy of a Rarita-Schwinger field in a sphere”. *Physical Review D* **108**, 086015 (2023). ArXiv: [2307.00057]. [5]
- **Daguerre L.**, Ginzburg M., Torroba G. “Holographic entanglement entropy inequalities beyond strong subadditivity”. *Journal of High Energy Physics* **10** (2022) 199. ArXiv: [2208.03334]. [6]

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Nomenclature

Symbols

$\mathcal{H}$	Hilbert space.
$ \psi\rangle$	Quantum state.
ρ	Density matrix.
F	Fidelity.
$1 - F$	Infidelity.
$[[n, k, d]]$	Quantum Error Correcting code.
$\mathcal{C}^{(1)}$ or $\mathcal{P}_n$	n -qubit Pauli group.
$\mathcal{C}^{(2)}$	Clifford group.
$\mathcal{C}^{(k)}$	k -th level Clifford Hierarchy.
$S(V)$	Entanglement Entropy.

Conventions

Space-time dimensions d ; code distance d (context dependent).

Natural units, $c = 1$ and $\hbar = 1$.

μ, ν, ρ, σ (Greek) with $\mu = 0, \dots, d - 1$ space-time indices.

i, j, m, n (Latin) with $i = 1 \dots, d - 1$ spatial indices only.

We employ the Einstein summation notation, e.g. $\sum_{\mu} x^{\mu} y_{\mu} \equiv x^{\mu} y_{\mu}$.

We employ the Feynman slash notation, e.g. $\not{A} = A_{\mu} \gamma^{\mu}$.

Acronyms and abbreviations

QEC	Quantum Error Correction.
FT	Fault Tolerant.
FTQC	Fault Tolerant Quantum Computer.
MSD	Magic State Distillation.
MSP	Magic State Preparation.
QFT	Quantum Field Theory.
CFT	Conformal Field Theory.
RG	Renormalization Group.
EE	Entanglement Entropy.
UV	Ultraviolet.
IR	Infrared.

Chapter 1

Introduction

The beginning of the 20th century overlapped with the discovery of Quantum Mechanics¹, a fundamental theory of nature that describes the dynamics and interplay of microscopic objects such as elementary particles, atoms, and molecules. While the principles of Quantum Mechanics lie at the core of a plethora of scientific fields, in this thesis, we focus on analyzing certain aspects of two paradigmatic fields: Quantum Computing and Quantum Field Theory (QFT).

Quantum computing arose in 1981 [8] when Feynman highlighted the importance of effectively simulating physical phenomena using a quantum mechanical system (a quantum computer). Since the discovery of Shor's factoring algorithm in 1994 [9], it has been established that quantum computers can solve certain computational problems exponentially faster than the best known classical algorithms [9–11]. However, the applications for which a quantum computer is expected to provide a substantial advantage tend to require a large number of physical operations [12]. Existing quantum computers are noisy, and taming the noise to the level low enough to run these algorithms remains as an outstanding open challenge.

¹Notably, this thesis also coincides with 100th anniversary of the discovery of the non-relativistic wave equation of Quantum Mechanics (Schrödinger equation) [7], which specifies the time evolution of a quantum state.

An essential step towards building a large-scale fault-tolerant quantum computer (FTQC) [13] is quantum error correction (QEC) [14, 15]. In principle, the overhead associated with fault-tolerance is merely polylogarithmic in the size of the computation [16], and can be even brought down to a constant [17]. However, the practical overhead needed for large-scale fault-tolerant quantum computation remains daunting, which this thesis seeks to reduce by studying one of its most resource-intensive components: the preparation of a logical magic state [18, 19]. Indeed, logical magic states are necessary to realize a universal gate set in a fault-tolerant quantum computer, since no error-correcting code can natively support such a universal gate set [20, 21]. Thus, Chapters 2, 3 and 4 are devoted to studying some features of logical magic state preparation protocols.

Besides seeking to reduce the overhead of FTQC by studying magic state preparation protocols, we also analyze efficient noise learning techniques needed to update in real-time prior benchmarks of quantum hardware. Indeed, techniques such as gate set tomography (GST) [22] and Pauli channel estimation [23] are time-consuming and are typically run infrequently. As a result, the descriptions of noise that they deliver might become inaccurate due to device and control drift during the execution of an algorithm. Hence, in Chapter 5, we propose a real-time noise estimate adaptation procedure for noisy quantum gates that does not interrupt algorithmic execution, which relies on Bayesian inference and extended flag gadgets [24, 25].

In the last part of this thesis, we investigate Quantum Field Theories (QFTs) using tools from quantum information theory. To begin with, QFT is a framework that describes quantum mechanical systems in the continuum with infinitely many degrees of freedom. Indeed, QFT unifies the principles of Quantum Mechanics and Special Relativity by assigning quantized fields to each point in space-time [26]. Methods of QFT have been successfully used in high energy physics [27] and condensed matter physics [28]. For instance, they have played a major role in the development of Quantum Electrodynamics (QED) [29–31], the Standard Model of Particle Physics [32, 33] and Superconductivity [34, 35]. More recently, certain types of QFTs were found to

have a deep connection with quantum gravity models, as exemplified by the notorious AdS/CFT correspondence [36, 37]. Relying on this correspondence, Ryu and Takayanagi proposed a formula [38, 39] to compute a quantum information measure known as entanglement entropy (EE) [40], providing an explicit geometric interpretation of EE. Furthermore, EE has been used to prove the irreversibility of the Renormalization Group (RG) flow for relativistic QFTs [41–43], to classify topologically-ordered phases of matter [44–46], and to diagnose confinement of strongly-coupled gauge theories [47]. Motivated by these findings, in Chapters 6 and 7, we analyze some QFT models, borrowing tools that are native to the quantum information community, and discuss their connection with the irreversibility of the RG flow.

1.1 Outline of the dissertation

The rest of this thesis is organized as follows. Chapters 2, 3, 4, 5, 6, and 7 constitute the main body of the thesis (see below for details). Chapter 8 provides an overall conclusion and outlook. Appendices A, B, C, D, and E provide supplemental material for Chapters 3, 4, 5, 6, and 7, respectively. The main body chapters are:

Part I: Magic States and Noise Learning in Quantum Computing

- **Chapter 2: “Code switching revisited: low-overhead magic state preparation using color codes”** is based on the publication [1]. In this chapter, we study one of the most resource-intensive components of a fault tolerant quantum computer: the creation of a logical magic state. We propose a low-overhead logical magic state preparation protocol via code switching between a three-dimensional (3D) and a two-dimensional (2D) color code. This protocol relies on a recently discovered transversal entangling gate between color codes, and a judicious use of flag based postselection. Additionally, we introduce a stabilizer-based numerical simulation method to avoid the use of a costly state-vector simulation. The latter, motivated a more general simulation approach which is discussed in Chapter 4.

- **Chapter 3: “Experimental demonstration of high-fidelity logical magic states from code switching”** is based on the publication [2]. In this chapter, we present an experimental realization on a trapped-ion quantum processor of the protocol from Chapter 2. This result provides the first experimental demonstration of code-switching between color codes, and produced a logical magic state with state-of-the-art fidelity. We also develop and realize a sample-efficient characterization method involving two copies of the logical magic state using a Bell basis measurement.
- **Chapter 4: “Efficient simulation of logical magic state preparation protocols”** is based on the publication [3]. In this chapter, we introduce the first scalable and efficient logical magic state preparation simulation technique, applicable to a vast group of protocols (magic state cultivation, magic state distillation at the logical level, and code switching). The efficiency of this technique is rooted on a curious fact: every circuit-level Pauli error propagates to an end-of-circuit Clifford error. To better formalize how errors propagate in cultivation-style protocols, we also develop a theory of Pauli-Square-Root Cliffords (PSC). These are (non-Pauli) Clifford unitaries that square to a Pauli. Indeed, the majority of magic states considered in the literature can be viewed as $+1$ -eigenstates of some PSC, hence motivating their study.
- **Chapter 5: “Real-time adaptation of quantum noise channel estimates”** is based on the publication [4]. In this chapter, we introduce a method to update in real-time prior estimates of noise channels associated with quantum gates on a quantum computer. The proposed technique relies on flag-gadgets, Bayesian inference and mid-circuit measurements, and provides a method to avoid off-line noise characterization techniques that interrupt algorithmic execution. We numerically demonstrate and evaluate its efficacy using a Dirichlet prior distribution in a Pauli error channel.

Part II: Entanglement Entropy in Quantum Field Theory

- **Chapter 6: “Entanglement entropy of a Rarita-Schwinger field in a sphere”** is based on the publication [5]. In this chapter, we compute the entanglement entropy (EE) of the vacuum in a spherical region for a relativistic free massless spin-3/2 (Rarita-Schwinger) field in a four dimensional Minkowski space-time. We do so by employing a dimensional reduction on a sphere, and comparing this mode decomposition with the spin-1/2 (Dirac) field case. As a consequence, we obtain from first principles the universal logarithmic coefficient for free fermionic fields with $\text{spin} \leq \frac{3}{2}$, with the aid of a geometric regularization induced by the mutual information. In conjunction with previous results for bosonic fields [48–50] and the spin-1/2 case [51], our findings contributed the culminating computation of universal logarithmic coefficients for relativistic free field theories with $\text{spin} \leq 2$.
- **Chapter 7: “Holographic entanglement entropy inequalities beyond strong subadditivity”** is based on the publication [6]. In this chapter, we compute the EE for field theories that admit a gravitational dual. We prove that in a large radius expansion and assuming the null-energy condition (NEC) in the bulk, some sub-leading terms of the EE can be physical. Indeed, we establish their irreversibility along holographic Renormalization Group (RG) flows, and reproduce known monotonicity theorems in particular cases [41–43]. This result goes beyond what has been proven in quantum field theory using strong subadditivity, and hints towards new methods for analyzing monotonicity of the RG in space-time dimensions bigger than four.

Part I: Magic States and Noise Learning in Quantum Computing

Chapter 2

Code switching revisited: low-overhead magic state preparation using color codes

In this chapter, we study the preparation of logical magic states on a quantum computer. In concrete, we propose a protocol to prepare a high-fidelity magic state on a two-dimensional (2D) color code using a three-dimensional (3D) color code. Our method modifies the known code switching protocol with (i) a recently discovered transversal gate between the 2D and the 3D code and (ii) a judicious use of flag-based postselection. We numerically demonstrate that these modifications lead to a significant improvement in the fidelity of the magic state. For instance, subjected to a uniform circuit-level noise of 10^{-3} (excluding idling noise), our code switching protocol yields a magic state encoded in the distance-3 2D color code with a logical infidelity of $4.6 \times 10^{-5} \pm 1.6 \times 10^{-5}$ (quantified by an error-corrected logical state tomography) with an 84% of acceptance rate. Used in conjunction with a postselection approach, extrapolation from a polynomial fit suggests a fidelity improvement to 5.1×10^{-7} for the same code. Our protocol is aimed for architectures that allow nonlocal connectivity and has been recently demonstrated on a trapped ion quantum processor [2]. Finally, we also present a simulation technique akin to an extended stabilizer simulator which

effectively incorporates the non-Clifford T -gate, that permits to simulate the protocol without resorting to a resource-intensive state-vector simulation. This simulation technique motivated to a more general method that is discussed in Chapter 4.

2.1 Introduction

General purpose quantum computation requires access to a universal gate set, which in a fault-tolerant architecture is often realized with the aid of magic states [18]. Historically, preparation of high-fidelity logical magic states has been one of the most costly parts of fault-tolerant quantum computation, due to the enormous complexity and overhead of magic state distillation (MSD) [18]. Traditional methods for magic state distillation relied on multi-level distillation of various protocols [18, 52–62]. Such analysis often led to an enormous overhead in preparing a magic state, motivating novel alternative methods. One of the important recent insights in reducing the overhead is that the size of the codes used at a lower level of distillation need not be as large [19, 63].

Even more recently, there has been a line of works that aim to prepare a higher-fidelity magic state before the distillation steps. An initial work in this direction is due to Li, who pointed out that the quality of the magic state can be improved by a judicious postselection [64]. Chamberland and Noh then used the flag-based methods [65–67] to prepare a magic state while detecting error with a small code [68]. While this work required a relatively challenging physical error rate of 10^{-4} , recent improvements in this direction led to protocols that can achieve substantial reduction in error even at a realistic physical error rate of 10^{-3} [69–71]. These protocols all boast a rather modest requirement on the number of qubits, which make them attractive quantum error correction protocols to implement and test in the near term; see Ref. [72] for a recent experiment, for instance. These methods, together with recent efficient magic state distillation protocols [19, 73] are expected to further reduce the overhead in magic state distillation. In particular, Ref. [71] reported a scheme that can reach an error

rate as low as 2×10^{-9} (with the post-selection success probability of 1%) under the same physical error rate. This is a level of error that is sufficient to run some quantum algorithms that have low resource requirement, e.g., Ref. [74], obviating the need for magic state distillation entirely for such applications.

However, it should be noted that there are important quantum algorithms requiring a number of T -gates that is still larger than the distillation-free methods can tolerate. For instance, the number of Toffoli gates used in quantum chemistry applications such as FeMoCo ranges between 5.3×10^9 [75] and 1.0×10^{10} [76]. Depending on the specifics of how the Toffoli gate is being used, each Toffoli can be converted to Clifford gates and between four and seven T gates [77]. Other applications in quantum chemistry tend to require even more T gates [78–80]. Even with the most recent method [71], a completely distillation-free approach cannot yet reach an error rate required for these applications. Therefore, an outstanding question is whether it is possible to bring down the cost of T gates even further, so that its cost is comparable to other Clifford gates in this regime.

This chapter introduces a different protocol that aims to achieve a similar goal. Unlike the recent protocols that aim to measure a transversal Clifford gate [70, 71], our approach aims to exploit a code with a non-Clifford transversal gate. Such an approach was proposed in Refs. [81, 82] and studied in detail in Ref. [83]. However, in light of the recent works that improved the fidelity using postselection [70, 71], it is natural to ask whether post-selection can also improve the fidelity of transversal-gate-based approaches.

To that end, we use the three-dimensional(3D) color code [81], and focus on its simplest instance, which is the 15-qubit quantum Reed-Muller code (qRM). We will aim to use the transversal gate of the 3D color code, which is then converted to the 2D color code [82, 84]. While a careful study has suggested that preparation of magic state using 3D color code using this approach is more costly than the multilevel distillation method [83], a more recent work exploited postselection and flag qubits [65–67] to improve the performance [69]. Our approach is similar in spirit, though we use the flag

qubits in a different way and also uses a transversal gate between 3D color code and 2D color code (that was recently discovered in Ref. [85]¹, which also appeared in Ref. [86] during the preparation of our manuscript.) Overall, our approach yields a high quality magic state on par with these prior results, which we discuss further in Sec. 2.2.

Although our protocol has a logical infidelity lower than what was reported in Refs. [70, 71] for similar setups (in terms of the code being used and the physical error rate), they are incomparable. References [70, 71] focused on quantum computing architectures equipped with nearest-neighbor gates on a two-dimensional grid, targeting superconducting qubit-based quantum computers [87]. Our approach uses gates that would require nonlocal connectivity. As such, our scheme, as it stands, cannot be used directly on these devices.

We emphasize, however, that our protocol is aimed at other types of quantum computers, such as the ones based on photons [88–90], ions [91–93], and neutral atoms [94, 95]. Non-local gates can be accommodated in these architectures, making them promising candidates to implement our protocol.

Lastly, we remark that we introduce a simulation method for Clifford+ T circuits that may be of an independent interest. The main strength of our method is that it is directly applicable to existing stabilizer circuit simulators, such as Stim [96]. The key ingredient relies on keeping track of the Pauli error frame associated to a logical stabilizer state. In this framework, a non-Clifford logical- T gate can be mimicked by introducing appropriate Clifford errors, which can be simulated easily using the existing simulators [96]. We provide more details in Sec. 2.5, and a more general approach in Chapter 4.

The rest of this chapter is organized as follows. In Sec. 2.2, we compare our protocol to the other related protocols in the literature. In Sec. 2.3, we review aspects of color codes. In Sec. 2.4, we describe our protocol. In Sec. 2.5 we describe our simulation method and present the result. We end with a Conclusion in Sec. 2.6.

¹We would like to thank an anonymous referee for pointing out this reference.

2.2 Comparison with prior work

A comparison of the infidelity of magic states prepared in our protocol with some recent results in the literature can be found in Tables 2.1 and 2.2.

Uniform depolarizing noise				
Method	Infidelity	Acceptance rate	Final code	Distance
Our protocol (error correction)	$4.6 \times 10^{-5} \pm 1.6 \times 10^{-5}$	84%	Steane code	3
Butt, <i>et al</i> [69]	10^{-4}	94%	Steane code	3
Our protocol ^(*) (postselection)	$\approx 5.1 \times 10^{-7}$	$\approx 84\%$	Steane code	3
Gidney, <i>et al</i> [71]	6×10^{-7}	65%	Steane code	3
Itogawa; <i>et al</i> [70]	10^{-4}	70%	Surface code	3

Table 2.1: Infidelity of magic states $|\bar{T}\rangle$ under a uniform depolarizing error model with strength $p = 10^{-3}$, for some state-of-the-art protocols, prepared in the final stage on distance $d = 3$ codes. Note that our error model does not include idling errors. The label “error correction/postselection” implies that the infidelity of the magic states is quantified via state tomography, where the final state in the postprocessing stage is either error corrected or postselected if syndromes are trivial, respectively. The first two rows use error correction, while the last three rows use postselection. ^(*)These results are *extrapolated* from the data points of Fig. 2.8, following the polynomial fits of (2.25) and (2.26), therefore the approximate symbol $\approx$ is utilized.

Multiparameter depolarizing noise				
Method	Infidelity	Acceptance rate	Final code	Distance
Our protocol (error correction)	$9 \times 10^{-5} \pm 2 \times 10^{-5}$	71%	Steane code	3
Butt, <i>et al</i> [69]	$1.6 \times 10^{-4} \pm 2 \times 10^{-5}$	82%	Steane code	3
Postler, <i>et al</i> [97]	$10^{-4} \pm 3 \times 10^{-5}$	85%	Steane code	3

Table 2.2: Infidelity of magic states $|\bar{T}\rangle$ ($|\bar{H}\rangle$ states for Ref. [97]) under a multiparameter depolarizing error model with initialization and measurement error $p_i = p_m = 10^{-3}$, single-qubit error $p_1 = 10^{-4}$, and two-qubit error $p_2 = 3 \times 10^{-3}$, for some state-of-the-art protocols, prepared in the final stage on the Steane code $[[7, 1, 3]]$. Note that our error model does not include idling errors and that Ref. [97] uses the single-qubit depolarizing noise model for initialization and measurement errors. The infidelity of these magic states are quantified via state tomography, where the final state in the post-processing stage is error corrected. The numerical values for the protocol [97] were obtained from Ref. [69].

A common feature of all these protocols is that they rely on some degree of postselection. However, there is also a difference in the overall approach. Our protocol (similar to Ref. [69]) uses a transversal non-Clifford gate, whereas Refs. [70, 71, 97] use the measurement of logical Clifford operators.

For our work, an important caveat is that the logical error rate estimate for the magic state was based on an “ungrown” patch of fixed distance $d = 3$. In order

to assess the quality of the magic state that will be used in practice, one needs to estimate the fidelity after converting this state to a magic state encoded in a larger-distance code [71]. We instead focus on estimating the fidelity for the $d = 3$ code; the error analysis related to the patch growth is left for future work.

Nonetheless, we can compare our protocols to the other protocols in the literature that studied the quality of the magic state on an ungrown patch. There are two types of works in the literature, depending on how one quantifies the quality of the magic state. In the first approach, one performs a logical state tomography at the final step, by performing noiseless measurement on all the qubits followed by an error correction. In the second approach, one instead post-selects on observing a trivial syndrome.

In the first approach, our numerical simulation reports an infidelity on par with other state-of-the-art results in the literature, using similar error models (no idling errors were included in our simulations); see Tables 2.1 and 2.2. For the second approach, we were unable to directly simulate at a physical error rate used in the literature; the infidelity resulting from the second approach is too low. Instead, we fitted the logical error rate with a polynomial at higher physical error rate and extrapolated. Needless to say, the result obtained this way cannot be directly compared to the results obtained from exact diagonalization [70, 71]. Nonetheless, it can serve as a proxy to understand how well our method would work.

2.3 Color codes

In this section, we provide a brief review of the two- and three-dimensional color codes [81, 84] that are relevant to this paper. This section will introduce a convention for the qubit labels we use, which shall be used throughout this paper; see Fig. 2.1.

Most of the results in this section are well known, but the discussion about a transversal gate between the two codes is relatively new, having recently appeared in Refs. [85] and [86] (the later gate is equivalent to ours up to a transversal unitary).

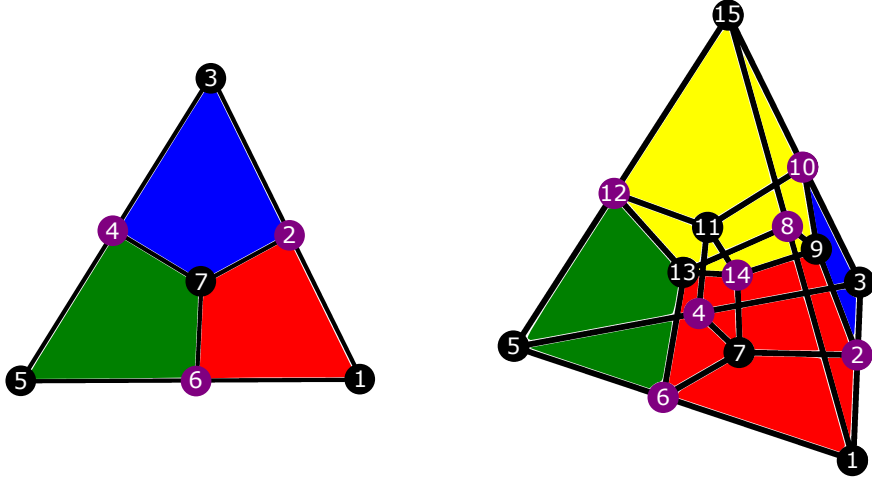


Figure 2.1: (Left) Pictorial representation of the $[[7, 1, 3]]$ Steane code including labels for the physical qubits. (Right) Pictorial representation of the $[[15, 1, 3]]$ qRM code including labels for the physical qubits.

2.3.1 2D color codes

The two-dimensional color code we consider is a CSS code with parameters $[[7, 1, 3]]$, also known as the Steane code [98]. The Steane code stabilizer group is generated by mutually commuting Z -type and X -type 2-cells (henceforth referred to as plaquettes) stabilizers, described in Table 2.3.

Steane: $Z(X)$ -type stabilizers			
p_1	$Z_1 Z_2 Z_6 Z_7$	p_4	$X_1 X_2 X_6 X_7$
p_2	$Z_2 Z_3 Z_4 Z_7$	p_5	$X_2 X_3 X_4 X_7$
p_3	$Z_4 Z_5 Z_6 Z_7$	p_6	$X_4 X_5 X_6 X_7$

Table 2.3: Z -type and X -type plaquette stabilizer generators for the $[[7, 1, 3]]$ Steane code.

The Steane code encodes a single logical qubit and has minimum weight-3 transversal logical $\bar{Z}$ and $\bar{X}$ operators

$$\bar{Z} = Z_1 Z_2 Z_3, \quad (2.1)$$

$$\bar{X} = X_1 X_2 X_3. \quad (2.2)$$

Given that the distance $d = 3$, the Steane code is capable of correcting arbitrary weight-1 errors, and detecting arbitrary weight-2 errors. Unfortunately, the Steane code does not support any transversal logical non-Clifford gate like the T gate. This is because the Steane code supports the full Clifford group transversally, however the no-

go Eastin-Knill theorem [20] states that no stabilizer quantum code exists that contains a transversal universal gate set.

2.3.2 3D color codes

The three dimensional color code we consider is a CSS code with parameters $[[15, 1, 3]]$. It is the smallest color code in three dimensions that admits a transversal T -gate and represents a specific instance of a family of codes known as quantum Reed-Muller codes (qRM).

The stabilizer group is generated by Z -type 2-cells (plaquettes) and X -type 3-cells. In total there are eighteen plaquettes (Table 2.4) and four 3-cells (Table 2.5). Since the qRM encodes a single logical qubit and $15 = 1 + 10 + 4$, there are only ten independent Z -type stabilizers, meaning that there are eight independent constraints (Table 2.6). Those are given by multiplying plaquettes around a cylinder, yielding a total of three constraints per 3-cell. In a given 3-cell, two such constraints give rise to the third one, thus, two constraints per 3-cell give the net result of eight independent ones.

qRM: Z -type stabilizers			
p_1	$Z_1 Z_2 Z_6 Z_7$	p_{10}	$Z_6 Z_7 Z_{13} Z_{14}$
p_2	$Z_2 Z_3 Z_4 Z_7$	p_{11}	$Z_2 Z_7 Z_9 Z_{14}$
p_3	$Z_4 Z_5 Z_6 Z_7$	p_{12}	$Z_4 Z_7 Z_{11} Z_{14}$
p_4	$Z_1 Z_6 Z_8 Z_{13}$	p_{13}	$Z_8 Z_{12} Z_{13} Z_{15}$
p_5	$Z_1 Z_2 Z_8 Z_9$	p_{14}	$Z_8 Z_9 Z_{10} Z_{15}$
p_6	$Z_2 Z_3 Z_9 Z_{10}$	p_{15}	$Z_{10} Z_{11} Z_{12} Z_{15}$
p_7	$Z_3 Z_4 Z_{10} Z_{11}$	p_{16}	$Z_8 Z_9 Z_{13} Z_{14}$
p_8	$Z_4 Z_5 Z_{11} Z_{12}$	p_{17}	$Z_9 Z_{10} Z_{11} Z_{14}$
p_9	$Z_5 Z_6 Z_{12} Z_{13}$	p_{18}	$Z_{11} Z_{12} Z_{13} Z_{14}$

Table 2.4: Z -type plaquette stabilizers for the $[[15, 1, 3]]$ qRM code. Only ten of them are independent due to the constraints of Table 2.6. In the simulations, we decided to measure the set of ten independent stabilizers $\{p_1, p_2, p_3, p_7, p_8, p_9, p_{13}, p_{16}, p_{17}, p_{18}\}$.

qRM: X -type stabilizers	
c_1	$X_1 X_2 X_6 X_7 X_8 X_9 X_{13} X_{14}$
c_2	$X_4 X_5 X_6 X_7 X_{11} X_{12} X_{13} X_{14}$
c_3	$X_2 X_3 X_4 X_7 X_9 X_{10} X_{11} X_{14}$
c_4	$X_8 X_9 X_{10} X_{11} X_{12} X_{13} X_{14} X_{15}$

Table 2.5: X -type 3-cell stabilizers for the $[[15, 1, 3]]$ qRM code.

qRM: Independent constraints			
Γ_1	$p_4 p_5 p_{10} p_{11}$	Γ_5	$p_6 p_7 p_{11} p_{12}$
Γ_2	$p_1 p_5 p_{10} p_{16}$	Γ_6	$p_2 p_6 p_{12} p_{17}$
Γ_3	$p_8 p_9 p_{10} p_{12}$	Γ_7	$p_{13} p_{15} p_{16} p_{17}$
Γ_4	$p_3 p_8 p_{10} p_{18}$	Γ_8	$p_{14} p_{15} p_{16} p_{18}$

Table 2.6: Independent set of constraints $\Gamma_i = I$ (identity) with $i = 1, 2, \dots, 8$ for the $[[15, 1, 3]]$ qRM code.

The minimum weight logical- Z operator $\bar{Z}$ has weight-3, and a representative lies at the edge of the tetrahedron

$$\bar{Z} = Z_1 Z_2 Z_3 . \quad (2.3)$$

The minimum weight logical- X operator $\bar{X}$ has weight-7, and a representative lies at the face of a boundary of the tetrahedron

$$\bar{X} = X_1 X_2 X_3 X_4 X_5 X_6 X_7 . \quad (2.4)$$

Hence, the distance $d = \min\{d_x, d_z\} = 3$, where $d_x = 7$ is the distance for X -type logical operators, and $d_z = 3$ is the distance for Z -type logical operators. In addition, the $[[15, 1, 3]]$ qRM code is capable of correcting arbitrary weight-1 Z -errors (phase flip) and up to weight-3 X -errors (bit flip).

The qRM code also admits a transversal T gate $\bar{T}$, consisting of single-qubit $T/T^\dagger$ gates applied to odd- and even labeled qubits, respectively,

$$\bar{T} = T_1 T_2^\dagger T_3 T_4^\dagger T_5 T_6^\dagger T_7 T_8^\dagger T_9 T_{10}^\dagger T_{11} T_{12}^\dagger T_{13} T_{14}^\dagger T_{15} , \quad (2.5)$$

where the single-qubit T gate is defined as

$$T_j = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix} . \quad (2.6)$$

Note that since the S gate $\bar{S} = \bar{T}^2$, the qRM code trivially supports a transversal

logical $\bar{S}$ gate in terms of single-qubit $S/S^\dagger$ gates, respectively,

$$\bar{S} = S_1 S_2^\dagger S_3 S_4^\dagger S_5 S_6^\dagger S_7 S_8^\dagger S_9 S_{10}^\dagger S_{11} S_{12}^\dagger S_{13} S_{14}^\dagger S_{15}. \quad (2.7)$$

Even though the $[[15, 1, 3]]$ qRM supports a transversal non-Clifford gate, it does not support a transversal Hadamard gate $\bar{H}$, as this would violate Eastin-Knill theorem [20]. Notably, both color codes described in this section achieve optimality between dimensionality and the Clifford hierarchy of the native transversal gates, saturating the bound proved for topological codes by the Bravyi-König theorem [21].

2.4 Protocol

Our protocol aims to prepare a magic state encoded in the Steane code. At the logical level, our approach uses the standard one-bit teleportation protocol [99] to teleport the magic state $|\bar{T}\rangle$ encoded in the qRM code to the Steane code, see Fig. 2.2.

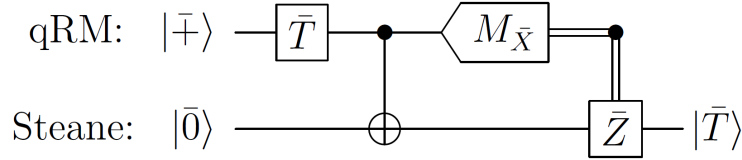


Figure 2.2: Protocol at the logical level. A qRM (quantum Reed-Muller) and a Steane codeblock are prepared in the $|\bar{+}\rangle$ and the $|\bar{0}\rangle$ state, respectively. The transversal logical $\bar{T}$ gate native to the qRM code is applied, creating a logical magic state $|\bar{T}\rangle = \bar{T}|\bar{+}\rangle$. The magic state is then teleported to the Steane code block by applying a logical $\overline{\text{CNOT}}$ gate, measuring the logical $\bar{X}$ operator and applying a logical $\bar{Z}$ correction in the case where $\bar{X} = -1$. At the end of the protocol, the logical magic state $|\bar{T}\rangle$ is prepared in the Steane code block.

We now describe each of the components in Fig. 2.2. By strategically combining various existing fault-tolerant constructions from the literature [66, 67, 81, 84], we succeed in giving an overall improvement compared to other known methods. Our main contribution is a novel protocol for the preparation of the $|\bar{+}\rangle$ state of the qRM code that uses parallel flagged syndrome extraction circuits with only a few extra ancillas and the utilization of a recently discovered $\overline{\text{CNOT}}$ gate.

For completeness, we first describe the standard methods we employ. For the logical

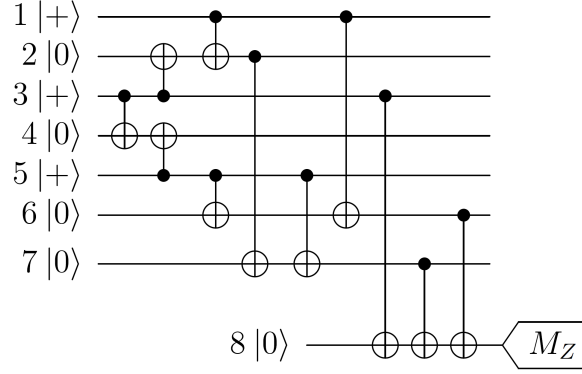


Figure 2.3: Preparation of the logical zero state $|\bar{0}\rangle$ in the Steane code. A non-fault-tolerant initialization involves preparing the physical qubits either in the zero $|0\rangle$ or plus $|+\rangle$ state, followed by a series of CNOT gates. A final verification step measures the logical $\bar{Z}$ operator and uses an ancilla qubit acting as a flag, detecting all weight-2 X errors originating from a single X error.

$\bar{T}$ gate of the qRM code, we apply the standard transversal gate (2.5) [18, 81]. For the logical- X measurement necessary for the teleportation, we first measure all the qubits of the qRM code in the X basis. Then, we compute the X syndrome (see Table 2.5) in postprocessing. At this point, we have a choice to either apply error correction, or instead postselect on measuring a trivial syndrome. We opt for the latter, since that yields a lower logical infidelity. After post-selecting for a trivial X syndrome, we extract the value of the logical- X operator $\bar{X}$, and we apply a logical- Z correction on the Steane code in the case where $\bar{X} = -1$. The $|\bar{0}\rangle$ state preparation of the Steane code follows the known protocol of Refs. [97, 100, 101]; see Fig. 2.3. The logical- Z correction on the Steane code uses the standard weight-3 logical operator (2.1).

Lastly, since the final magic state is encoded in the Steane code, an additional round of flag-based error correction could be used to detect further errors as in Refs. [66, 97], at the expense of increasing the overhead cost of the protocol. Given the depth of syndrome extraction circuits of Sec. 2.4.1, we decided not to incorporate this variation.

2.4.1 Preparation of $|\bar{+}\rangle$ for qRM code

The most involved part of our protocol is the preparation of the $|\bar{+}\rangle$ for the qRM code. At a high level, our approach prepares the logical $|\bar{+}\rangle$ state using the encoding method of Ref. [69], followed by an adapted version of flag-based error detection [65–67, 102]. Our adapted flag-based error detection scheme employs a scheme inspired by Ref. [66],

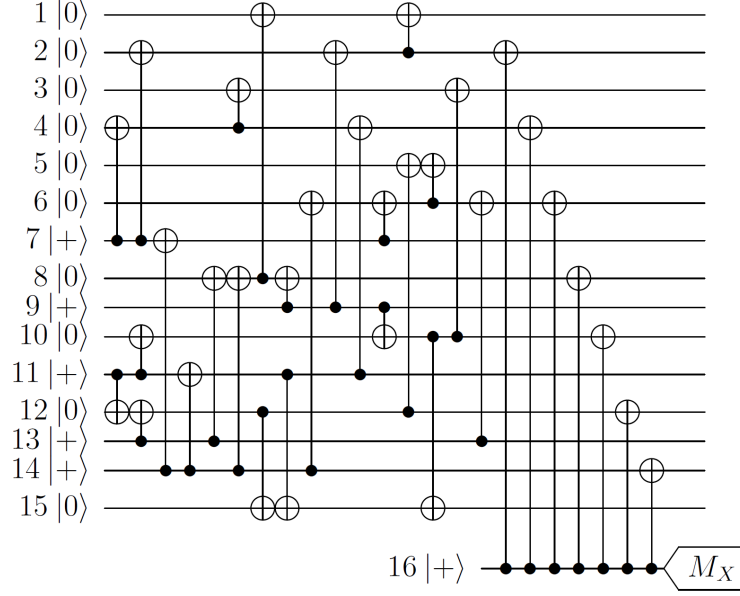


Figure 2.4: Preparation of the logical plus state $|\bar{+}\rangle$ in the qRM code. A non-fault-tolerant initialization involves preparing the physical qubits either in the zero $|0\rangle$ or plus $|+\rangle$ state, followed by a series of CNOT gates.

which is appropriately modified to the qRM code.

The first step of this protocol is described in Fig. 2.4. The final verification step measures the logical $\bar{X}$ operator and uses an ancilla qubit acting as a flag, detecting all uncorrectable weight-2 Z errors originating from a single Z error.

At this point, the state prepared may have additional X errors. If we do not correct them, they will propagate through the transversal T gate to a XS error, which will lead to an error in the final measurement $M_{\bar{X}}$ of the qRM code. In order to mitigate this effect, one must measure the Z -type syndromes. Such measurements should be chosen carefully. If we were to measure each Z -type syndrome using the standard approach (i.e., using a single ancilla and four CNOTs), a single fault can propagate to weight-2 errors in the data block.

We can avoid this problem by using the parallel flag-based syndrome-extraction circuits for the *Steane code* [66], adapted to the qRM code. In that paper, the authors introduced two types of syndrome extraction circuits, one extracting two syndromes at once and the other extracting three syndromes at once; see Fig. 2.5. In the qRM code, there are ten independent Z -type stabilizers, see Table 2.4, which we can organize as follows. First, we can measure $(Z_8 Z_{12} Z_{13} Z_{15}, Z_5 Z_6 Z_{12} Z_{13})$ and $(Z_3 Z_4 Z_{10} Z_{11}, Z_4 Z_5 Z_{11} Z_{15})$

2.4 Protocol

using Fig. 2.5 (left). Then we can measure $(Z_1Z_2Z_6Z_7, Z_2Z_3Z_4Z_7, Z_4Z_5Z_6Z_7)$ and $(Z_8Z_9Z_{13}Z_{14}, Z_9Z_{10}Z_{11}Z_{14}, Z_{11}Z_{12}Z_{13}Z_{14})$ using Fig. 2.5 (right). The advantage of using this new scheme is that instead of employing ten ancilla qubits to flag each syndrome extraction circuit individually, we reduce the number to four. Moreover, the number of time steps needed to run a full syndrome extraction cycle is also reduced, which is desirable for experimental demonstrations. Flags and syndromes are postselected to be +1. We remark that there are other sets of stabilizers one may choose to measure². We leave such studies for future work.

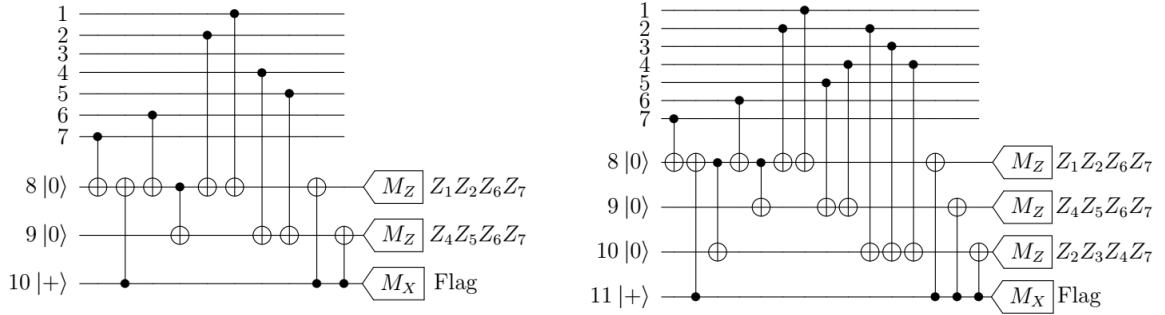


Figure 2.5: (Left) Simultaneous flagged syndrome extraction circuit for *two* Z -type stabilizers in the Steane code. (Right) Simultaneous flagged syndrome extraction circuit for *three* Z -type stabilizers in the Steane code. In both cases, an additional qubit prepared in the plus state $|+\rangle$ acts as a flag and detects higher weight data Z -errors originating from arbitrary single qubit ancilla Z -errors.

2.4.2 Transversal CNOT gate

The logical $\overline{\text{CNOT}}$ gate in Fig. 2.2 can be implemented using a transversal gate. With respect to the convention described in Fig. 2.1, we can apply the following operation:

$$\overline{\text{CNOT}} = \bigotimes_{i=1}^7 \text{CNOT}_i, \quad (2.8)$$

where CNOT_i is the CNOT gate whose control and target is the i 'th qubit of the qRM and Steane code, respectively (see Fig. 2.6). The qubits belonging to the qRM code

²It turns out that four is the minimum number of Z -type stabilizers needed to *detect* all propagated weight-2 or higher X errors after the initialization of Fig. 2.4. For instance, a set of plaquette stabilizers that satisfy this condition is $\{p_2, p_3, p_8, p_{13}\}$. In an experiment, this reduction can decrease the space-time cost of the protocol (see Sec. 2.4.3). We thank an anonymous referee for suggesting to inspect this property.

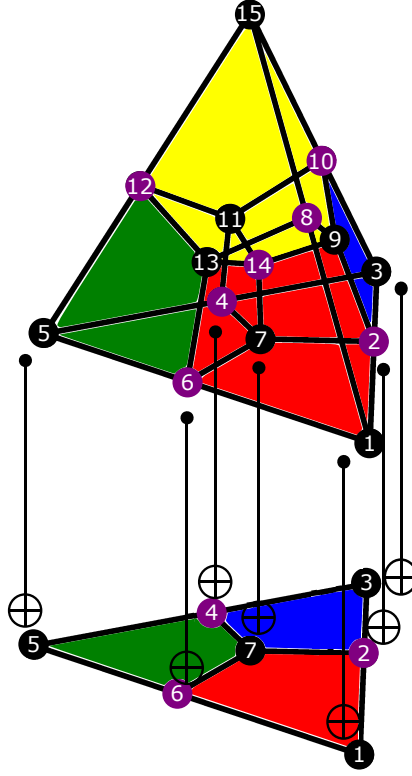


Figure 2.6: Logical $\overline{\text{CNOT}}$ gate between the Steane and qRM codeblocks, consisting of physical CNOT gates acting on the base of the tetrahedron as controls and on the Steane codeblock as targets.

that participate in the CNOT gate span the bottom face of the tetrahedron of Fig. 2.1 (right). In addition, the other orientation of the CNOT gate not used in this protocol is not available via the transversal method of (2.8).

This gate preserves the stabilizer group and satisfies the following relations:

$$\begin{aligned}\overline{\text{CNOT}}\bar{X}_{\text{qRM}}\overline{\text{CNOT}} &= \bar{X}_{\text{qRM}}\bar{X}_{\text{S}} \\ \overline{\text{CNOT}}\bar{Z}_{\text{S}}\overline{\text{CNOT}} &= \bar{Z}_{\text{qRM}}\bar{Z}_{\text{S}}\end{aligned}\tag{2.9}$$

up to stabilizers, where $\bar{X}_{\text{qRM}}$ and $\bar{Z}_{\text{qRM}}$ are logical X and Z operators of the qRM code, (2.4) and (2.3); similarly, $\bar{X}_{\text{S}}$ and $\bar{Z}_{\text{S}}$ are logical X and Z operators of the Steane code, (2.2) and (2.1). Thus, Eq. (2.8) is a logical CNOT from the qRM code to the Steane code. A generalization of this construction to the entire 3D and 2D color code family is discussed in Refs. [85, 86].

2.4.3 Space-time Cost

In this section, we summarize the overall space-time cost of our protocol. The majority of the cost comes from $|\bar{\pm}\rangle$ state preparation (Fig. 2.4) and the syndrome extraction circuits (Fig. 2.5). Overall, we estimate the total space-time volume to be at most $\approx 1.3 \times 10^3$; see Table 2.7 for a breakdown.

It is interesting to note that the overall space-time cost is significantly smaller than methods based on magic state distillation. For instance, consider a recent distillation protocol based on 2D color codes, studied in Ref. [73]. In Fig. 14 of Ref. [73], the authors report an overall space-time cost needed to achieve a target infidelity. At a physical error rate of 10^{-3} , for an infidelity of order 10^{-6} , there is no distillation-based protocol with a space-time cost less than 10^6 . On the other hand, our protocol achieves an infidelity of 5.1×10^{-7} (with a postselection approach) using a space-time volume of $\approx 1.3 \times 10^3$, which is a significant improvement.

Furthermore, we note that our estimate of 1.3×10^3 is likely an overestimate. For instance, the circuits of Fig. 2.5 (right) could be implemented in parallel in our protocol. So, the space-time cost of the most resource-intensive individual part of the protocol in principle can be at least halved.

Protocol	Volume	2-qubit gates	Measurements	Depth
$ \bar{0}\rangle$ State preparation (Fig. 2.3)	75	11	1	10
$ \bar{\pm}\rangle$ State preparation (Fig. 2.4)	309	32	1	20
Syndrome extraction (Fig. 2.5 left)	360	20	6	20
Syndrome extraction (Fig. 2.5 right)	532	30	8	28
Transversal T gate	15	—	—	1
Transversal CNOT gate	22	7	—	1
Logical- X measurement	22	—	15	1
Total	1335	100	31	81

Table 2.7: Summary of the total space-time cost estimate of the protocol, together with the number of 2-qubit CNOT gates, single-qubit destructive measurements, and circuit depth. The space-time cost (volume) is defined as the number of qubits times the number of time steps. For the syndrome extraction circuits, the estimates contemplate two uses for each type of circuit (see Sec. 2.4.1).

2.5 Simulation

The protocol described in Sec. 2.4 uses 22 data qubits and 16 ancilla qubits. If the ancilla qubits are reused, it is possible to reduce the ancilla qubit requirements to four, which is bottlenecked by the flag circuit in Fig. 2.5 (right). Even so, an exact *mixed state* simulation of 26 qubits is challenging.

As such, we resort to a Monte Carlo sampling-based approach. We keep track of the Pauli errors, which after passing through $\bar{T}$, become Clifford errors. Thus, by studying an *ensemble* of circuits, each suffering from a random Clifford error, we can simulate the performance of our protocol. This is a simulation technique akin to an extended stabilizer simulator, which effectively incorporates the non-Clifford T gate.

To incorporate the stochastic Clifford errors into the simulation, we first initialize the noisy logical plus state $|\bar{+}\rangle$ in the qRM code as in Fig. 2.2 and extract the Pauli error frame P ,

$$|\bar{+}\rangle = P|\bar{+}\rangle_{\text{noiseless}}, \quad (2.10)$$

where $|\bar{+}\rangle_{\text{noiseless}}$ is the noiseless plus state. Since the T gate has to be applied to the noisy plus state,

$$\bar{T}|\bar{+}\rangle = (\bar{T}P\bar{T}^\dagger)\bar{T}|\bar{+}\rangle_{\text{noiseless}} = C(P)|\bar{T}\rangle_{\text{noiseless}}. \quad (2.11)$$

The state $|\bar{T}\rangle_{\text{noiseless}} = \bar{T}|\bar{+}\rangle_{\text{noiseless}}$ is a noiseless magic state in the qRM code and $C(P) = \bar{T}P\bar{T}^\dagger$ is the Clifford error frame. If $P \sim \bigotimes_{i=1}^{15} X_i^{a_i} Z_i^{b_i}$ for $a_i, b_i \in \{0, 1\}$, then the Clifford error frame becomes

$$C(P) \sim \left(\bigotimes_{i \text{ odd}} S_i^{a_i} \right) \left(\bigotimes_{i \text{ even}} S_i^{\dagger a_i} \right) P, \quad (2.12)$$

up to a global phase. The ordering of the gates appearing in (2.12) is important, with the Pauli error frame P (2.10) acting first, followed by the phase gates.

After updating the Pauli errors to Clifford errors, we effectively have an ensemble of encoded $|\bar{T}\rangle_{\text{noiseless}}$ states of the qRM code followed by a stochastic Clifford noise.

2.5 Simulation

Note that for a magic state $|\bar{T}\rangle$, the density matrix $|\bar{T}\rangle\langle\bar{T}|$ can be written as a linear combination of pure stabilizer states:

$$\begin{aligned} |\bar{T}\rangle\langle\bar{T}| &= \frac{1}{2}I + \frac{\sqrt{2}}{4}(|\bar{+}\rangle\langle\bar{+}| - |\bar{-}\rangle\langle\bar{-}|) \\ &\quad + \frac{\sqrt{2}}{4}(|\bar{Y}_+\rangle\langle\bar{Y}_+| - |\bar{Y}_-\rangle\langle\bar{Y}_-|). \end{aligned} \quad (2.13)$$

All these states can be implemented by applying logical transversal gates to the logical plus state in the qRM code: $|\bar{-}\rangle = \bar{Z}|\bar{+}\rangle$, $|\bar{Y}_+\rangle = \bar{S}|\bar{+}\rangle$ and $|\bar{Y}_-\rangle = \bar{S}^\dagger|\bar{+}\rangle$. For each of the stabilizer states appearing in Eq. (2.13), we can estimate the fidelity between the logical noiseless magic state in the Steane code $|\bar{T}\rangle_{\text{Steane}}$ (after teleportation) and the given noisy final state $\bar{\rho}$ using the following relation:

$$\langle\bar{T}|\bar{\rho}|\bar{T}\rangle_{\text{Steane}} = \frac{1}{2} + \frac{\sqrt{2}}{4}(\langle\bar{X}\rangle_{\bar{\rho}} + \langle\bar{Y}\rangle_{\bar{\rho}}), \quad (2.14)$$

where $\langle\bar{X}\rangle_{\bar{\rho}}$ and $\langle\bar{Y}\rangle_{\bar{\rho}}$ are the expectation values of the logical X and Y operators evaluated with respect to the code state $\bar{\rho}$, i.e., $\langle\mathcal{O}\rangle_{\bar{\rho}} = \text{Tr}(\mathcal{O}\bar{\rho})$.

In our simulation, the state $\bar{\rho}$ is chosen to be the (normalized) postselected state that we obtain at the very end of the protocol. Because the postselection probability is identical for every stabilizer state appearing in Eq. (2.13), we can estimate Eq. (2.14) by taking the expectation value of the logical X and Y operator of the Steane code only for the post-selected events. Indeed, by combining (2.13) and (2.14), the fidelity can be conveniently written as

$$\langle\bar{T}|\bar{\rho}|\bar{T}\rangle_{\text{Steane}} = \frac{1}{2} + \frac{1}{8}\Delta, \quad (2.15)$$

where

$$\begin{aligned} \Delta &= \left(\langle\bar{X}\rangle_{|\bar{+}\rangle} - \langle\bar{X}\rangle_{|\bar{-}\rangle} + \langle\bar{X}\rangle_{|\bar{Y}_+\rangle} - \langle\bar{X}\rangle_{|\bar{Y}_-\rangle} \right) \\ &\quad + \left(\langle\bar{Y}\rangle_{|\bar{+}\rangle} - \langle\bar{Y}\rangle_{|\bar{-}\rangle} + \langle\bar{Y}\rangle_{|\bar{Y}_+\rangle} - \langle\bar{Y}\rangle_{|\bar{Y}_-\rangle} \right). \end{aligned} \quad (2.16)$$

A proof of (2.15) and (2.16) can be found in Section 2.5.1. We stress that the described

simulation method is well suited for our protocol because we only employ once a logical transversal T gate, thus, it is applied in a single layer at the physical level. However, in a more general scenario where two or more non-Clifford gates act on some subset of qubits (as in Refs. [68, 101]), it is unclear if our proposed method is applicable. This is because Pauli errors become Clifford errors after the first non-Clifford gate, and subsequently non-Clifford errors after the remaining non-Clifford gates.

We quantify the quality of the magic state using two different methods. In the first approach, we compute the fidelity using Eqs. (2.15) and (2.16) assuming that at the final step we perform logical measurement. That is, we measure all the qubits in the X -, or Y - basis and obtain the syndrome information from the measurement outcomes (recall that in the Steane code, since the stabilizer generators have weight-4, it is possible to get the Z syndrome by multiplying the X and Y syndromes, respectively). From the syndrome information, a correction is deduced using a look-up table, after which we obtain the logical measurement outcome. This approach roughly quantifies the quality of the magic state encoded in the Steane code.

In the second approach, in the last step we postselect on measuring a trivial syndrome. This can be used as a proxy for the lowest error rate one can achieve if one were to later enlarge the code to a larger one whilst post-selecting [70, 71]. However, as pointed out in Ref. [71], the logical error rate obtained after such enlargement process is often higher than the one obtained prior to that stage. How the logical error rate changes under such a process is beyond the scope of this paper, and we leave it for a future work.

2.5.1 Fidelity formula derivation

In this section we give additional details about the derivation of (2.15) and (2.16) from (2.13) and (2.14). Notice that the final noisy state produced by the protocol $\bar{\rho}$ can be interpreted as the result of an effective linear map $\mathcal{E}$ acting on the noisy magic state $|\bar{T}\rangle\langle\bar{T}|$ prepared on the qRM code (2.11), i.e., $\bar{\rho} = \mathcal{E}(|\bar{T}\rangle\langle\bar{T}|)$. Expressing the noisy

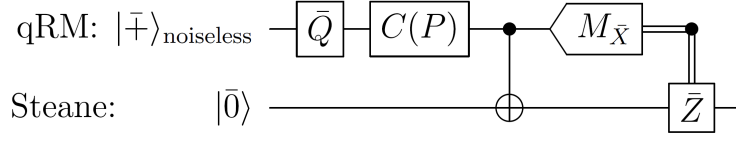


Figure 2.7: Diagram of logical circuits utilized for the numerical simulations. $C(P)$ represents the Clifford error (2.12) for a Pauli frame P (2.10), and $\bar{Q} \in \{I, \bar{Z}, \bar{S}, \bar{S}^\dagger\}$ represents the Pauli rotations which produces the stabilizer states $|\bar{+}\rangle, |\bar{-}\rangle = \bar{Z}|\bar{+}\rangle, |\bar{Y}_+\rangle = \bar{S}|\bar{+}\rangle$ and $|\bar{Y}_-\rangle = \bar{S}^\dagger|\bar{+}\rangle$. At the end of each circuit, after an ideal round of error correction (or post-selection), the expected value $\langle \bar{M} \rangle_{\bar{\rho}'_Q}$ with $\bar{M} \in \{\bar{X}, \bar{Y}\}$ of the final noisy stabilizer state $\bar{\rho}'_Q$ is computed.

magic state using (2.13) leads to

$$\begin{aligned} \mathcal{E}(|\bar{T}\rangle\langle\bar{T}|) &= \frac{1}{2}I + \frac{\sqrt{2}}{4} \left(\mathcal{E}(|\bar{+}\rangle\langle\bar{+}|) - \mathcal{E}(|\bar{-}\rangle\langle\bar{-}|) \right) \\ &\quad + \frac{\sqrt{2}}{4} \left(\mathcal{E}(|\bar{Y}_+\rangle\langle\bar{Y}_+|) - \mathcal{E}(|\bar{Y}_-\rangle\langle\bar{Y}_-|) \right). \end{aligned} \quad (2.17)$$

Therefore, the expected value $\langle \bar{X} \rangle_{\bar{\rho}} = \text{Tr}(\bar{X}\bar{\rho})$ appearing in (2.14) can be written as

$$\langle \bar{X} \rangle_{\bar{\rho}} = \frac{\sqrt{2}}{4} \left(\langle \bar{X} \rangle_{|\bar{+}\rangle} - \langle \bar{X} \rangle_{|\bar{-}\rangle} + \langle \bar{X} \rangle_{|\bar{Y}_+\rangle} - \langle \bar{X} \rangle_{|\bar{Y}_-\rangle} \right), \quad (2.18)$$

and similarly for $\langle \bar{Y} \rangle_{\bar{\rho}}$. The lower index label indicates that the expected value is computed with respect to the respective noisy stabilizer state prepared on the qRM code subject to the linear map $\mathcal{E}$ (a process which has an associated circuit that we present in Fig. 2.7). Equations (2.15) and (2.16) follow directly from (2.18) and its analogous expression for $\langle \bar{Y} \rangle_{\bar{\rho}}$.

2.5.2 Noise model

We use the noise model in which every operation is followed or preceded by a noisy process; we use the uniform depolarizing noise model of strength p . For state preparation, we assume that there is a probability p of flipping the initial state. Hence, we model the preparation of a $|0\rangle$ state as perfect $|0\rangle$ followed by a bit flip X applied with probability p . Similarly, the preparation of a $|+\rangle$ state is modeled as a perfect $|+\rangle$ state followed by a phase flip Z with probability p .

For measurements, we follow a similar recipe as for state preparation. We model a Z -type measurement as a bit flip X applied with probability p , followed by a perfect

Z -type measurement. Similarly, we model an X -type measurement as a phase flip Z applied with probability p , followed by a perfect X -type measurement.

For single- and two-qubit gates, we model them as perfect gates followed by the depolarizing error model. For 1-qubit gates, the depolarizing error model leaves the state unaltered with probability $1 - p$, and applies a Pauli error $P \in \{X, Y, Z\}$ (denoted as $\mathcal{P}_1$) with probability $\frac{p}{3}$. For 2-qubit gates, the depolarizing error model leaves the state unaltered with probability $1 - p$, and applies a Pauli error $P \otimes Q$ with $P, Q \in \{I, X, Y, Z\}$ (denoted as $\mathcal{P}_2$) and $P \otimes Q \neq I \otimes I$ with probability $\frac{p}{15}$. Specifically, these channels can be written as follows

$$\mathcal{D}_1(\rho) = (1 - p)\rho + \sum_{P \in \mathcal{P}_1/\{I\}} \frac{p}{3} P\rho P, \quad (2.19)$$

$$\mathcal{D}_2(\rho) = (1 - p)\rho + \sum_{P \in \mathcal{P}_2/\{I \otimes I\}} \frac{p}{15} P\rho P. \quad (2.20)$$

Here, $\mathcal{D}_1$ and $\mathcal{D}_2$ are a single- and two-qubit depolarizing noise model, respectively.

Regarding idling errors, we do not consider them in our simulations. Given the depths of the different circuits present in our protocol, their contribution might not be entirely insignificant in a experimental demonstration, which we ultimately expect to give a conclusive assessment of the protocol. We plan to study this effect in more detail in a future work.

In order to compare our findings with other state-of-the-art results in the literature, some simulations are done with the multiparameter depolarizing error model too, see Table 2.2. This model is defined similarly as the uniform counterpart, with the only difference that each type of error can be tuned independently, and they are parametrized by p_i initialization error, p_m measurement error, and p_1 and p_2 single- and two-qubit error gate.

2.5.3 Simulation Methods

Our simulations are done using the stabilizer simulator package Stim [96] for Python. Specifically, using Pauli frames obtained from the functions `FlipSimulator()` and `peek_pauli_flips()`, we generated random instances of Clifford errors, each of which are later incorporated to the full circuit using again Stim. For a given simulation, we run N_{tot} Monte Carlo shots, and postselected N_{post} of them. Hence, the acceptance rate of the protocol is given by

$$p_{\text{accept}} = \frac{N_{\text{post}}}{N_{\text{tot}}} . \quad (2.21)$$

For later reference, the postselection rejection probabilities are defined as the complement of the acceptance rate (2.21), in other words ,

$$p_{\text{reject}} = 1 - p_{\text{accept}} . \quad (2.22)$$

Similarly, the infidelity of the magic state quantifies the logical failure and is defined as the complement of the infidelity (2.15) and (2.16),

$$p_{\text{fail}} = 1 - \langle \bar{T} | \bar{\rho} | \bar{T} \rangle_{\text{Steane}} . \quad (2.23)$$

The total number of shots N_{tot} ranges from 10^7 up to 3×10^8 . To compute the uncertainty of the fidelity, we define first the uncertainty of the expectation values $\langle \bar{P} \rangle_{\bar{\rho}}$ for $P = X, Y$, which is given by

$$\sigma_{P, \bar{\rho}} = \sqrt{\frac{\text{Var}(\langle \bar{P} \rangle_{\bar{\rho}})}{N_{\text{post}}}} . \quad (2.24)$$

We observe that at low error rates, the major contribution to the variance comes from the intrinsic probabilistic nature of the measurement of an eigenstate of a Pauli P in another basis P' . More precisely, this occurs when computing in (2.15) and (2.16) the expected values $\langle \bar{X} \rangle_{|\bar{Y}_{\pm}\rangle}$ and $\langle \bar{Y} \rangle_{|\bar{X}_{\pm}\rangle}$. In a noiseless scenario, we can model the

2.5 Simulation

measurement outcomes as a Bernoulli distribution that returns $+1$ and -1 with even probability $1/2$, which has variance 1, thus, yielding an error of $\sigma_{P,\bar{\rho}} \gtrsim 1/\sqrt{N_{\text{post}}}$ for the aforementioned four expected values. Finally, taking into account normalization factors in (2.15) and (2.16), this implies that the propagated fidelity error is roughly given by $\sigma_{\langle \bar{T} | \bar{\rho} | \bar{T} \rangle_{\text{Steane}}} \gtrsim 1/(4\sqrt{N_{\text{post}}})$.

2.5.4 Results

As we stated before in Sec. 2.5, we consider two approaches. The first approach performs error correction when measuring the logical X and Y used in Eqs. (2.15) and (2.16). The second approach uses postselection on measuring trivial syndrome at this step.

The results of the simulation for both approaches are plotted in Fig. 2.8. In the first and the second approach, our circuit can detect all faults of weight 1 and 2, respectively; this difference comes from the final logical measurement stage. We have fitted the logical infidelity and the postselection probability to a polynomial. From the fitted polynomial for the infidelity we obtained at leading order,

$$p_{\text{fail}} \approx \begin{cases} 25.5p^2 - 1266.7p^3 + 165884.4p^4 \\ \quad - 4339823.2p^5 + 39742917.9p^6 \\ \qquad \qquad \qquad (\text{error correction}), \\ 508.5p^3 + 4477.1p^4 \\ \qquad \qquad \qquad (\text{postselection}). \end{cases} \quad (2.25)$$

2.5 Simulation

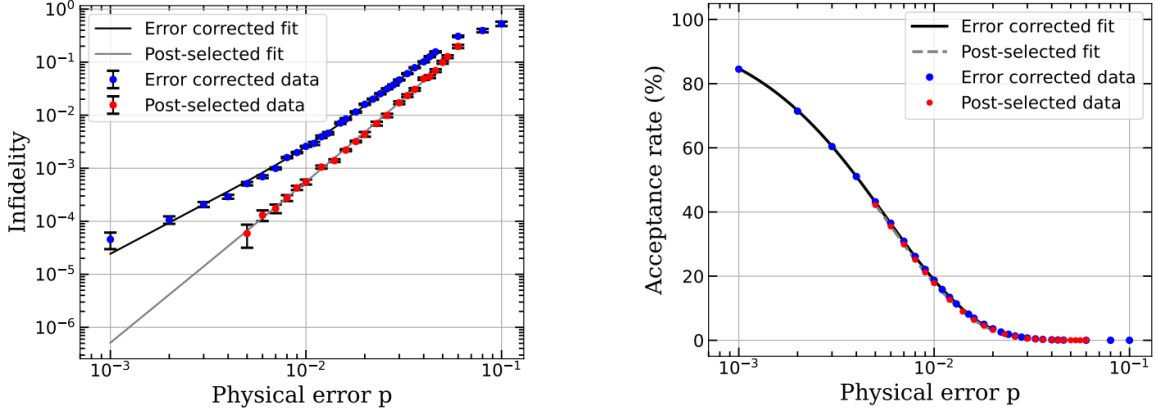


Figure 2.8: (Left) Infidelity of magic states $|\bar{T}\rangle$ as a function of physical error rate for a uniform depolarizing error model (excluding idling errors) of strength p . The polynomial fits with their respective parameters are explicitly given in Eq. (2.25). (Right) Acceptance rate of magic states $|\bar{T}\rangle$ as a function of physical error rate for a uniform depolarizing error model (excluding idling errors) of strength p . The polynomial fits with their respective parameters are explicitly given in Eq. (2.26). A plot of the difference between acceptance rates in logarithmic scale can be found in Fig. 2.9.

In addition, at leading order the polynomial fits for the rejection rates yield,

$$p_{\text{reject}} \approx \begin{cases} 164.6p - 12362.8p^2 + 477206.9p^3 \\ -7518868.5p^4 \\ \text{(error correction),} \\ 166.4p - 12352.7p^2 + 462706.3p^3 \\ -7014618.5p^4 \\ \text{(postselection).} \end{cases} \quad (2.26)$$

The acceptance rate plots in Fig. 2.8 (right) suggest a small difference between the error-corrected and the postselected simulation results. Hence, in Fig. 2.9 we show a plot in logarithmic scale of the difference between the acceptance rate using error correction p_{accept}^{EC} and postselection/error-detection p_{accept}^{ED} , respectively. Their difference gives an estimate of the number of accepted shots with non trivial syndrome in the final decoding since

$$p_{\text{accept}}^{EC} - p_{\text{accept}}^{ED} = \frac{N_{\text{post}}^{EC}}{N_{\text{tot}}} - \frac{N_{\text{post}}^{ED}}{N_{\text{tot}}}, \quad (2.27)$$

Moreover, in Fig. 2.9 we also show a plot of the difference of the weighted infidelities,

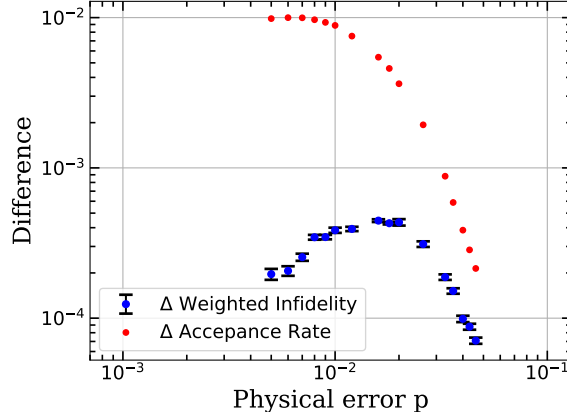


Figure 2.9: Plot of the difference between acceptance rates (2.27) (in red) and weighted infidelities (2.29) (in blue) for the error-correction and postselection analysis, as a function of physical error rate for a uniform depolarizing error model (excluding idling errors) of strength p . Note that the vertical axis is in logarithmic scale and that the acceptance rate is not expressed in percent.

which are defined as the infidelity times the acceptance rate

$$p_{\text{fail}}^{\alpha} p_{\text{accept}}^{\alpha} = \left(\frac{N_{\text{fail}}^{\alpha}}{N_{\text{post}}^{\alpha}} \right) \left(\frac{N_{\text{post}}^{\alpha}}{N_{\text{tot}}} \right) = \frac{N_{\text{fail}}^{\alpha}}{N_{\text{tot}}}, \quad (2.28)$$

where N_{fail}^{α} indicates the number of shots with a logical failure and $\alpha = EC, ED$ (standing from error-correction and error-detection/postselection, respectively). The difference between the weighted infidelities gives an estimate of the number of logical failures with non-trivial syndrome in the final decoding

$$p_{\text{fail}}^{EC} p_{\text{accept}}^{EC} - p_{\text{fail}}^{ED} p_{\text{accept}}^{ED} = \frac{N_{\text{fail}}^{EC}}{N_{\text{tot}}} - \frac{N_{\text{fail}}^{ED}}{N_{\text{tot}}}. \quad (2.29)$$

A complementary check of the previous results, which is corroborated in Fig. 2.9, is that the difference of weighted infidelities (2.29) is always smaller than the difference of acceptance rates (2.27).

It is worth pointing out that for $p \in [10^{-3}, 10^{-2}]$ the leading and sub-leading terms of the polynomial fits (2.25) have the same order of magnitude. Hence, even though the polynomial interpolates the data points in that regime, extrapolation for even lower probabilities $p \ll 10^{-3}$ might lead to unreliable results. A similar note should be addressed in relation to our reported result of 5.1×10^{-7} in Table 2.1 for the infidelity

of the post-selected state when $p = 10^{-3}$. Notwithstanding, the extrapolation was done from a nearby error rate $p = 5 \times 10^{-3}$, and roughly twenty data points with different error rates were simulated in order to account for a robust interpolating fitting polynomial.

2.6 Conclusion

In this chapter, we introduced a method for preparing a high-fidelity magic state using color codes. Our approach employs a judicious use of flag-based post-selection and a transversal gate (that was recently discovered in Ref. [85], which also appeared in Ref. [86] during the preparation of our manuscript.) An important question at this point is whether one can achieve an even higher-fidelity magic state by using a similar protocol, with a flag-based postselection approach on a larger 3D color code. There are several problems that need to be solved for such a study. First of all, we need to generalize our syndrome extraction circuit to the higher distance of the 3D codes. Secondly, a better simulation method must be developed. The infidelity of the magic state produced this way is expected to be multiple orders of magnitude lower than what is reported in this manuscript. Simulation of such a low error rate will be extremely challenging using a Monte Carlo approach. (For instance, Ref. [71] reported weeks of performing a Monte Carlo simulation and it is not even clear if that will be enough for this study.) And, a naive density matrix simulation of the full circuit is likely out of reach for classical computers. Perhaps a tensor network calculation can be useful for this purpose. We leave these studies for future work.

Another important future research direction is an end-to-end analysis of the fidelity of the magic state. In order to use our high-fidelity magic state, one must convert the given state on the original 2D color code to a larger 2D lattice, employing postselection in this process. It was found in a recent study that there is a non-negligible difference between the logical error rate obtained before and after this process [71]. The ratio between the two should depend on the details about the effective error model induced

on the 2D color code patch which is influenced by the protocol. As such, it is not completely clear if the ratio reported in Ref. [71] would remain the same whether their growing process is applied to our setup. Understanding this would require yet another challenging large-scale simulation.

Lastly, we note that our approach should be readily implementable in platforms that allow all-to-all connectivities such as the ion trap [103, 104] and neutral atom-based quantum computers [95]. Indeed, in Chapter 3 we describe the results of the first experimental demonstration of code-switching between color codes, based on the article [2].

Chapter 3

Experimental demonstration of high-fidelity logical magic states from code switching

In this chapter, we present an experimental realization of the logical magic state preparation protocol detailed in Chapter 2. Recall that preparation of high-fidelity logical magic states has remained as a necessary but daunting step towards building a large-scale fault-tolerant quantum computer. One approach is to fault-tolerantly prepare a magic state in one code and then switch to another, a method known as code switching. We experimentally demonstrate this protocol on an ion-trap quantum processor, yielding a logical magic state encoded in an error-correcting code with state-of-the-art logical fidelity. Our experiment is based on the first demonstration of code switching between color codes, from the fifteen-qubit quantum Reed-Muller code to the seven-qubit Steane code. We prepare an encoded magic state in the Steane code with 82.58% probability, with an infidelity of at most $5.1(2.7) \times 10^{-4}$. The reported infidelity is lower than the leading infidelity of the physical operations utilized in the protocol by a factor of at least 2.7, indicating the quantum processor is below the pseudo-threshold. Furthermore, we create two copies of the magic state in the same quantum processor and perform a logical Bell basis measurement for a sample-efficient certification of the

encoded magic state. The high-fidelity magic state can be combined with the already-demonstrated fault-tolerant Clifford gates, state preparation, and measurement of the 2D color code, completing a universal set of fault-tolerant computational primitives with logical error rates equal or better than the physical two-qubit error rate.

3.1 Introduction

Theoretically, the threshold theorem asserts that a noisy quantum computer can simulate a noiseless quantum computer with a moderate overhead, if the physical error rate is sufficiently low [16]. Bridging the gap between the requirement of the threshold theorem and what is experimentally feasible has been one of the central efforts in quantum computing that spanned multiple decades of work. A large body of recent literature demonstrated different aspects of fault-tolerant quantum computation, e.g., logical state preparation, memory, and gates [95, 97, 105–110]. In particular, recently Ref. [111] demonstrated that the fidelity of logical controlled-NOT gates and state preparation are equal or better than their physical counterparts in a trapped ion quantum processor. However there was one logical operation whose fidelity was worse than that of the involved physical operations: T -gate, or equivalently, a preparation of logical magic state [18]. This is a necessary ingredient for building a universal set of fault-tolerant gates.

Historically, preparation of high-fidelity magic state has been one of the most costly and challenging parts of fault-tolerant quantum computation. A common approach has been to inject a noisy magic state into a code, which is then distilled [18]. Injection of a magic state is not fault-tolerant, so to reduce the error rate to a level comparable to the other logical operations, it is necessary to carry out magic state distillation [18], which can lead to a considerable amount of extra complexity and overhead; see Ref. [19] and the references therein.

An alternative approach is to use code switching [82, 83, 112]. In this approach, the magic state is prepared in a code that admits a transversal logical non-Clifford

gate, such as the T -gate. Then the code is switched to another code that admits a complementary set of fault-tolerant logical gates; see Ref. [72] for a recent experiment. Code switching had been deemed less practical than magic state distillation in the past [83], but a more recent work [1] suggests that it can be improved further than previously thought possible.

In this chapter, we experimentally demonstrate that code switching can be used to prepare a high-fidelity magic state encoded in a quantum error-correcting code, using a modest amount of resources. To that end, we present the first experimental demonstration of magic state preparation that employs a code switching between color codes [81, 113], from the $[[15, 1, 3]]$ quantum Reed-Muller code [114] to the $[[7, 1, 3]]$ Steane code [98]. We report the state-of-the-art logical infidelity of at most $5.1(2.7) \times 10^{-4}$, using error-corrected logical quantum state tomography. Indeed, this infidelity is lower than all the reported results in the literature [72, 97, 105, 115–121], even the ones whose infidelity is estimated using post-selected logical quantum state tomography [121], while only using 28 qubits in total. In a similar line of research, another experiment done by some of the authors, which uses an error-detecting code and post-selected logical quantum state tomography, will appear elsewhere [122].

Aside from achieving the state-of-the-art infidelity for the logical magic state encoded in a quantum error-correcting code, this experiment also shows that the error rates of the existing quantum processor is below the pseudothreshold of our protocol. The dominant source of errors are the two-qubit error ($1.05(8) \times 10^{-3}$) and the state preparation and measurement (SPAM) error ($1.38(12) \times 10^{-3}$), which are higher than the infidelity of the reported magic state by a factor of 2 and 2.7, respectively. Thus, continued improvement in physical layer fidelities should improve the infidelity of the magic state at an even faster rate.

Due to the high fidelity of our magic state, the number of samples needed to certify its fidelity becomes rather large. In order to reduce this complexity, we perform a Bell basis measurement over two copies of the encoded magic state. It was recently shown that such a measurement can lead to an asymptotic improvement in the number of

3.2 Magic state preparation protocol

Year	Reference	State	Fidelity	AR (%)	Codes	Platform
2025	This work	$ \bar{T}\rangle$	0.99949^{+27}_{-27}	82.58	Steane, [[15,1,3]]	Trapped-ion
2024	(PS)Lacroix, et al [121]	$ \bar{T}\rangle$	0.9992^{+3}_{-15}	75.2	Steane	Superconducting qubits
		$ \bar{H}\rangle$	0.9959^{+38}_{-37}	74.6		
	Rodriguez, et al [120]	$ \bar{M}\rangle$	0.994^{+3}_{-4}	1	Steane, [[5,1,3]]	Neutral atoms
	(PS)Pogolero et al [72]	$ \bar{T}\rangle$	0.963^{+3}_{-4}	19	Steane, [[10,1,2]]	Trapped-ion
	Kim, et al [119]	$ \bar{H}\rangle$	0.8806^{+2}_{-2}	36.3	Surface code	Superconducting qubits
2023	Ye, et al [118]	$ \bar{T}\rangle$	0.8771^{+9}_{-9}	73.41	Surface code	Superconducting qubits
		$ \bar{H}\rangle$	0.9090^{+9}_{-9}	73.41		
	Gupta, et al [117]	$ \bar{CZ}\rangle$	0.9877^{+11}_{-11}	17	Surface code	Superconducting qubits
2021	Anderson, et al [105]	$ \bar{T}\rangle$	0.978^{+6}_{-6}	100	Steane	Trapped-ion
	Postler, et al [97]	$ \bar{H}\rangle$	0.994^{+5}_{-14}	13.7	Steane	Trapped-ion
	Marques, et al [116]	$ \bar{T}\rangle$	0.966	<25	Surface code	Superconducting qubits
2020	Egan, et al [115]	$ \bar{H}\rangle$	0.972^{+12}_{-12}	100	Bacon-Shor	Trapped-ion

Table 3.1: Comparison of experimental magic state fidelities for quantum codes with distance $d \leq 3$, including acceptance rate (AR) and experimental platform. The magic states correspond to: $|\bar{T}\rangle = \frac{1}{\sqrt{2}}(|\bar{0}\rangle + e^{i\pi/4}|\bar{1}\rangle)$, $|\bar{H}\rangle = \cos(\pi/8)|\bar{0}\rangle + \sin(\pi/8)|\bar{1}\rangle$, $|\bar{M}\rangle = \cos(\theta/2)|\bar{0}\rangle + e^{i\pi/4} \cos(\theta/2)|\bar{1}\rangle$ with $\theta = \cos^{-1}(1/\sqrt{3})$, and $|\bar{CZ}\rangle = \frac{1}{\sqrt{3}}(|\bar{00}\rangle + |\bar{10}\rangle + |\bar{01}\rangle)$. Our reported value $0.99949(27)$ is a lower bound for the fidelity (see Section 3.4). Results marked with (PS) indicate that post-selection is further utilized in the logical state tomography measurements. Using post-selected logical state tomography measurements, our reported fidelity lower bound is $0.99985(11)$ with 81.26% of acceptance rate.

samples needed, assuming the two copies are identical [123]. We use a simple variant of this method with a more relaxed set of assumptions, yielding a rigorous upper bound on the infidelity. A comparison of our results with other experiments in the literature can be found in Table 3.1.

3.2 Magic state preparation protocol

We prepare a magic state $|\bar{T}\rangle = \frac{1}{\sqrt{2}}(|\bar{0}\rangle + e^{i\pi/4}|\bar{1}\rangle)$ using the code switching protocol of Chapter 2. This protocol utilizes two different quantum error-correcting codes: the Steane code [[7,1,3]] [98] and the quantum Reed-Muller [[15,1,3]] (qRM) code [114]. These codes require $n = 7$ and $n = 15$ physical qubits, respectively, and encode a single logical qubit $k = 1$. They are also distance $d = 3$ instances of the two-dimensional (2D) [113] and three-dimensional (3D) [81] color code families, respectively. Indeed, they are capable of correcting arbitrary single-qubit errors and detecting arbitrary two-qubit errors. While the Steane code supports the full Clifford group transversally, it does not admit any transversal non-Clifford gate [20, 21]. In contrast, the qRM code

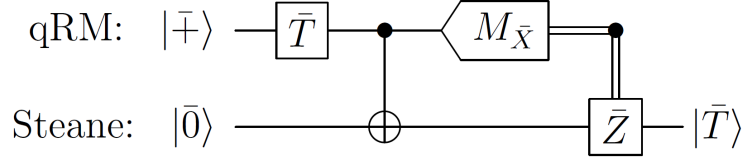


Figure 3.1: The magic state preparation protocol at the logical level [1]. A qRM (quantum Reed-Muller) and a Steane codeblock are prepared in $|\bar{+}\rangle$ and $|\bar{0}\rangle$, respectively. The transversal logical $\bar{T}$ gate is applied, creating a logical magic state $|\bar{T}\rangle = \bar{T}|\bar{+}\rangle$ in the qRM code. The magic state is then teleported to the Steane codeblock by applying a logical $\overline{\text{CNOT}}$ gate, measuring the logical $\bar{X}$ operator and applying a logical $\bar{Z}$ correction if $\bar{X} = -1$. The output of the protocol is a logical magic state $|\bar{T}\rangle$ in the Steane codeblock.

supports a transversal non-Clifford $\bar{T} = \text{diag}(1, e^{i\pi/4})$ gate [81]. Because of this, the code-switching protocol of Chapter 2, described at the logical level in Fig. 3.1, allows the preparation of a magic state $|\bar{T}\rangle = \bar{T}|\bar{+}\rangle$ in the Steane code. Hence, the magic state can be used to implement a logical $\bar{T}$ gate to an arbitrary logical state encoded in the Steane code via gate teleportation [99], effectively circumventing the restrictions imposed by [20, 21].

The protocol of Fig. 3.1 comprises of several different logical components; refer to Section 2.4 of Chapter 2 for further details. Regarding state initialization, a Steane codeblock is prepared in the logical $|\bar{0}\rangle$ state, and a qRM codeblock is prepared in the logical $|\bar{+}\rangle$ state. Their initialization is done using verification flag-based gadgets [1, 66, 69, 101]. Although this process is often viewed as post-selection, we instead refer to this as a *pre-selection* [110] gadget. Because the magic state preparation protocol can be repeated until success, without affecting the other parts of the computation.

After initializing the two code blocks, a magic state is prepared in the qRM codeblock using the native transversal logical $\bar{T}$ gate given by

$$\bar{T} = T_1 T_2^\dagger T_3 T_4^\dagger T_5 T_6^\dagger T_7 T_8^\dagger T_9 T_{10}^\dagger T_{11} T_{12}^\dagger T_{13} T_{14}^\dagger T_{15}. \quad (3.1)$$

Once the magic state is prepared in the qRM codeblock, its logical information is transferred to the Steane codeblock using a logical one-bit teleportation gadget [99]. Correspondingly, an entangling logical $\overline{\text{CNOT}}$ gate between both codeblocks is ap-

plied [85, 86]

$$\overline{\text{CNOT}} = \bigotimes_{i=1}^7 \text{CNOT}_i, \quad (3.2)$$

which consist of physical CNOT gates between qubits at the bottom face of the qRM codeblock acting as controls, and the Steane codeblock acting as targets. Finally, the logical $\bar{X}$ operator is destructively measured in the qRM codeblock, where further pre-selection is employed (see Appendix A.2). In cases where the measurement outcome $\bar{X} = -1$, a logical $\bar{Z}$ correction has to be applied, which in practice it can be taken into account in software post-processing without being physically applied (see Appendix A.2).

3.3 Logical magic state certification

In order to quantify the quality of the noisy magic state $\bar{\rho}$ produced in the experiments, we perform quantum state tomography at the logical level to estimate the fidelity $F(\bar{\rho}, |\bar{T}\rangle\langle\bar{T}|)$. The fidelity can be simplified to the following expression (see (3.9) in Section 3.3.1):

$$F(\bar{\rho}, |\bar{T}\rangle\langle\bar{T}|) = \frac{1}{2} + \frac{1}{2\sqrt{2}} (\langle\bar{X}\rangle_{\bar{\rho}} + \langle\bar{Y}\rangle_{\bar{\rho}}), \quad (3.3)$$

where $\langle\bar{P}\rangle_{\bar{\rho}} = \text{Tr}(\bar{\rho}\bar{P})$ is the expected value of $\bar{P} \in \{\bar{X}, \bar{Y}\}$. We refer to the method of determining $\langle\bar{P}\rangle_{\bar{\rho}} = \text{Tr}(\bar{\rho}\bar{P})$ for $\bar{P} \in \{\bar{X}, \bar{Y}, \bar{Z}\}$ as the *single-copy experiment*, see Fig. 3.2a. These expected values can be estimated by applying physical measurements in the X , Y , or Z eigenbasis and applying error-correction or error-detection/post-selection to the measurement outcomes. For more details, see Appendix A.2.

A drawback of determining the fidelity solely from (3.3) is that neither $\bar{X}$ nor $\bar{Y}$ possess the target magic state as an eigenstate. Thus, their variance is of order unity. If we obtain N_{shots} independent shots to determine the expected values, the fidelity can be bounded only up to $F \geq 1 - O(1/\sqrt{N_{\text{shots}}})$. This is unpractical if the infidelity $1 - F$ is small, which is precisely the case at hand.

In order to lower the sample complexity, we employ an alternative method that can

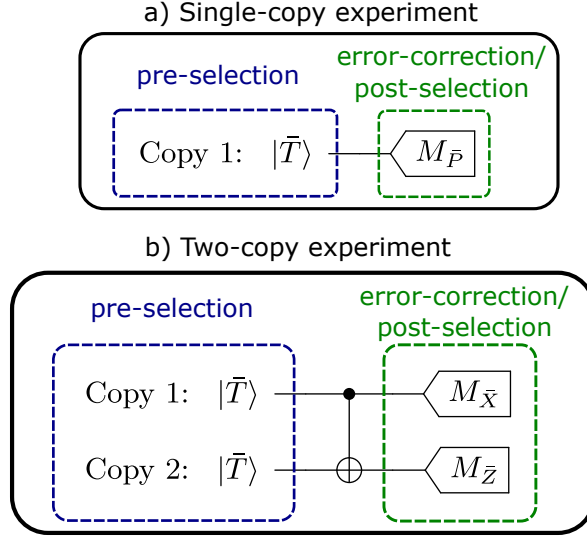


Figure 3.2: Single-copy (a) and two-copy experiments (b), respectively. In both experiments, the magic states are prepared using pre-selection as in Fig. 3.1. In (a) the logical $\bar{P}$ operators with $\bar{P} \in \{\bar{X}, \bar{Y}, \bar{Z}\}$ are measured, whereas in (b) the logical $\bar{X}_1 \otimes \bar{Z}_2$ operator is measured. The overlap with the singlet ϵ (3.4) is given by the fraction of measurement outcomes such that $(m_{\bar{X}}, m_{\bar{Z}}) = (-1, -1)$. In both cases, the logical operators can be determined either with an ideal round of error-correction or error-detection/post-selection.

achieve $F \geq 1 - O(1/N_{\text{shots}})$. This involves performing an additional experiment using two copies of the state, which we refer to as the *two-copy experiment*. The main idea is to perform a simplified version of the SWAP test [124] to estimate the purity of the state; see Fig. 3.2b for the circuit diagram. This process lets us determine the purity of an experimental state by quantifying the overlap with the singlet (anti-symmetric) state $|\bar{\Phi}_1\rangle = \frac{1}{\sqrt{2}}(|\bar{0}\bar{1}\rangle - |\bar{1}\bar{0}\rangle)$,

$$\begin{aligned} \epsilon &\equiv \langle \bar{\Phi}_1 | \bar{\rho}_1 \otimes \bar{\rho}_2 | \bar{\Phi}_1 \rangle \\ &= \langle -1 | \overline{\text{CNOT}}_s (\bar{\rho}_1 \otimes \bar{\rho}_2) \overline{\text{CNOT}}_s | -1 \rangle, \end{aligned} \quad (3.4)$$

where $|\bar{-1}\rangle \equiv |\bar{-}\rangle_1 |\bar{1}\rangle_2$. Here the logical $\overline{\text{CNOT}}_s$ gate is implemented between two copies of the Steane code, unlike the logical $\overline{\text{CNOT}}$ (3.2) gate; see Fig 3.3. For the experimental details of the two-copy experiment, see Appendix A.2.

Combining the results from one- and two-copy experiments, we can obtain a rigorous lower bound on the fidelity:

$$F(\bar{\rho}, \bar{\sigma}_T) \geq 1 - \left(\epsilon + \frac{\delta_X^2 + \delta_Y^2 + \delta_Z^2}{4} \right). \quad (3.5)$$

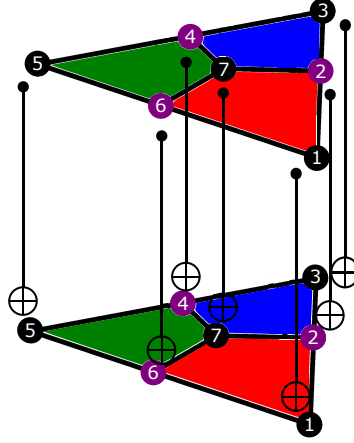


Figure 3.3: Logical $\overline{\text{CNOT}}_s$ gate between Steane codes, consisting of physical CNOT gates between corresponding physical qubits.

The values $\vec{\delta} = (\delta_X, \delta_Y, \delta_Z)$ correspond to the difference of the vectors associated to the Bloch sphere representation of the experimental state $\bar{\rho} = \frac{I + \vec{v} \cdot \vec{\sigma}}{2}$ and the target logical pure state $\bar{\sigma}_T = \frac{I + \vec{u} \cdot \vec{\sigma}}{2}$,

$$\vec{v} = \vec{u} + \vec{\delta}, \quad (3.6)$$

where $\vec{\sigma}$ is the vectorial representation of the Pauli matrices. Note that the vector $\vec{v} = (\langle \bar{X} \rangle_{\bar{\rho}}, \langle \bar{Y} \rangle_{\bar{\rho}}, \langle \bar{Z} \rangle_{\bar{\rho}})$ and for magic $|\bar{T}\rangle\langle\bar{T}|$ states $\vec{u} = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$; see Section 3.3.1 for a derivation. The formula (3.5) holds regardless of the logical pure target state $\bar{\sigma}_T$, and achieves the desired $F \geq 1 - O(1/N_{\text{shots}})$ scaling.

We remark that a recent work also proposed a method with the same scaling in sample complexity [123]. Our approach differs from that work in two aspects. First, unlike Ref. [123], our result can be extended to the setup in which the states are not necessarily identical, only assuming they are in a product state. In this case, Eq. (3.5) applies to at least one of the two copies. For the worst-case fidelity between the two copies, we obtain a similar bound, albeit with a worse constant appearing in front of ϵ . Second, Ref. [123] proposes to twirl both copies of the magic states before applying the entangling $\overline{\text{CNOT}}_s$ gate. We forgo the twirling operation and instead perform the single-copy experiments. For future work, it will be interesting to compare the estimated fidelity using these two different approaches.

3.3.1 Fidelity bound proof

In this section we prove a lower bound for the fidelity $F(\bar{\rho}, \bar{\sigma}_T) = \text{Tr}(\bar{\rho}\bar{\sigma}_T)$, between an experimental state $\bar{\rho}$ and a target ideal pure state $\bar{\sigma}_T$, both with Bloch sphere decompositions

$$\bar{\rho} = \frac{I + \vec{v} \cdot \vec{\sigma}}{2} \quad , \quad \bar{\sigma}_T = \frac{I + \vec{u} \cdot \vec{\sigma}}{2} \quad , \quad |\vec{u}|^2 = 1 . \quad (3.7)$$

We define the difference between their vector representation $\vec{\delta}$ as

$$\vec{v} = \vec{u} + \vec{\delta} . \quad (3.8)$$

The vector $\vec{v} = (\langle \bar{X} \rangle_{\bar{\rho}}, \langle \bar{Y} \rangle_{\bar{\rho}}, \langle \bar{Z} \rangle_{\bar{\rho}})$. For a magic $|\bar{T}\rangle\langle\bar{T}|$ state $\vec{u} = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$. The fidelity $F(\bar{\rho}, \bar{\sigma}_T)$ is

$$F(\bar{\rho}, \bar{\sigma}_T) = \frac{1}{2} (1 + \vec{u} \cdot \vec{v}) = 1 + \frac{1}{2} \vec{u} \cdot \vec{\delta} . \quad (3.9)$$

On the other hand, the trace of the state squared is

$$\text{Tr}(\bar{\rho}^2) = \frac{1}{2} (1 + |\vec{v}|^2) = 1 + \frac{1}{2} |\vec{\delta}|^2 + \vec{u} \cdot \vec{\delta} . \quad (3.10)$$

Thus, combining (3.9) and (3.10) yields

$$\text{Tr}(\bar{\rho}^2) = 1 + \frac{1}{2} |\vec{\delta}|^2 + 2(F(\bar{\rho}, \bar{\sigma}_T) - 1) . \quad (3.11)$$

The values of $\vec{\delta}$ can be obtained from the single-copy experiment. However, the trace of the state squared has to be estimated from an experiment involving at least two-copies. Indeed, similarly to the SWAP test [124], which determines the purity of a state, the projection onto the singlet (anti-symmetric) state $|\bar{\Phi}_1\rangle = \frac{1}{\sqrt{2}}(|\bar{01}\rangle - |\bar{10}\rangle)$ is equal to

$$\begin{aligned} \text{Tr}(\bar{\rho}_1 \bar{\rho}_2) &= \text{Tr}(\overline{\text{SWAP}}(\bar{\rho}_1 \otimes \bar{\rho}_2)) \\ &= 1 - 2\langle \bar{\Phi}_1 | \bar{\rho}_1 \otimes \bar{\rho}_2 | \bar{\Phi}_1 \rangle . \end{aligned} \quad (3.12)$$

3.4 Experimental results

Note that we do not assume that both copies $\bar{\rho}_1$ and $\bar{\rho}_2$ are identical, even though they were produced using the same quantum circuits. The projection ϵ is defined as

$$\begin{aligned}\epsilon &\equiv \langle \bar{\Phi}_1 | \bar{\rho}_1 \otimes \bar{\rho}_2 | \bar{\Phi}_1 \rangle \\ &= \langle \overline{-1} | \overline{\text{CNOT}_s} (\bar{\rho}_1 \otimes \bar{\rho}_2) \overline{\text{CNOT}_s} | \overline{-1} \rangle ,\end{aligned}\tag{3.13}$$

where $|\overline{-1}\rangle \equiv |-\rangle_1 |\bar{1}\rangle_2$. Due to the Cauchy-Schwarz inequality

$$\sqrt{\text{Tr}(\bar{\rho}_1^2) \text{Tr}(\bar{\rho}_2^2)} \geq \text{Tr}(\bar{\rho}_1 \bar{\rho}_2) = 1 - 2\epsilon .\tag{3.14}$$

Moreover, because of the AM-GM inequality

$$\frac{\text{Tr}(\bar{\rho}_1^2) + \text{Tr}(\bar{\rho}_2^2)}{2} \geq \sqrt{\text{Tr}(\bar{\rho}_1^2) \text{Tr}(\bar{\rho}_2^2)} \geq 1 - 2\epsilon .\tag{3.15}$$

Then, $1 - 2\epsilon$ is a lower bound for the maximum (or average) trace of the experimental state squared

$$\max \left\{ \text{Tr}(\bar{\rho}_i^2) \right\} \geq 1 - 2\epsilon .\tag{3.16}$$

Finally, combining (3.11) and (3.16) we prove the lower bound on the fidelity for at least one copy

$$F(\bar{\rho}, \bar{\sigma}_T) \geq 1 - \left(\epsilon + \frac{\delta_X^2 + \delta_Y^2 + \delta_Z^2}{4} \right) .\tag{3.17}$$

3.4 Experimental results

The logical state certification experiments were carried out on the Quantinuum H2-1 trapped-ion quantum processor [125, 126] using 28 qubits total (22 data and 6 ancilla qubits) for the single-copy experiments, and 56 qubits total (44 data and 12 ancilla qubits) for the two-copy experiments. The previous numbers assume mid-circuit measurement and qubit reuse since the single-copy experiments require 31 qubits (22 data and 9 ancilla qubits), whereas the two-copy experiments require 62 qubits (44 data and 18 ancilla qubits). A virtue of the trapped-ion quantum processor is its all-to-all

3.4 Experimental results

connectivity, capable of implementing requisite non-local gates with little additional error. Technical information about the Quantinuum H2-1 quantum processor can be found in Appendix A.1.

The fidelity lower bound for the magic state $|\bar{T}\rangle$ is computed using (3.5). The result gives for an error-corrected magic state an infidelity $1 - F \leq 5.1(2.7) \times 10^{-4}$. With a total of $N_{\text{shots}} = 10,000$ shots for each Pauli basis, the average acceptance rate across all single-copy experiments is 82.58%. The dominant contribution to the fidelity bound comes from the two-copy experiments since $\epsilon = 4.56(2.63) \times 10^{-4}$. We also perform $N_{\text{shots}} = 10,000$ shots of the two-copy experiments. The acceptance rate is 65.73% and 3 logical $|\bar{-1}\rangle$ states are detected in the experiments. The magnitude of ϵ , which quantifies the purity of the state, is one order of magnitude larger than the single-copy experiments contribution to (3.5), which is $\frac{1}{4}(\delta_X^2 + \delta_Y^2 + \delta_Z^2) = 5.24(5.60) \times 10^{-5}$. A summary of the experimental results can be also found in Table A.1 in Appendix A.2.

If we employ error-detection/post-selection in the decoding step, the infidelity bound becomes $1 - F \leq 1.5(1.1) \times 10^{-4}$, with an acceptance rate of 81.26%. The two-copy experiment yields $\epsilon = 9.28(9.28) \times 10^{-5}$ with an acceptance rate of 61.82% (no logical $|\bar{-1}\rangle$ states are detected). The contribution to the fidelity bound due to ϵ is still dominant, because it is almost twice as large as the single-copy experiment contribution $\frac{1}{4}(\delta_X^2 + \delta_Y^2 + \delta_Z^2) = 5.76(5.93) \times 10^{-5}$. Thus, the infidelity may be estimated to be even lower if we take more samples. We leave such studies for future work.

The reported infidelity of $5.1(2.7) \times 10^{-4}$ is below the leading error rate of the involved physical operations. For comparison, the two-qubit error rate is $p_2 = 1.05(8) \times 10^{-3}$ and the SPAM error rate $1.38(12) \times 10^{-3}$. Thus these error rates are below the pseudo-threshold of our scheme. Moreover, preparation of the encoded magic state and its characterization has an infidelity expected to be lower than the infidelity of the same process at the physical level. (Such a process is essentially limited by the SPAM error of $1.38(12) \times 10^{-3}$.) Lastly, the reported infidelity is the new state-of-the-art, even compared against the other methods in the literature that use post-selection; see Table 3.1. Thus our experiment serves as a new frontier for preparing high-fidelity magic

states in experiments, an essential ingredient of fault-tolerant quantum computation.

3.5 Conclusion

In this chapter, we experimentally demonstrate one of the key building blocks of fault-tolerant quantum computation: preparation of high-fidelity encoded magic states. We use code switching from the 15-qubit qRM code to the 7-qubit Steane code [82, 83, 112], employing a verified pre-selection protocol [1]. The reported infidelity of the logical magic state is the new state-of-the-art result for magic states encoded in a quantum error-correcting code. Moreover, this infidelity is lower than the leading physical error rate (dominated by SPAM) by a factor of 2.7, indicating that the quantum processor is below the pseudo-threshold of the protocol.

Combined with the fault-tolerant Clifford gates, state preparation and measurement using the same code [111], we complete a universal set of logical operations whose logical error rates are all equal or better than the physical two-qubit error rate.

It is notable that the state-of-the-art fidelity was achieved using a rather modest number of qubits (22 data and 6 ancilla qubits). The modest resource requirement suggests that the realistic cost of magic-state distillation may be reduced substantially in the near future. For instance, if we use the standard 15-to-1 magic state distillation protocol [18], the error rate of the magic state can be reduced from p to $\sim 35p^3$. Plugging in the infidelity of our magic state, we obtain an expected magic state infidelity of at most 4.6×10^{-9} . This is a number low enough to study the challenging 2D Hubbard model [127] and it is even lower than the inverse of the number of T -gates to run quantum algorithms for FeMoco [128–130]. We anticipate this finding to affect future studies of resource estimate for quantum algorithms on a realistic quantum computer.

Our work also highlights the importance of verified pre-selection in designing fault-tolerant quantum computation protocols [1, 70, 71, 101, 110]. Certain parts of quantum computations can be repeated probabilistically until success, without affecting other parts of the computation. Our work shows that there is a large design space for

improving the existing protocols this way, even in the near-term.

One might suggest the next frontier is to demonstrate a logical $\bar{T}$ -gate with an infidelity lower than the physical T -gate error rate. Because the physical single-qubit error rate of H2-1 quantum processor is $1.9(4) \times 10^{-5}$, the magic state created in this experiment is not sufficient for this goal. If the logical error rate is dominated by two-qubit gate errors p , and we assume the logical error rate is proportional to $\propto p^2$ in the $d = 3$ protocol, the two-qubit gate error would need to improve by approximately $\sqrt{\frac{5.1 \times 10^{-4}}{1.9 \times 10^{-5}}} \sim 5\times$ for this goal. Improving the two-qubit gate fidelity by 5x is not inconceivable, as trapped-ions have achieved gate errors near this level using microwave gates [104]; however, such gates have yet to be demonstrated in a system of many interacting qubits.

Extending our approach to a higher-distance instance of the color code may prove to be the most straightforward approach once more qubits are available in next-generation devices. In such a case, because the number of physical qubits scales as $\Theta(d^3)$, and the post-selection rate is going to be exponentially suppressed (although strategies with a partial level of post-selection could be engineered), we expect the role of our protocol to be slightly different than magic state distillation, since the size of the 3D color code should be capped. Indeed, our protocol can be seen as a source of high-fidelity magic states for 2D color codes at some finite distance, which will need to be further complemented with a procedure that increases the code distance, together with at least one round of magic state distillation.

Furthermore, we advise some healthy skepticism in the definition of the next frontier regarding a logical $\bar{T}$ -gate breaking-even the physical T -gate error rate, as one can imagine this goal being easier to achieve in a system with a slightly worse single-qubit gate error (since the logical error could still be dominated by the two-qubit gate error), and it seems troublesome to define milestones that are easier to achieve with lower performance machines. Another approach to gauging progress is that once all logical operations have error rates below the dominant source of noise in the physical layer (which we have now achieved), the next frontier is to demonstrate algorithmic break-

3.5 Conclusion

even through lower circuit infidelities, where the circuits use a universal gate set in a standardized way. Of course, defining such a family of circuits is a complex task and beyond the scope of this work.

Finally, extending our approach to other code families that admit a transversal logical non-Clifford gate such as $\overline{CCZ}$ [131], could be another interesting direction to pursue in the future.

Chapter 4

Efficient simulation of logical magic state preparation protocols

Developing space- and time-efficient logical magic state preparation protocols will likely be an essential step towards building a large-scale fault-tolerant quantum computer. Motivated by this need, we introduce a scalable method for simulating logical magic state preparation protocols under the standard circuit-level noise model. When applied to protocols based on code switching, magic state cultivation, and magic state distillation, our method yields a complexity polynomial in (i) the number of qubits and (ii) the non-stabilizerness, e.g., stabilizer rank or Pauli rank, of the target encoded magic state. The efficiency of our simulation method is rooted in a curious fact: every circuit-level Pauli error in these protocols propagates to a Clifford error at the end. This property is satisfied by a large family of protocols, including those that repeatedly measure a transversal Clifford that squares to a Pauli. We provide a proof-of-principle numerical simulation that prepares a magic state using such logical Clifford measurements. Our work enables practical simulation of logical magic state preparation protocols without resorting to approximations or resource-intensive state-vector simulations.

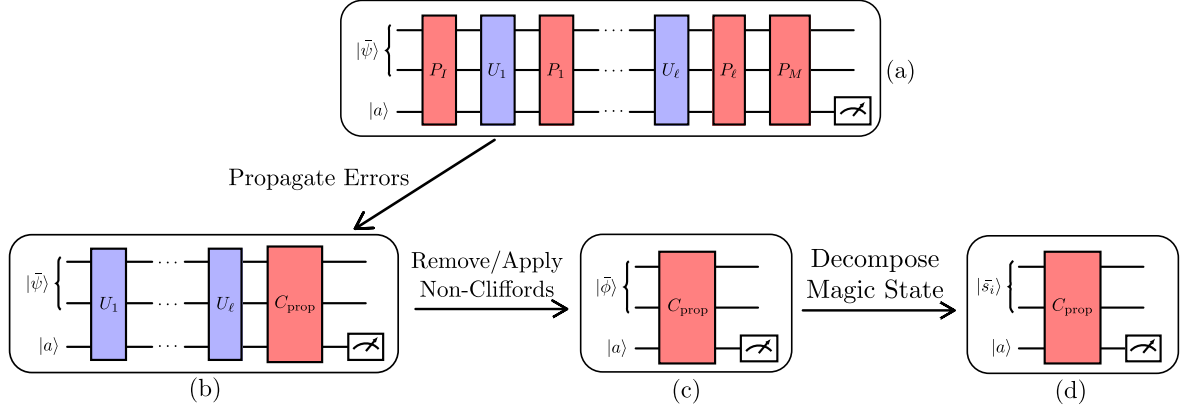


Figure 4.1: Schematic representation of the simulation technique for a magic state preparation (MSP) protocol. (a) This is the general form of the MSP protocol considered in this chapter. Here $U_1, \dots, U_\ell$ are layers of unitary gates that comprise the protocol. Circuit-level Pauli noise is denoted $P_1, \dots, P_\ell$, P_I , and P_M , representing the errors associated with $U_1, \dots, U_\ell$, initialization, and measurement, respectively. Upon measuring the ancilla register (denoted by $|a\rangle$), one either post-selects or error-corrects the logical magic state. (b) For our circuit family, all circuit-level Pauli errors can be propagated to an end-of-circuit Clifford error C_{prop} . (c) Because a noiseless circuit would have prepared a noiseless magic state, the original noisy protocol circuit can be recast as a Clifford error C_{prop} acting on a noiseless logical magic state $|\bar{\phi}\rangle \otimes |a\rangle = \Pi_i U_i(|\bar{\psi}\rangle \otimes |a\rangle)$. (d) To enable efficient simulation, the logical magic state is decomposed into a linear combination of stabilizer states $|\bar{s}_i\rangle$. The fidelity of the output noisy logical magic state can be obtained by simulating an ensemble of logical stabilizer states subjected to stochastic Clifford errors and measurements in the Pauli basis; see Section 4.7 for more details.

4.1 Introduction

In the textbook model of quantum computation, one often considers a continuous gate set consisting of arbitrary one- and two-qubit gates. However, to combat noise present in quantum computers, one must use quantum error correction [14] to encode quantum information in a logical subspace. This logical subspace must not only protect quantum information, but also support quantum computation with a set of fault-tolerant logical gates, i.e., logical gates that are robust to noise [16].

Such fault-tolerant gates are often classified into two categories: Clifford and non-Clifford gates. While there are many methods for implementing Clifford gates [84, 132–135], non-Clifford gates are more difficult to realize. To this end, non-Clifford gates are often carried out by preparing a special resource state called a *magic state* [18]. For many existing fault-tolerant quantum computing architectures, it is commonly assumed that preparing magic states is significantly more costly than Clifford gates [18, 52–62]. For this reason, quantum algorithm development had been rooted in a model in which

non-Clifford gates are significantly more costly than their Clifford counterparts [128].

However, in recent years there has been significant progress in improving the efficiency of magic state preparation (MSP) protocols [1, 64–68, 70, 71, 136–139]. A common feature of these protocols are carefully designed circuits that can efficiently detect errors during the preparation of a magic state. With this progress, the cost of preparing logical magic states is getting closer to that of preparing logical Clifford gates. Moreover, a series of experimental demonstrations for preparing logical magic states have been performed on various quantum devices [2, 72, 97, 105, 117–122, 140], some of which are based on these new protocols (see Chapter 3). These recent developments call for a careful study of more general MSP protocols, which will in turn inform future architectures for fault-tolerant quantum computers and algorithms.

Unfortunately, understanding the exact performance of these MSP protocols is significantly more challenging than for protocols implementing Clifford gates. For the latter, classical simulation can be carried out using the standard Gottesman-Knill theorem [141, 142]. However, MSP protocols involve non-Clifford gates and therefore cannot be simulated this way. In principle, extended stabilizer simulation methods may be used to simulate these protocols [143–150]. However, the complexity of these simulation methods generally scale exponentially with the number of non-Clifford gates. In conjunction, the number of non-Clifford gates used in these protocols scales with the code size, ultimately making the cost of simulation exponential in the number of qubits. To the best of our knowledge, there is no known efficient method for simulating these protocols.

In this chapter, we propose an efficient and broadly applicable method to simulate MSP protocols. When applicable, our method yields a computational complexity scaling polynomially with the number of qubits and a quantity that quantifies the non-stabilizerness of the target encoded magic state, e.g., stabilizer rank [145] or Pauli rank [146]. As a concrete example, our method can be used to efficiently simulate the magic state cultivation protocol [71]. Using a distance- d color code [84], this protocol applies $\Omega(d^2)$ non-Clifford gates on $\Theta(d^2)$ qubits. As such, the simulation cost would

naively scale exponentially in d . However, because the target encoded magic state has a stabilizer rank of 2 independent of d , our method can enable the simulation of this protocol in time polynomial in d .

More broadly, our method is applicable to (i) protocols based on a measurement of certain logical Clifford operator and (ii) protocols based on a transversal non-Clifford gate in the third level of the Clifford hierarchy. Note that there are many different ways of implementing these protocols in practice. They may be used at the logical level to perform magic state distillation [18, 52]. Alternatively, one may opt to employ them at the physical level [1, 68–71, 101, 151, 152], using flag qubits to suppress errors [65–67]. Either way, the simulation cost ends up being polynomial in the number of qubits and the stabilizer/Pauli rank [145, 146] of the target encoded magic state.

The main insight that enables efficient simulation is the special structure of the propagated circuit-level error. More precisely, we observe that circuit-level Pauli errors in these protocols propagate to a Clifford error at the end of the protocol [Fig. 4.1], despite the presence of many non-Clifford gates. In turn, noisy circuits containing non-Clifford gates can be effectively described by a noiseless logical magic state subjected to a Clifford error. We note that this fact was used in the simulation of protocols based on transversal non-Clifford gates [1]; see Chapter 2. However, for the protocols based on measurements of a logical Clifford, this fact is much less obvious.

To better formalize how errors propagate in these protocols, we develop a theory of *Pauli-Square-Root Cliffords* (PSC). These are (non-Pauli) Clifford unitaries that square to a Pauli. Indeed, the majority of magic states considered in the literature can be viewed as $+1$ -eigenstates of some PSC, hence motivating their study. We prove several mathematical facts concerning the structure of PSCs, which can be used to study error propagation through MSP protocols based on measuring logical PSCs in a systematic way. Additionally, we believe PSCs may be of interest independent of simulating MSP protocols.

Compared to existing simulation approaches, ours provide several advantages. Let us focus on cultivation-based protocols [71, 136–139], which are relatively more nontriv-

ial to simulate. In these works, the authors use the fidelity of preparing certain logical stabilizer states as a proxy for determining the fidelity of target logical magic states. For instance, Ref. [71] estimates fidelities for the logical $|T\rangle = T|+\rangle$ and $|Y_+\rangle = S|+\rangle$ state for the distance-3 codes using state-vector simulation. The ratio between the two is then used to deduce the fidelity of the logical $|T\rangle$ state at higher code distances. However, the assumption that this ratio remains approximately the same as a function of increasing code distance is a nontrivial one. By contrast, our method is free of such ambiguities. More recently, some works also proposed a simulation method for magic state cultivation protocols based on the ZX-calculus formalism [153, 154], whereby non-Clifford ZX-diagrams are decomposed into superpositions of a few Clifford ZX-diagrams [155]. However, the number of Clifford ZX-diagrams in this decomposition depends on the circuit-level error configuration, in contrast to our method which employs a superposition of two logical stabilizers states irrespective of the error configuration.

The rest of this chapter is organized as follows. In Section 4.2, we introduce our notations and definitions. In Section 4.3, we describe a simple example that demonstrates the key ideas behind our approach. In Section 4.4, we introduce the notion of Pauli-Square-Root Cliffords (PSC) and describe their salient properties. In Section 4.5, we show that many existing MSP protocols in the literature, such as cultivation-like methods [68, 70, 71, 101, 136–138, 152], logical magic state distillation [18, 52–61] and code-switching [1, 69, 82, 83, 112], propagate circuit-level Pauli errors to an end-of-circuit Clifford error. In Section 4.6, we describe our phase-insensitive method to estimate the fidelity of a target magic state. In Section 4.7, we provide a final overview of the simulation technique. In particular, as a proof-of-concept, we numerically simulate the protocol from Ref. [97, 101, 152] in Section 4.7.2. We end with a conclusion in Section 4.8.

4.2 Preliminaries

We begin by introducing some useful definitions and formalisms. The n -qubit *Pauli group*, denoted by $\mathcal{P}_n$, is generated by the n -fold tensor product of single-qubit Pauli matrices (including a global phase) $\mathcal{P}_n = \{\pm 1, i\} \times \{I, X, Y, Z\}^{\otimes n}$.

The *Clifford hierarchy* [156] is defined recursively for $k \geq 2$ as

$$\mathcal{C}^{(k)} = \{V \in U(2^n) : V P V^\dagger \in \mathcal{C}^{(k-1)}, \forall P \in \mathcal{P}_n\}, \quad (4.1)$$

where $\mathcal{C}^{(1)} = \mathcal{P}_n$ is the Pauli group, and $\mathcal{C}^{(2)}$ is the *Clifford group*. Note that for $k \geq 3$, $\mathcal{C}^{(k)}$ does not form a group. Unitary gates that do not belong to $\mathcal{C}^{(2)}$ are *non-Clifford gates*.

A *Clifford circuit* is defined as a circuit of the following form. Without loss of generality, we consider an initial state prepared in a computational basis state $|0\rangle^{\otimes n}$. The gates in the circuit belong to the Clifford group $\mathcal{C}^{(2)}$ and measurements are performed in the Pauli basis. Moreover, *Pauli stabilizer states* are states of the form $|\psi\rangle = U|0\rangle^{\otimes n}$ for $U \in \mathcal{C}^{(2)}$. These states are +1-eigenvectors of $U Z_i U^\dagger \in \mathcal{P}_n$ for $i = 1, \dots, n$, where Z_i acts non-trivially on the i -th qubit. The single-qubit Pauli stabilizer states are $|P\rangle \in \{|+\rangle, |-\rangle\} \cup \{|Y_+\rangle, |Y_-\rangle\} \cup \{|0\rangle, |1\rangle\}$, which are ± 1 eigenvectors of X , Y and Z , respectively. *Controlled gates* are unitary gates $C(U)$ (or CU) constructed from another unitary gate U such that $C(U) = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U$.

Magic states are resource states that can be consumed to implement a non-Clifford gate [18], up to a Clifford correction. Importantly, a common approach for realizing a universal gate set is to augment the Clifford gate set with the preparation of such magic states. We note that a large class of magic states studied in the literature are +1-eigenstates of Clifford unitaries that we call *Pauli-square-root Clifford* (PSC) [Definition 1]. These are Cliffords that square to a Pauli, whose salient features relevant to our work shall be described in Section 4.4.

For single-qubit magic states, the following examples are well-known:

$$\begin{aligned}
 |T\rangle &= T|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{i\frac{\pi}{4}}|1\rangle), \\
 |H\rangle &= e^{-i\pi/8}SH|T\rangle \\
 &= \cos(\pi/8)|0\rangle + \sin(\pi/8)|1\rangle,
 \end{aligned} \tag{4.2}$$

which are +1-eigenstates of $TXT^\dagger = e^{-\frac{\pi}{4}i}SX$ and H , respectively. (We use the convention of $T = \text{diag}(1, e^{i\frac{\pi}{4}})$ and $S = \text{diag}(1, i)$). For multi-qubit magic states, the following are standard examples

$$|CCZ\rangle = CCZ|+\rangle^{\otimes 3}, \quad |CS\rangle = CS|+\rangle^{\otimes 2}. \tag{4.3}$$

Note that these are +1 eigenstates of the sets spanned by $\{X_1CZ_{2,3}, X_2CZ_{1,3}, X_3CZ_{1,2}\}$ and $\{X_1S_2CZ_{1,2}, X_2S_1CZ_{1,2}\}$, respectively. These examples (except for $|H\rangle$) all have the form of $|V\rangle = V|+\rangle^{\otimes l}$, where V is a diagonal gate in $V \in \mathcal{C}^{(3)}$ [145]. These states are stabilized by the set of $C_i = VX_iV^\dagger \in \mathcal{C}^{(2)}$. Another example is $|CZ\rangle \propto \frac{I+CZ}{2}|+\rangle^{\otimes 2}$, which is a +1 eigenstate [117, 157] of CZ .

All these examples can be written in the following form. Let S_C be an abelian group generated by a commuting set of PSCs, i.e., $S_C = \langle U_i : U_i \text{ is PSC for } 1 \leq i \leq l \wedge [U_i, U_j] = 0 \forall i, j \rangle$. These magic states can be then expressed as

$$|\phi\rangle \propto \sum_{c \in S_C} c|\Omega\rangle, \tag{4.4}$$

where $|\Omega\rangle$ is a stabilizer state. It follows from the definition that $|\phi\rangle$ is a joint +1 eigenstate of all the elements of S_C .

The *stabilizer rank* [144, 145] of an n -qubit state $|\phi\rangle$ is the minimum number q of stabilizer states $|s_i\rangle$ whose linear combination yields $|\phi\rangle$, with $\alpha_i \in \mathbb{C}$,

$$|\phi\rangle = \sum_{i=1}^q \alpha_i |s_i\rangle. \tag{4.5}$$

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From Eq. (4.4), it follows that the stabilizer rank of a magic state is at most $|S_C| \leq 8^l$. For (possibly) mixed quantum states, a natural magic monotone to consider is *Pauli rank* [146], which for an n -qubit state ρ is the minimum number p of non-trivial Paulis P_i whose linear combination yields ρ ,

$$\rho = \frac{1}{2^n} I^{\otimes n} + \frac{1}{2^n} \sum_{i=1}^p \beta_i P_i, \quad (4.6)$$

where $P_i \in \{I, X, Y, Z\}^{\otimes n} \setminus \{I^{\otimes n}\}$ and $\beta_i = \text{Tr}(\rho P_i)$. Our definition of Pauli rank differs from [146] by an additive factor of one since we only account for non-trivial Paulis in the expansion.

Lastly, we comment on the error model we consider. We will focus on arbitrary *circuit-level* Pauli noise in which each quantum operation is modeled as a noiseless operation, preceded or followed by some stochastic Pauli error occurring with a given probability. For our simulations, we utilize the error model described in Appendix B.1.

4.3 A Toy Example

In this Section, we describe a toy example that demonstrates the key ideas behind our simulation method. This example is based on the $[[4, 2, 2]]$ code [52] (also known as the C_4 code). Its stabilizer group is generated by $\{X_1 X_2 X_3 X_4, Z_1 Z_2 Z_3 Z_4\}$ and the logical Pauli-operators are generated by $\{X_1 X_2, X_1 X_3, Z_1 Z_2, Z_1 Z_3\}$ [Fig. 4.2].

This code has two transversal Clifford gates, namely $H_1 H_2 H_3 H_4$ and $S_1 S_2 S_3 S_4$. We will focus on the former, whose action on the logical subspace is $(\bar{H}_1 \otimes \bar{H}_2) \overline{SWAP}_{1,2}$, where $\bar{H}_k$, for $k \in \{1, 2\}$, is the logical Hadamard on the k 'th qubit and $\overline{SWAP}_{1,2}$ is the logical swap gate.

The $[[4, 2, 2]]$ code is a useful guiding example for understanding simulations of the protocols in Refs. [70, 71, 136–138] under circuit-level noise. In these works, the authors studied a protocol to prepare a logical magic state using the following approach:

1. Prepare an encoded magic state (in a manner that is not necessarily fault-tolerant).

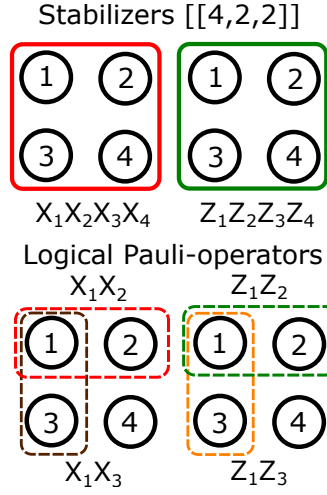


Figure 4.2: Pictorial representation of the $[[4,2,2]]$ code. Each circle corresponds to a physical qubit with their respective labels. The stabilizer group generators (solid lines) and logical Pauli-operators (dashed lines) are highlighted.

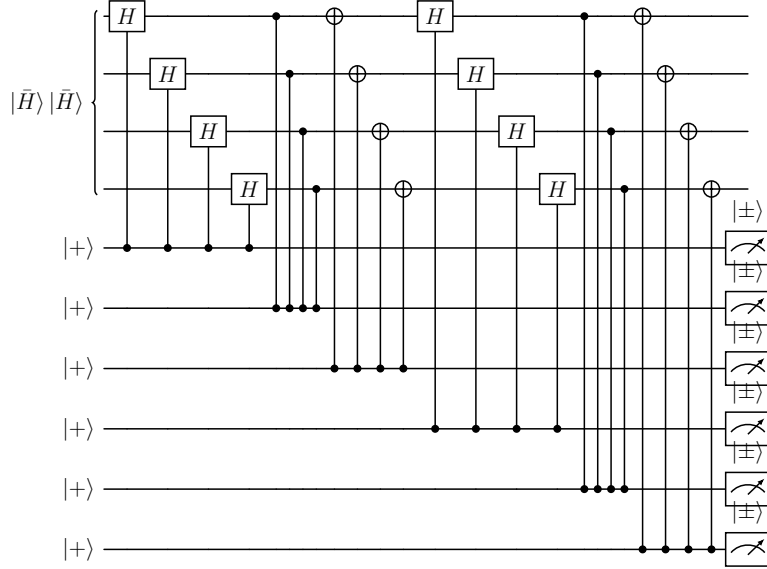


Figure 4.3: A toy example protocol for preparing an encoded magic state $|\bar{H}\rangle|\bar{H}\rangle$ in the $[[4,2,2]]$ code. The logical magic state is prepared, followed by two rounds of logical Clifford and stabilizer measurements.

2. Measure a logical Clifford whose eigenstate is the encoded magic state.
3. Measure the stabilizers.
4. Repeat Step 2 and 3 judiciously, and post-select on detecting no error.

Because the $[[4,2,2]]$ code has a non-trivial transversal logical Clifford gate, we can envision a similar protocol using the same template.

One toy example of such a circuit is shown in Figure 4.3. In this protocol, an

4.3 A Toy Example

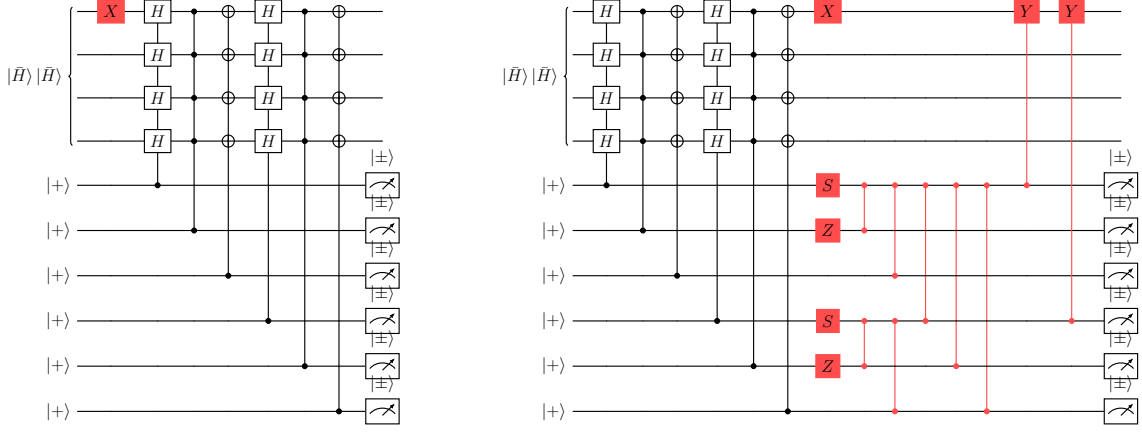


Figure 4.4: Example of X-error propagation in $|\bar{H}\rangle|\bar{H}\rangle$ -state measurement protocol on $[[4, 2, 2]]$ code. Left: Injection of a Pauli X-error. Right: The X-error propagates to a Clifford error at the end of the circuit. To better visualize the propagated error, we compress the sequentially-applied controlled gates from Fig. 4.3.

encoded magic state $|\bar{H}\rangle|\bar{H}\rangle$ is first prepared, where $|\bar{H}\rangle$ is the $+1$ eigenstate of the Hadamard operator. Then, this state is verified using two rounds of logical Clifford and stabilizer measurements. We note that one should not use this circuit as is to prepare a logical magic state. One reason is that weight-1 circuit-level error may propagate to a weight-2 error.¹ Another reason is that the logical Clifford measurement would not distinguish between $|\bar{H}\rangle|\bar{H}\rangle$ and $|-\bar{H}\rangle|-\bar{H}\rangle$, where $|-\bar{H}\rangle = \bar{Y}|\bar{H}\rangle$. Nonetheless, the purpose of this example is to demonstrate the error propagation rule explicitly in a simplified setup.

The simulation of Fig. 4.3 in the absence of circuit-level noise is trivial. Because the initial state is stabilized by the logical Clifford and the stabilizers, the state obtained at the end of the protocol will be $|\bar{H}\rangle|\bar{H}\rangle$. Thus, the main question is how to simulate the circuit in Fig. 4.3 in the presence of circuit-level noise without using a state-vector simulator.

Our central claim is that in the presence of arbitrary circuit-level Pauli errors, the state resulting from this protocol is $\mathcal{C}_m|\bar{H}\rangle|\bar{H}\rangle$, for some stabilizer operation $\mathcal{C}_m$ that can be readily computed from the circuit-level Pauli noise. Here, $\mathcal{C}_m$ may include a Clifford gate, but more generally, a projection onto a ± 1 eigenspace of some Pauli operator.

¹If needed, this issue can be dealt with by using a $|\text{CAT}\rangle$ state ancilla $|\text{CAT}\rangle = \frac{1}{\sqrt{2}}(|0\rangle^{\otimes 4} + |1\rangle^{\otimes 4})$ [13].

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Because stabilizer operations do not increase the stabilizer rank, the stabilizer rank of the noisy state is, for every possible circuit-level Pauli error, at most the stabilizer rank of the noiseless final state. This is the main observation that will generalize to the protocols in Refs. [1, 2, 68, 70, 71, 81–83, 101, 136–138, 152].

Before we proceed, let us comment on why we are assuming only Pauli errors during the preparation of the $|\bar{H}\rangle|\bar{H}\rangle$ state, prior to the verification step. We envision preparing the logical state $|\bar{H}\rangle|\bar{H}\rangle$ by applying a Clifford encoding circuit to a noisy physical $|H\rangle|H\rangle$ state. The key point is that one can randomly apply H at the physical level, decohering the state in the eigenbasis of H . Then, the only possible error acting on this state is the Y error, which is a Pauli. This error, when propagated through a Clifford, remains as a Pauli error; see Appendix B.1.1 for a generalization of this fact to other physical magic states.

We now explain how circuit-level errors propagate in Fig. 4.3. Given we are considering circuits with many non-Clifford gates, the main complication we must deal with is how individual circuit-level Pauli errors propagate through such circuits. If such an error only encounters a *single* non-Clifford gate in $\mathcal{C}^{(3)}$, it simply propagates to a Clifford error, which is manageable. However, if this Pauli error encounters two or more non-Clifford gates, it may propagate to a non-Clifford error, which is harder to deal with.

Surprisingly though, in the circuit shown in Fig. 4.3, any circuit-level Pauli error *always* propagates to a Clifford error. Let us see why this is the case. As an example, consider a circuit-level X -error injected at one of the data qubits at the beginning, which is then propagated to an error at the end of the circuit [Fig. 4.4]. The propagated error can be computed by sequentially passing it through the gates in the circuit. To

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H errors

$$\begin{array}{c} \text{---} [X] \text{---} \bullet \text{---} \\ | \\ \text{---} [H] \text{---} \end{array} = \begin{array}{c} \text{---} \bullet \text{---} [X] \text{---} \\ | \\ \text{---} [H] \text{---} [H] \text{---} \end{array} . \quad (4.11)$$

Given the previous circuit identity introduces H errors, we must also analyze how such errors propagate. Note the following:

$$\begin{array}{c} \text{---} \bullet \text{---} \\ | \\ \text{---} [H] \text{---} \bullet \text{---} \end{array} = \begin{array}{c} \text{---} \bullet \text{---} \bullet \text{---} [S] \text{---} \\ | \quad | \\ \text{---} \bullet \text{---} [H] \text{---} [Y] \text{---} \end{array} , \quad (4.12)$$

$$\begin{array}{c} \text{---} \bullet \text{---} \\ | \\ \text{---} [H] \text{---} \oplus \text{---} \end{array} = \begin{array}{c} \text{---} \bullet \text{---} \bullet \text{---} [S^\dagger] \text{---} \\ | \quad | \\ \text{---} \oplus \text{---} [H] \text{---} [Y] \text{---} \end{array} . \quad (4.13)$$

Thus, propagating H errors introduce additional gates, namely a controlled- Y and phase gates. The phase gate remains in the ancilla register without affecting data qubits. Remarkably, the controlled- Y can be again propagated to the end as a Clifford error, using Eq. (4.8). Therefore, any circuit-level Pauli error injected on the syndrome qubits also propagates to a Clifford error at the end of the circuit. To summarize, *any* circuit-level Pauli error propagates to a Clifford error at the end of the circuit.

Thus, prior to measurement, we have a state of the following form:

$$C_{\text{prop}}(E)(|\bar{H}\rangle|\bar{H}\rangle|+\rangle^{\otimes 6}), \quad (4.14)$$

where $C_{\text{prop}}(E)$ is a Clifford that depends on the error configuration E . Then, we can proceed by simulating each of the 6 measurements. To that end, note that $|\bar{H}\rangle|\bar{H}\rangle$ is a linear combination of at most $q = 4$ stabilizer states (as in Eq.(4.5)):

$$|\bar{H}\rangle|\bar{H}\rangle = \sum_{i=1}^4 \alpha_i |\bar{s}_i\rangle, \quad (4.15)$$

where $\{|\bar{s}_i\rangle : i = 1, \dots, 4\}$ is a set of stabilizer states and α_i complex coefficients. The protocol can be simulated by computing the probability of measuring ± 1 for each

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individual measurement and calculating the post-measurement state. This state can be obtained from a post-selection of the stabilizer states in some fixed basis (say $|0\rangle, |1\rangle$), all of which can be done using the standard extended stabilizer simulation method [145]. Finally, one can apply a Pauli (or even Clifford, if necessary) correction based on these measurement outcomes and compute the overlap with the state $|\bar{H}\rangle|\bar{H}\rangle$. Crucially, the overall cost of the simulation depends only on the stabilizer rank of the final state, not the number of non-Clifford gates used in the protocol. We review this stabilizer rank-based simulation approach in Appendix B.5.

One can also express the ideal logical magic state and its noisy counterparts as density matrices

$$\bar{\rho} = (|\bar{H}\rangle\langle\bar{H}|)^{\otimes 2}, \quad (4.16)$$

and

$$\hat{\rho}_m = \mathcal{C}_m(E) \left[(|\bar{H}\rangle\langle\bar{H}|)^{\otimes 2} \right], \quad (4.17)$$

respectively, where $\mathcal{C}_m(E)$ is a stabilizer operation that depends on the error E and the measurement outcome m . After applying a decoding operation $\mathcal{D}$ that maps $\hat{\rho}_m$ to a state in the code subspace $\bar{\rho}_N = \mathcal{D}(\hat{\rho}_m)$ (up to a potential logical error), we can compute the fidelity $F = \text{Tr}(\bar{\rho}\bar{\rho}_N)$ in the following way. Note the following decomposition (as in Eq.(4.6)):

$$(|\bar{H}\rangle\langle\bar{H}|)^{\otimes 2} = \frac{1}{4}\bar{I}^{\otimes 2} + \frac{1}{4}\sum_{i=1}^8 \beta_i \bar{P}_i, \quad (4.18)$$

where $\bar{P}_i$ are non-trivial 2-qubit Pauli operators and β_i are $p = 8$ real non-negative coefficients. Thus, the fidelity can be computed from expectation values of Pauli logical operators since $\langle \bar{P}_i \rangle_{\bar{\rho}_N} = \text{Tr}(\bar{P}_i \bar{\rho}_N)$. In Section 4.6, we provide further detail about how these expectation values can be estimated by running 8×2^2 stabilizer circuits for each $\bar{P}_i$ (and more generally, $p \times 2^k$ circuits for k logical qubits and Pauli rank p).

This example may raise more questions than answers as the way in which a circuit-level Pauli error propagates to an end-of-circuit Clifford error may seem mysterious. A natural question is whether there is a more general theory that underlies this observation. This is the topic of Section 4.4.

The following are a few key circuit identities that drive our discussion

$$\begin{array}{c} \text{---} X \text{---} \bullet \text{---} \\ | \\ \text{---} \text{---} U \text{---} \end{array} = \begin{array}{c} \bullet \text{---} \bullet \text{---} X \text{---} \\ | \quad | \\ \text{---} U \text{---} U^{+2} \text{---} U \text{---} \end{array}, \quad (4.20)$$

For reasons we make clear in Section 4.4.1, we will choose U to be a Clifford which is a *square root* of a Pauli [Definition 1].

4.4.1 Cliffords that square to Paulis (PSC)

We study a special class of Cliffords that square to a Pauli and elucidate its properties. The main results of this Section concern complete characterization of these Cliffords from two different perspectives: controlled-unitary [Lemma 1] and its canonical form [Proposition 1]. We begin by introducing a formal definition.

Definition 1. *A unitary is Pauli-Square-Root Clifford (PSC) if it is a (non-Pauli) Clifford that squares to a Pauli.*

PSCs are special in that they satisfy a number of extra properties that are not universally true for all Cliffords. For instance, controlled versions of Cliffords are not necessarily in the third level of the Clifford hierarchy, with the Clifford HS being one such counterexample [158]. However, PSCs are precisely those unitaries whose controlled version lie in the third level of the Clifford hierarchy.

Lemma 1. *Let U be a unitary. U is a PSC if and only if controlled- U is in the third level of the Clifford hierarchy $\mathcal{C}^{(3)}$.*

Moreover, there is a canonical form for any PSC, which will turn out to be convenient for proving the circuit identities in Section 4.4.2.

Proposition 1. *A unitary U is a PSC if and only if it can be written in the following form:*

$$U = \alpha P \exp \left(\frac{\pi i}{4} \sum_{j=1}^m Q_j \right), \quad (4.21)$$

where P is a Pauli and $\{Q_j : j = 1, \dots, m\}$ is a commuting set of Paulis $[Q_i, Q_j] = 0$, and α is a complex number such that $\alpha^8 = 1$.

It is possible to check these statements individually for well-known PSCs, such as $H, CZ, X \otimes CZ, TST^\dagger$. However, the advantage of these statements is that those properties can be verified by simply checking if a given Clifford squares to a Pauli, something that can be done much more straightforwardly in many cases.

The proofs of Lemma 1 and Proposition 1 can be found in Appendix B.2.

4.4.2 Circuit identities

In this Section, we derive circuit identities involving PSCs that generalize the circuit identities discussed in Section 4.3. These follow straightforwardly from the canonical form [Eq. (4.21)]. For details, see Appendix B.2.

Proposition 2. *Let C and P be a PSC and a Pauli respectively, supported on t qubits*

$$\begin{array}{c} \text{---} \\ | \\ \text{---}^t \text{---} [P] \text{---} [C] \text{---} \end{array} = \begin{array}{c} \text{---} \\ | \\ \text{---}^t \text{---} [C] \text{---} [P] \text{---} [Q] \text{---} \end{array}, \quad (4.22)$$

where Q is a t -qubit Pauli that either commutes or anticommutes with C . Furthermore, $\text{Supp}(Q) \subseteq \text{Supp}(C)$.

Proposition 3. *Let C and P be a PSC and a Pauli respectively, supported on t qubits*

$$\begin{array}{c} \text{---} \\ | \\ \text{---}^t \text{---} [C] \text{---} [P] \text{---} \end{array} = \begin{array}{c} \text{---} \\ | \\ \text{---}^t \text{---} [P] \text{---} [C] \text{---} [Q] \text{---} \end{array}, \quad (4.23)$$

where Q is a t -qubit Pauli that either commutes or anticommutes with C . Furthermore, $\text{Supp}(Q) \subseteq \text{Supp}(C)$.

The proof of Proposition 2 uses the circuit identity from Eq. (4.22), in addition to the canonical form of PSCs [Proposition 1]. The details of the proof can be found in Appendix B.2. Proposition 3 is proved using a similar argument.

Theorem 1. *Let C be a PSC on t qubits and P be a $(t+1)$ -qubit Pauli*

$$\begin{array}{c} \text{---} \\ | \\ \text{---}^t \text{---} [P] \text{---} [C] \text{---} \end{array} = \begin{array}{c} \text{---} \\ | \\ \text{---}^t \text{---} [C] \text{---} [P'] \text{---} [Q] \text{---} [C^b] \text{---} \end{array}, \quad (4.24)$$

for some $(t+1)$ -qubit Pauli P' , t -qubit Pauli Q , and $b \in \{0, 1\}$, where Q either commutes or anticommutes with C . Furthermore, $\text{Supp}(Q) \subseteq \text{Supp}(C)$.

Proof. If P does not contain an X or Y on the control qubit, the claim follows immediately from Proposition 2. If the Pauli on the control qubit is X , using Eqs. (4.20) and (4.22), we obtain:

$$\begin{array}{c} \text{---} \boxed{X} \text{---} \\ \text{---} \text{---} \end{array} \begin{array}{c} \bullet \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \end{array} \begin{array}{c} \boxed{P} \text{---} \boxed{C} \text{---} \\ \text{---} \end{array} = \begin{array}{c} \text{---} \text{---} \end{array} \begin{array}{c} \bullet \\ | \end{array} \begin{array}{c} \text{---} \boxed{X} \text{---} \\ \text{---} \end{array} \begin{array}{c} \bullet \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \end{array} \begin{array}{c} \boxed{C} \text{---} \boxed{PQ^\dagger C^2} \text{---} \boxed{Q^\dagger C^2} \text{---} \boxed{C} \text{---} \\ \text{---} \end{array}, \quad (4.25)$$

where $Q' = CPC^\dagger P^\dagger$ is a t -qubit Pauli that either commutes or anticommutes with C [Proposition 2]. In particular, $[C^2, Q'^\dagger] = 0$. Therefore, C and $Q = Q'^\dagger C^2$ either commutes or anticommutes. Moreover, since C is a PSC, $Q'^\dagger C^2$ and $PQ'^\dagger C^2$ are Paulis, concluding the proof for this case. This argument also applies to the case in which the Pauli on the control qubit is Y .

□

Theorem 1 is important because it establishes a nontrivial structural property of a Pauli error propagating through a controlled-Clifford. Since the controlled-Clifford is in the third level of the Clifford hierarchy [Lemma 1], the error may propagate to a Clifford error. However, the non-Pauli part of the error consists of two components that have nontrivial algebraic relations with the original controlled-Clifford.

For instance, because Q and C in Eq. (4.24) either commute or anticommute, we have

$$\begin{array}{c} \text{---} \text{---} \end{array} \begin{array}{c} \bullet \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \end{array} \begin{array}{c} \boxed{Q} \text{---} \boxed{C} \text{---} \\ \text{---} \end{array} = \begin{cases} \begin{array}{c} \text{---} \text{---} \end{array} \begin{array}{c} \bullet \\ | \end{array} \begin{array}{c} \text{---} \boxed{Z} \text{---} \\ \text{---} \end{array} \begin{array}{c} \bullet \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \end{array} \begin{array}{c} \boxed{C} \text{---} \boxed{Q} \text{---} \\ \text{---} \end{array} & \text{if } \{Q, C\} = 0, \\ \begin{array}{c} \text{---} \text{---} \end{array} \begin{array}{c} \bullet \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \end{array} \begin{array}{c} \boxed{C} \text{---} \boxed{Q} \text{---} \\ \text{---} \end{array} & \text{if } [Q, C] = 0. \end{cases} \quad (4.26)$$

and

$$\begin{array}{c} \text{---} \text{---} \end{array} \begin{array}{c} \bullet \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \end{array} \begin{array}{c} \boxed{Q} \text{---} \boxed{C} \text{---} \\ \text{---} \end{array} = \begin{cases} \begin{array}{c} \text{---} \text{---} \end{array} \begin{array}{c} \bullet \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \end{array} \begin{array}{c} \bullet \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \end{array} \begin{array}{c} \boxed{C} \text{---} \boxed{Q} \text{---} \\ \text{---} \end{array} & \text{if } \{Q, C\} = 0, \\ \begin{array}{c} \text{---} \text{---} \end{array} \begin{array}{c} \bullet \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \end{array} \begin{array}{c} \boxed{C} \text{---} \boxed{Q} \text{---} \\ \text{---} \end{array} & \text{if } [Q, C] = 0. \end{cases} \quad (4.27)$$

Therefore, if the controlled- Q encounters another controlled- C gate later, they commute up to a potential CZ gate on the controls. Similarly, because Q is a Pauli, it will also commute with any other controlled-Pauli up to a potential CZ gate on the controls. Moreover, if we were to propagate C in Eq. (4.24) through a controlled-Pauli, we only get an additional controlled-Pauli whose underlying Pauli either commutes or

anticommutes with C [Proposition 3].

4.5 Error propagation in magic state preparation protocols

In this Section, we summarize families of MSP protocols for which arbitrary circuit-level Pauli errors propagate through them to an end-of-circuit Clifford error. We consider protocols based on measuring logical PSCs [Section 4.5.1], magic state distillation at the logical level [Section 4.5.2] and protocols based on the implementation of a transversal non-Clifford gate [Section 4.5.3]. Before diving into details, we would like to highlight that error propagation for protocols from Section 4.5.1 is in general more involved than for protocols from Sections 4.5.2 and 4.5.3. This is due to the complex error propagation properties of logical PSC measurements [Section 4.4]. We also note that, compared to Section 4.5.1, the discussions in Sections 4.5.2 and 4.5.3 do not rely heavily on the properties of PSCs. Nonetheless, we discuss these protocols for completeness.

We note that all protocols discussed in this Section can be equivalently recast with measurements postponed to the end. For convenience, we stick to this convention throughout this Section. One *can* simulate mid-circuit measurements and ancilla resets explicitly without having to postpone them to the end. However, in this case, the propagated error also includes projections by stabilizer states, which are more cumbersome (though still efficient) to simulate. For instance, the MSP protocol of Ref. [157] requires mid-circuit measurements and feed-forward Pauli corrections to guarantee fault-tolerance. We leave analysis of error propagation through mid-circuit measurements and ancilla resets to future work.

4.5.1 Canonical family 1: logical PSC measurement

We describe a general framework for a family of protocols preparing logical magic states that are +1-eigenstates of logical PSC operators. Such protocols interleave layers of logical PSC measurements with stabilizer measurements [68, 70, 71, 101, 136–138, 152].

We show that the error propagation observed from the toy example of Section 4.3 can be generalized to these cases.

As a warm-up, we first consider a non fault-tolerant (non-FT) version of PSC measurement protocols. We then discuss a FT version using $|\text{CAT}\rangle$ states (where $|\text{CAT}\rangle = \frac{1}{\sqrt{2}}(|0\rangle^{\otimes s} + |1\rangle^{\otimes s})$ for some natural number s). Additionally, we also briefly discuss the use of flag qubits [66–68, 151, 152] for achieving fault-tolerance in lieu of $|\text{CAT}\rangle$ states to improve ancilla overhead.

Our discussion will center around logical PSC gates, defined as follows.

Definition 2 (Transversal PSC gate). *A logical unitary gate $\bar{U}$ is a transversal PSC if it can be written as a tensor product of PSC gates V_i with disjoint support,*

$$\bar{U} = \bigotimes_{i=1}^{\ell} V_i. \quad (4.28)$$

Note that we are using a liberal definition of transversality in that V_i may act on more than one qubit. We make this choice in order to include logical Cliffords that are tensor products of multi-qubit PSCs. For example, in the folded surface code [159], the full set of logical Cliffords can be realized by a transversal PSC gate, wherein some V_i act on two qubits instead of just one.

In the rest of this Section, we focus on protocols that measure a transversal PSC $\bar{U} = \bigotimes_{i=1}^{\ell} V_i$ with the following additional properties:³

1. Every V_i acts on at most $O(1)$ qubits.
2. The PSC $\bar{U}$ has order 2, i.e., $\bar{U}^2 = I$.

Let us briefly justify these choices. Without the first property, $\bar{U}$ may spread low-weight errors to undesirable high-weight errors. Indeed, to the best of our knowledge, all known protocols that measure a logical Clifford obey this assumption. The second

³Note that eigenstates of PSCs are not automatically magic states. For instance, the eigenstates of the S gate are $|0\rangle$ and $|1\rangle$. Therefore, checking whether a measurement of a logical PSC yields a magic state must be done on a case-by-case basis.

assumption is imposed due to the fact that many existing protocols for preparing logical magic states measure PSCs of order 2.⁴ We also note that generalizing to the case where $\bar{U}$ is of order 4 is straightforward. Given $\bar{U}$ is a PSC, its square is a logical Pauli. The eigenphase of $\bar{U}$ can be determined by performing quantum phase estimation with $\bar{U}$, which involves applying both controlled- $\bar{U}$ and controlled- $\bar{U}^2$. The propagation of errors we discuss generalizes to this setting in a straightforward way. We also note that cases where $\bar{U}^4 = -I$ (due to a global phase) are redundant as this does not change U 's eigenstate.

Now we introduce various protocols for measuring logical PSCs and prove that circuit-level Pauli errors propagate to an end-of-circuit Clifford error [Theorem 2] with polynomially-many one- and two-qubit gates. To provide some context, recall the MSP protocol discussed in Section 4.3. Here, a logical PSC and stabilizers of the $[[4, 2, 2]]$ code were measured twice (non-fault tolerantly) in an alternating fashion. We envision generalizing this idea to protocols that repeatedly measure an arbitrary subset of a code's stabilizers and an available logical PSC, in an arbitrary order.

More formally, consider measuring a subset of stabilizers $S_M = \{g_1, \dots, g_m\} \subseteq S$, which can be specified in terms of a parity check matrix H . We define sparsity parameters w_c and w_q associated with H as the maximum row and column weights of this matrix, respectively. In particular, these are the maximum weight of the elements of S_M and the maximum number of elements in S_M acting nontrivially on a single qubit, respectively.

Given a logical PSC $\bar{U}$, we consider three types of protocols for measuring $\bar{U}$:

1. **Standard protocol.** A protocol is *standard* if every stabilizer/PSC is measured in a non-fault tolerant manner with single ancilla qubits; see Fig. 4.5.
2. **Shor-style protocol.** A protocol is *Shor-style* if every stabilizer/PSC is measured fault tolerantly with $|\text{CAT}\rangle$ states; see Fig. 4.6

⁴However, exceptions do exist, e.g., Ref. [137]. The Clifford being measured in this work is not a PSC.

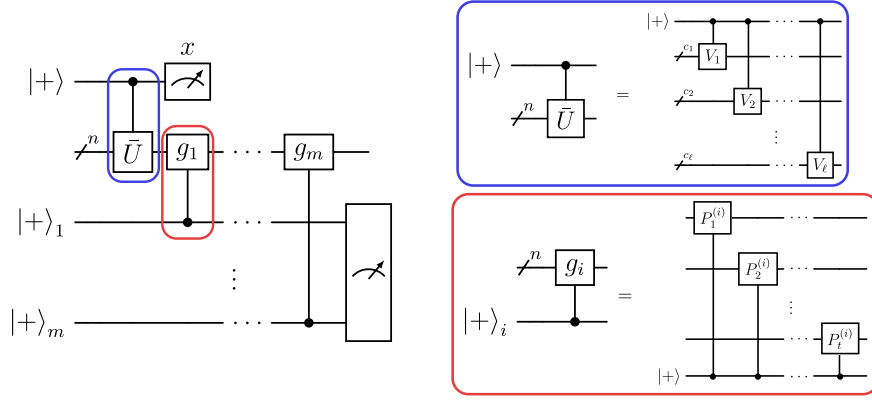


Figure 4.5: Non-FT standard measurement gadget. Measurement of a transversal logical PSC $\bar{U} = \bigotimes_{i=1}^{\ell} V_i$, for PSCs V_i , is followed by single-ancilla measurements of Pauli stabilizer generators $\{g_1, \dots, g_m\}$ where $g_i = \bigotimes_{j=1}^t P_j^{(i)}$ for single-qubit Paulis $P_j^{(i)}$.

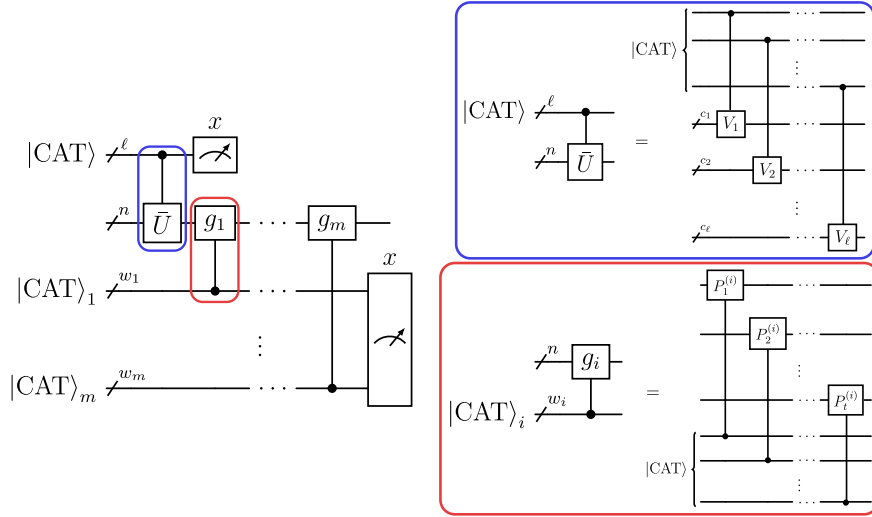


Figure 4.6: Shor-style measurement gadget. Measurement of a transversal logical PSC $\bar{U} = \bigotimes_{i=1}^l V_i$ for PSCs V_i controlled by a weight- ℓ $|\text{CAT}\rangle$ state is followed by Shor-style measurements of Pauli stabilizer generators $\{g_1, \dots, g_m\}$ where $g_i = \bigotimes_{j=1}^t P_j^{(i)}$ for single-qubit Paulis $P_j^{(i)}$ using weight- w_i $|\text{CAT}\rangle$ states.

3. **Flag-based.** A protocol is *flag-based* if the stabilizer/PSC measurements involve flag qubits; see Fig. 4.9 for an example measuring $\bar{H}$ on the Steane code.

For each type of protocol, we show that circuit-level Pauli errors propagate to Clifford errors with sufficiently-small gate descriptions, in effect enabling efficient simulation (since it is difficult to systematically cover all flag-based protocols, we only provide a general remark and an example.) At a high-level, we consider propagating a circuit-level error originating at a data or ancilla qubit and give a coarse upper bound on the one- and two-qubit gate count of the resulting Clifford error. In particular,

4.5 Error propagation in magic state preparation protocols

we show this upper-bound to be polynomial in the number of rounds of stabilizer and logical PSC measurements, the sparsity parameters w_q and w_c of parity-check matrix H , and the number of PSC tensor factors V_i in $\bar{U}$ [Definition 2].

Theorem 2. *Let w_c and w_q be the maximum row and column weight of a parity check matrix H . Consider a standard protocol consisting of $r = r_S + r_L$ rounds of stabilizer (r_S) and PSC (r_L) measurements. Any single-qubit circuit-level error propagates through this protocol to a Clifford error consisting of $O(r^2 w_q(w_c + \ell))$ one- and two-qubit Clifford gates, for ℓ the number of PSC tensor factors V_i in $\bar{U}$.*

We provide an in-depth proof of Theorem 2 in Appendix B.3.1. Given Theorem 2, we can straightforwardly extrapolate to an average-case upper-bound on the number of gates in a Clifford error due to propagating *all* sampled circuit-level errors. In particular, if a protocol circuit has M error locations, the one- and two-qubit gate count of the total propagated Clifford error scales as $O(Mr^2 w_q(w_c + \ell))$.

Corollary 1. *Consider a standard protocol consisting of $r = r_S + r_L$ rounds of stabilizer (r_S) and PSC (r_L) measurements, with M error locations. Any error configuration on these M error locations propagates through this protocol to an end-of-circuit Clifford error consisting of $O(Mr^2 w_q(w_c + \ell))$ one- and two-qubit Clifford gates.*

Additionally, the result from Theorem 2 naturally upper-bounds the size of a Clifford error propagated through a Shor-style protocol. For instance, a circuit-level error on a stabilizer measurement ancilla qubit will spread to at most a *single* data qubit rather than w_c qubits due to transversality of the stabilizer measurement. Likewise, an error on a PSC measurement ancilla qubit would also only spread to at most *single* data qubit instead of ℓ disjoint subsystems. As a result, the number of gates in a Clifford error propagated through a Shor-style protocol, originating from an ancilla qubit, would no longer have a dependence on w_c or ℓ . Hence we obtain the following result:

Corollary 2. *Consider a Shor-style protocol⁵ consisting of $r = r_S + r_L$ rounds of stabilizer (r_S) and PSC (r_L) measurements, with M' error locations. Any error config-*

⁵Corollary 2 holds similarly for Steane and Knill-type error correction.

uration on these M' error locations propagates through this protocol to a Clifford error consisting of $O(M'r^2w_q)$ one- and two-qubit Clifford gates.

One practical downside of using $|\text{CAT}\rangle$ states is its sizable ancilla overhead. Additionally, each $|\text{CAT}\rangle$ state has to be prepared and verified prior to performing measurements to maintain fault-tolerance [13]. If post-selection is being employed, this would mean incurring a much lower acceptance rate to prepare high-fidelity magic states.

As such in many practical scenarios, it is helpful to use flag qubits [65–68, 151]. Flag qubit-based syndrome measurement schemes are engineered to detect when low-weight (correctable) faults propagate to faults with weight larger than $\lfloor (d-1)/2 \rfloor$, for code distance d . More precisely, a circuit is called a *t-flag circuit* [151], for $t = \lfloor (d-1)/2 \rfloor$, if all $v \leq t$ circuit faults that propagate to an error weight $> v$ are detected. Hence, such a *t-flag circuit* would require *at most* t ancilla qubits to detect an adversarial spread of errors.

Once again, just like the standard and Shor-style FT protocols, circuit-level Pauli noise propagates to end-of-circuit Clifford errors with sufficiently-few one- and two-qubit gates. This is because flag-based methods only introduce additional controlled-Pauli gates and at most an extra t ancilla qubits per PSC measurement and stabilizer check. Indeed, we demonstrate a concrete example of such a flag-based PSC measurement protocol in Section 4.7.2.

In conjunction with the above results, we note that rules for error propagation can be conveniently packaged into a directed graph structure. Recall that logical PSC measurement protocols are comprised entirely of controlled-PSC gates $C(V)$ and controlled-Pauli gates $C(M)$. To this end, Fig. 4.7 specifies a complete set of recursive error propagation rules for circuit-level Pauli noise under these gates and shows that *only certain* Clifford errors are propagated through to the end of a PSC measurement-based protocol. Thus, the propagated error is necessarily Clifford.

A motivation for Fig. 4.7 is as follows: starting with Pauli errors (denoted by P), propagation through PSC measurements is given by Theorem 1. Subsequently, propagation of the resulting controlled-Pauli errors through future PSC and stabilizer

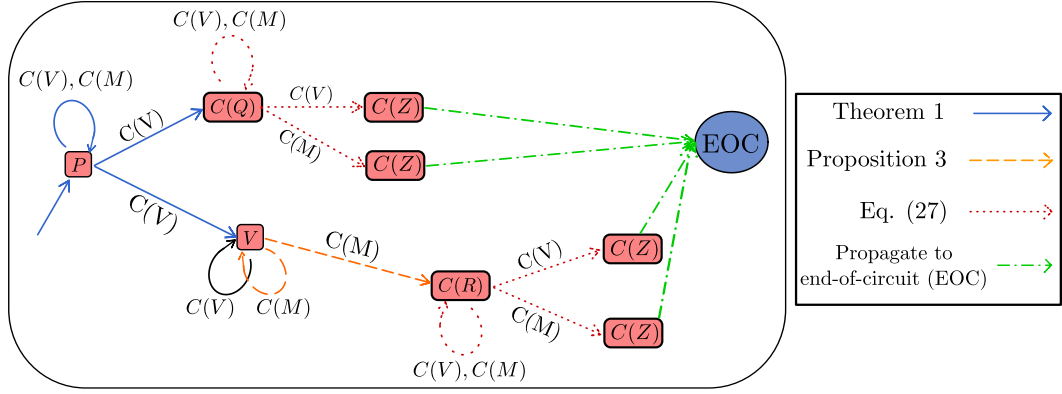


Figure 4.7: Error propagation rules for canonical PSC measurement protocols. Here, P is a Pauli and V is a PSC. $C(R)$ and $C(Q)$ are controlled-Paulis where Q and R either commute or anticommute with V . This diagram only shows nontrivial propagation of errors. For instance, an error (vertices) and a gate (edges) may have disjoint supports, in which case the error will remain the same. Such propagations are not included in this diagram.

measurements is given by Eq. (4.27), incurring $C(Z)$ gates between ancilla qubits. Since we consider a circuit model in which ancillas are never reused, these $C(Z)$ errors can trivially be commuted to the end of the circuit. Finally, PSC errors (denoted V) can be commuted past further stabilizer measurements by Proposition 3.

4.5.2 Canonical family 2: magic state distillation

Magic state distillation (MSD) protocols [18, 52–61] based on stabilizer codes also propagate circuit-level Pauli errors to an end-of-circuit Clifford error. In light of [160], all known MSD protocols can be recast using the Stabilizer Reduction formalism [161]. Indeed, given an $[[n, k, d]]$ stabilizer code, a decoder U_D consisting of Clifford operations acts on a k -qubit logical state $|\bar{\phi}\rangle$ as

$$U_D|\bar{\phi}\rangle = |\phi\rangle \otimes |0\rangle^{\otimes(n-k)}. \quad (4.29)$$

An n -to- k MSD protocol for such a code can be engineered by non-fault-tolerantly preparing n copies of the magic state as input $\rho_{in} = \rho_i^{\otimes n}$, followed by the application of the decoder U_D and by a final round of $n - k$ measurements in the Z basis. Upon post-selecting the +1 measurement outcomes, the protocol outputs a distilled k -qubit magic state $\rho_{out} = \text{Tr}_{anc}(U_D \tilde{\rho} U_D^\dagger)$ with higher fidelity, where $\tilde{\rho} \propto \Pi \rho_{in} \Pi$ and Π is the

projector onto the codespace.

MSD protocols described this way do not apply any non-Clifford gates during the distillation process. Instead, one only applies Clifford gates to non-Pauli stabilizer inputs. Thus, all circuit-level Pauli noise propagates to a Pauli error at the end. The fidelity of this noisy magic state can be estimated using extended stabilizer simulation, as we explain in more detail in Section 4.6. Importantly, the simulation cost is polynomial in the stabilizer rank/Pauli rank of the *output* logical magic state. Note that in many protocols of practical interest, e.g., 15-to-1 protocol [18], the stabilizer/Pauli rank of the output is significantly smaller than that of the input. Therefore, this observation may lead to faster simulation of magic state distillation protocols.

4.5.3 Canonical family 3: transversal non-Clifford gate

Another family of protocols that propagate circuit-level Pauli errors to an end-of-circuit Clifford error are those that rely on quantum error correcting codes admitting a transversal non-Clifford gate from the third level of the Clifford hierarchy. Examples of such codes are 3D color codes [81, 162, 163] and 3D surface codes [164], which admit transversal $\bar{T}$ and $\overline{CCZ}$ gates, respectively. In general, to realize universal quantum computation, such codes are not used alone as several no-go theorems restrict the set of available fault-tolerant, logical gates [20, 21]. Instead, one can use a *pair* of codes with a complementary, fault-tolerant, and universal set of logical gates to circumvent these restrictions. Namely, this is done by switching back and forth between them in a technique known as code-switching [1, 2, 69, 82, 83, 112]. For instance, MSP protocols can use 3D color codes to prepare a magic $|\bar{T}\rangle = \bar{T}|\bar{+}\rangle$ state fault-tolerantly, which can then be teleported to a 2D color code [1] using a transversal entangling gate between both codes [85, 86] [Fig. 4.8],

The structure of propagated Clifford errors for the family of MSP protocols described in Fig. 4.8 is simple. First, in a circuit-level noise model, the fault-tolerant preparation of the noisy $|\bar{+}\rangle$ state solely produces an initialization Pauli error frame P_I such that $|\bar{+}\rangle = P_I|\bar{+}\rangle_{\text{noiseless}}$, for a noiseless plus state $|\bar{+}\rangle_{\text{noiseless}}$. In binary repre-

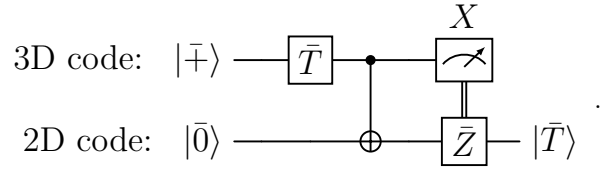


Figure 4.8: Code-switching protocol between 3D and 2D color codes to prepare logical $|\bar{T}\rangle$ states [1] (Chapter 2). The logical non-Clifford $\bar{T}$ gate is transversal in the 3D color code.

sensation, $P_I \sim \bigotimes_{i=1}^n X_i^{a_i} Z_i^{b_i}$ for $a_i, b_i \in \{0, 1\}$ (up to a global phase). Moreover, the transversal $\bar{T}$ gate in 3D color codes is such that

$$\bar{T} = \left(\bigotimes_{i \in A} T_i \right) \left(\bigotimes_{i \in A^C} T_i^\dagger \right), \quad (4.30)$$

for a disjoint partition $M = A \cup A^C$ of the set of physical qubits M of the 3D color code [162, 163]. The Clifford error frame $C_{\text{prop}}(P_I)$ is obtained upon propagating the Pauli error frame P_I through $\bar{T}$. Indeed,

$$\bar{T}|\bar{+}\rangle = (\bar{T}P_I\bar{T}^\dagger)\bar{T}|\bar{+}\rangle_{\text{noiseless}} = C_{\text{prop}}(P_I)|\bar{T}\rangle_{\text{noiseless}}, \quad (4.31)$$

where

$$C_{\text{prop}}(P_I) = \bar{T}P_I\bar{T}^\dagger = \left(\bigotimes_{i \in A} S_i^{a_i} \right) \left(\bigotimes_{i \in A^C} S_i^{b_i^\dagger} \right) P_I. \quad (4.32)$$

Hence, Eq. (4.31) shows that a logical $\bar{T}$ gate acting on a noisy $|\bar{+}\rangle$ state can be effectively described by a noiseless encoded logical magic state $|\bar{T}\rangle_{\text{noiseless}}$ subjected to a propagated Clifford error (4.32).

4.6 Fidelity estimation

In the previous Section, we showed how circuit-level Pauli noise propagates to a Clifford error on the final state [Fig. 4.1(b)] for various MSP protocols. In this Section, we give a detailed account on how to use the propagated Clifford error to estimate the fidelity of the output noisy logical magic state.

First, note that once errors are propagated to the end of the circuit, the noiseless

circuit containing non-Clifford gates can freely act on the initial logical state to prepare a *noiseless* logical magic state. Hence, the circuit can be effectively described as a noiseless logical magic state followed by the propagated Clifford error [Fig. 4.1(c)]. In order to estimate the fidelity of such a noisy magic state using stabilizer simulations, we must circumvent the inability of such simulators to encode a non-Pauli stabilizer state.

One approach is to decompose the magic state as a linear combination of stabilizer states, namely its stabilizer rank decomposition [Eq. (4.5)], and evolve each stabilizer state independently. We describe this method, which was originally proposed in Ref. [145], in further detail in Appendix B.5. This method keeps track of the global phase of stabilizer states, which is used to determine the relative phases needed in computing the overlaps between two such linear combinations of stabilizer states.

A second approach we consider relies on decomposing the magic state density matrix into a linear combination of Pauli matrices, namely its Pauli rank decomposition [Eq. (4.6)] (which can be further decomposed into a linear combination of stabilizer state projectors) [146]. This technique allows for simulating MSP protocols with a stabilizer simulator without the need to keep track of global phases. As such, it is readily applicable to commonly-used simulation tools such as **Stim** [96]. Although the technique was originally introduced in Ref. [1] for the special case of $|T\rangle$ states, here we provide a general framework suitable for arbitrary multi-qubit magic states.

We now describe how to efficiently estimate the fidelity $F = \text{Tr}(\bar{\rho}\bar{\rho}_N)$ of a noisy k -qubit logical state $\bar{\rho}_N$ with respect to a target logical pure state $\bar{\rho}$. The noisy logical state is defined as

$$\bar{\rho}_N = \mathcal{E}_L(\bar{\rho}) = (\mathcal{D} \circ \mathcal{E} \circ \mathcal{U})(\bar{\rho}), \quad (4.33)$$

for an effective logical noise channel $\mathcal{E}_L$. The channel $\mathcal{E}_L$ is composed of the encoding channel $\mathcal{U}$ which maps a logical k -qubit state onto an n -qubit state, a circuit-level noise channel $\mathcal{E}$ acting on an n -qubit state, and the decoding channel $\mathcal{D}$ that maps the noisy n -qubit state back onto a k -qubit logical state (up to a potential logical error).

Since k -qubit Pauli operators form a basis for $2^k \times 2^k$ complex-valued matrices, one

4.6 Fidelity estimation

can re-express the magic state $\bar{\rho}$ as a linear combination of them as in Eq. (4.6),

$$\bar{\rho} = \frac{1}{2^k} \bar{I}^{\otimes k} + \frac{1}{2^k} \sum_{i=1}^p \beta_i \bar{P}_i, \quad (4.34)$$

where $\bar{P}_i \in \{\bar{I}, \bar{X}, \bar{Y}, \bar{Z}\}^{\otimes k} \setminus \{\bar{I}^{\otimes k}\}$ and $\beta_i = \text{Tr}(\bar{\rho} \bar{P}_i)$. The number of non-trivial Paulis p is known as the *Pauli rank* of $\bar{\rho}$ [146]. Thus, by linearity of trace, it follows that

$$F = \frac{1}{2^k} + \frac{1}{2^k} \sum_{i=1}^p \beta_i \langle \bar{P}_i \rangle_{\bar{\rho}_N}, \quad (4.35)$$

for expected values $\langle \bar{P}_i \rangle_{\bar{\rho}_N} = \text{Tr}(\bar{P}_i \bar{\rho}_N)$. Recall that our goal is to efficiently estimate the fidelity F . Additionally, recall that we cannot specify non-stabilizer input states $\bar{\rho}_N$ in a stabilizer simulator. As such, we further decompose $\bar{\rho}_N$ into a linear combination of stabilizer state projectors. In particular, we can insert Eq. (4.34) into Eq. (4.33) and then further decompose each logical Pauli $\bar{P}_i$ into such a linear combination. First, we write each k -qubit Pauli $\bar{P}_i$ as a tensor product of single-qubit Paulis

$$\bar{P}_i = \bigotimes_{j=1}^k P_i^{(j)}, \quad (4.36)$$

where $P_i^{(j)} \in \{\bar{I}, \bar{X}, \bar{Y}, \bar{Z}\}$. Each single-qubit Pauli $P_i^{(j)}$ is thus either the identity or a non-convex combination of Pauli stabilizer states

$$\bar{X} = |\bar{+}\rangle\langle\bar{+}| - |\bar{-}\rangle\langle\bar{-}|, \quad (4.37)$$

$$\bar{Y} = |\bar{Y}_+\rangle\langle\bar{Y}_+| - |\bar{Y}_-\rangle\langle\bar{Y}_-|, \quad (4.38)$$

$$\bar{Z} = |\bar{0}\rangle\langle\bar{0}| - |\bar{1}\rangle\langle\bar{1}|, \quad (4.39)$$

$$\bar{I} = |\bar{s}\rangle\langle\bar{s}| + |\bar{s}^\perp\rangle\langle\bar{s}^\perp|, \quad \langle\bar{s}|\bar{s}^\perp\rangle = 0, \quad (4.40)$$

for $|\bar{s}\rangle$ a Pauli stabilizer state (for instance, $|\bar{s}\rangle = |\bar{+}\rangle$ and $|\bar{s}^\perp\rangle = |\bar{-}\rangle$). Therefore, a non-trivial Pauli $\bar{P}_i$ can be written as a *non-convex* combination of tensor products of

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Pauli stabilizer states

$$\bar{P}_i = \sum_{l=1}^{2^k} (-1)^{\gamma_l} \left(\bigotimes_{j=1}^k |\bar{s}_l^{(j)}\rangle \langle \bar{s}_l^{(j)}| \right) = \sum_{l=1}^{2^k} (-1)^{\gamma_l} \Pi_l^i, \quad (4.41)$$

where $\gamma_l \in \{0, 1\}$, $|\bar{s}_l^{(j)}\rangle \langle \bar{s}_l^{(j)}|$ is a single logical-qubit stabilizer state projector acting on the j -th logical qubit and Π_l^i is a k -qubit stabilizer state projector, both corresponding to the l -th term of the decomposition associated to $\bar{P}_i$. Hence, by the linearity of trace and the logical noise channel $\mathcal{E}_L$,

$$\langle \bar{P}_i \rangle_{\bar{\rho}_N} = \frac{1}{2^k} \sum_{j=1}^p \sum_{l=1}^{2^k} (-1)^{\gamma_l} \langle \bar{P}_i \rangle_{\mathcal{E}_L(\Pi_l^j)}, \quad (4.42)$$

where $\langle \bar{P}_i \rangle_{\mathcal{E}_L(\Pi_l^j)} = \text{Tr}(\mathcal{E}_L(\Pi_l^j) \bar{P}_i)$. Finally, the fidelity (4.35) can be written as

$$F = \frac{1}{2^k} + \frac{1}{4^k} \sum_{i,j=1}^p \sum_{l=1}^{2^k} \beta_i \beta_j (-1)^{\gamma_l} \langle \bar{P}_i \rangle_{\mathcal{E}_L(\Pi_l^j)}. \quad (4.43)$$

Thus, to estimate the fidelity of the noisy logical magic state $\bar{\rho}_N$, it suffices to run $O(p^2 2^k)$ different logical stabilizer circuits subjected to a propagated Clifford error. This is quadratic in the Pauli rank and exponential in the number of logical qubits.

As a concrete example, consider the $k = 1$ magic state $|\bar{T}\rangle \langle \bar{T}|$ with Pauli rank $p = 2$, which can be written as

$$|\bar{T}\rangle \langle \bar{T}| = \frac{1}{2} \bar{I} + \frac{1}{2\sqrt{2}} (\bar{X} + \bar{Y}). \quad (4.44)$$

The fidelity (4.43) has the following expression [1]

$$F_{|\bar{T}\rangle \langle \bar{T}|} = \frac{1}{2} + \frac{1}{8} \Delta, \quad (4.45)$$

where

$$\begin{aligned} \Delta = & \langle \bar{X} \rangle_{|\bar{+}\rangle} - \langle \bar{X} \rangle_{|\bar{-}\rangle} + \langle \bar{X} \rangle_{|\bar{Y}_+\rangle} - \langle \bar{X} \rangle_{|\bar{Y}_-\rangle} \\ & + \langle \bar{Y} \rangle_{|\bar{+}\rangle} - \langle \bar{Y} \rangle_{|\bar{-}\rangle} + \langle \bar{Y} \rangle_{|\bar{Y}_+\rangle} - \langle \bar{Y} \rangle_{|\bar{Y}_-\rangle} . \end{aligned} \quad (4.46)$$

In the last equation, the lower index $|\bar{s}\rangle$ stands for $\mathcal{E}_L(|\bar{s}\rangle\langle\bar{s}|)$, where the $|\bar{s}\rangle$ states are $|\bar{s}\rangle \in \{|\bar{+}\rangle, |\bar{-}\rangle, |\bar{Y}_+\rangle, |\bar{Y}_-\rangle\}$.

4.7 Simulation overview

Having described the families of MSP protocols that propagate circuit-level Pauli errors to an end-of-circuit Clifford error in Section 4.5 and a fidelity estimation method in Section 4.6, in this Section we provide a holistic overview of our simulation technique (including a summary in Section 4.7.1). In Section 4.7.2, we present a proof-of-principle numerical simulation of a MSP protocol that measures a transversal Clifford operator. Finally, in Section 4.7.3, we analyze the space and time complexity of our method.

4.7.1 Summary

Below, we provide an executive summary of our simulation technique.

Protocol definition: MSP protocol, specified as a sequence of one- and two-qubit unitaries $\{U_i\}$ with $U_i \in \mathcal{C}^{(2)}$ or $\mathcal{C}^{(3)}$, acting on a logical input state $|\bar{\psi}\rangle$ to produce a logical magic output state $|\bar{\phi}\rangle$ ⁶ such that $\prod_i U_i(|\bar{\psi}\rangle \otimes |a\rangle) = |\bar{\phi}\rangle \otimes |a\rangle$ for an ancilla register $|a\rangle$. Deferred projective measurements in the Pauli basis $\{M\}$ [Fig. 4.1].

Simulation input: MSP protocol. Circuit-level noise model of strength p , accounting for initialization P_I , gate-specific $\{P_i\}$ and measurement P_M errors [Appendix B.1].

Total number of Monte Carlo shots N_{tot} .

⁶For protocols based on measurements of a logical PSC, the encoded state $|\bar{\psi}\rangle$ is equal to the output logical magic state $|\bar{\phi}\rangle$ stabilized by the PSC. For code-switching protocols described in this chapter, $|\bar{\psi}\rangle = |\bar{+}\rangle$ which differs from the the output magic state $|\bar{\phi}\rangle$.

Simulation Output: Fidelity $F = \langle \bar{\phi} | \bar{\rho}_N | \bar{\phi} \rangle = \text{Tr}(\bar{\rho} \bar{\rho}_N)$ of the output logical noisy magic state $\bar{\rho}_N$ with respect to the noiseless logical $\bar{\rho} = |\bar{\phi}\rangle\langle\bar{\phi}|$ magic state. Acceptance rate $p_{\text{acc}} = N_{\text{acc}}/N_{\text{tot}}$, for a number of accepted (pre-selected) shots N_{acc} .

Simulation Method:

- **Error sampling [Fig. 4.1(a)]:** Sample circuit-level Pauli errors at every location; see Appendix B.1 for the error model. Of N_{tot} samples, a fraction f [Eq. (4.47)] of them contain non-trivial errors (non-identity Pauli strings).
- **Error propagation [Fig. 4.1(b)]:** If non-trivial circuit-level Pauli errors are sampled, propagate these errors to an end-of-circuit Clifford error C_{prop} [Fig. 4.1(b)].⁷

Upon error propagation, circuits containing non-Clifford gates can be effectively described by a noiseless logical magic state $|\bar{\phi}\rangle \otimes |a\rangle$ subjected to a Clifford error C_{prop} [Fig. 4.1(c)].

- **State decomposition [Fig. 4.1(d)]:** Decompose the noiseless logical magic state into a form that enables stabilizer simulation. For instance, $\bar{\rho} = |\bar{\phi}\rangle\langle\bar{\phi}|$ may be decomposed into a linear combination of logical Pauli matrices [Eq. (4.6)], which can be further decomposed as a linear combination of logical stabilizer projectors. Alternatively, $|\bar{\phi}\rangle$ may be decomposed into a linear combination of stabilizer states [Eq. (4.5)].
- **Stabilizer-based simulation:** Apply the Clifford error C_{prop} to a stabilizer state appearing in the aforementioned decomposition. Simulate measuring the $|a\rangle$ register, sampling over the post-selected state. The logical error rate can be expressed as a linear combination of random variables that can be computed from such states and the noiseless magic state $|\bar{\phi}\rangle$; see Section 4.6 and Appendix B.5 for details. Take the sum of each expected value and renormalize by the acceptance rate p_{acc} , which yields the logical error probability.

⁷In practice, it is enough to propagate Clifford errors up the last U_i that belongs to $\mathcal{C}^{(3)}$.

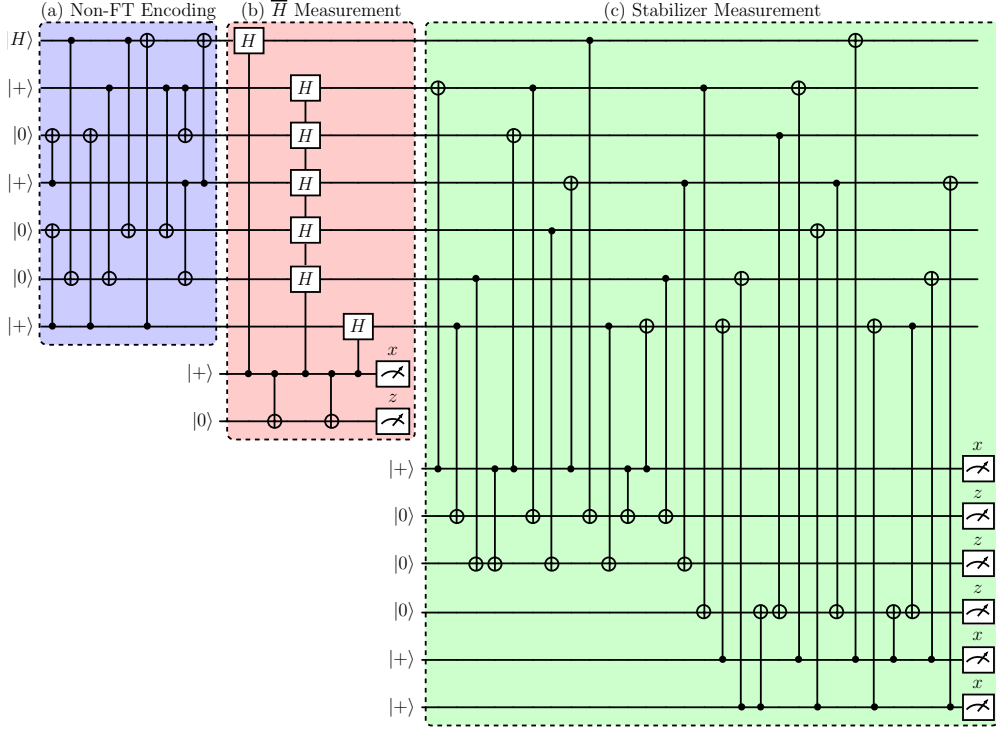


Figure 4.9: Magic $|\bar{H}\rangle$ state preparation protocol on the $[[7,1,3]]$ Steane code. (a) Implements a unitary non-fault-tolerant encoding of the magic state $|\bar{H}\rangle$. (b) Measures the $\bar{H}$ operator using a 1-flag fault-tolerant gadget. (c) Performs a final round of fault-tolerant stabilizer measurements. Steps (b) and (c) correspond to a flag-based measurement with $(r_L, r_S) = (1, 1)$. For the purposes of simulation, measurements are deferred to the end of the circuit and shots are post-selected on +1 outcomes. See Figs. 4.10 and 4.11 for numerical results from simulating this protocol.

4.7.2 Numerical results: $|\bar{H}\rangle$ state preparation on the Steane code

As a proof-of-principle demonstration, we consider an MSP protocol [97, 101, 152] that prepares an $|\bar{H}\rangle$ state [Eq.(4.2)] stabilized by the Hadamard operator $\bar{H}$ in the $[[7,1,3]]$ Steane code [98]; see Fig. 4.9 for the circuit description of this protocol. This protocol is composed of a non-FT encoding of $|\bar{H}\rangle$ followed by a flag-based measurement of $\bar{H}$ with $r_L = 1$ PSC and $r_S = 1$ stabilizer measurement rounds, respectively. We compare our phase-insensitive simulation technique with a state-vector simulation and achieve comparable results with sizable runtime improvements; see Figs. 4.10 and 4.11). The slight difference in fidelity at low error rates is due to finite sampling effects.

We make a few remarks about our simulation. First, our phase-insensitive simulations rely on an explicitly-defined distribution for the propagated Clifford errors C_{prop}

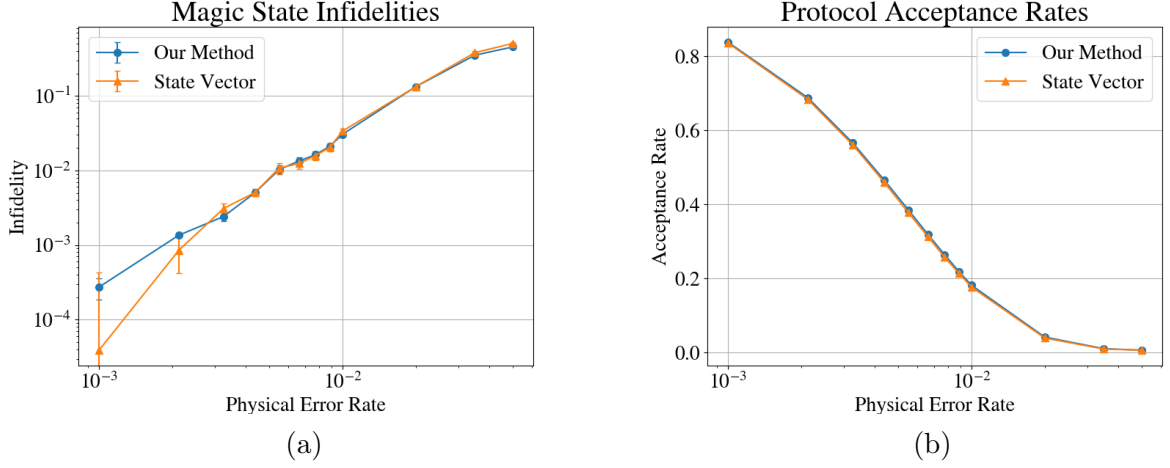


Figure 4.10: Numerical simulations for the magic state $|\bar{H}\rangle$ preparation protocol on the $[[7, 1, 3]]$ Steane code under uniform circuit-level noise with physical error rate p . Numerical simulations were performed with our phase-insensitive technique for $\bar{\rho} = |\bar{H}\rangle\langle\bar{H}|$ using the stabilizer-based simulator Stim [96] (blue) and for $|\bar{H}\rangle$ using the state-vector simulator Cirq [165] (orange). (a) Infidelity of the magic state as a function of the physical error rate p . At lower error rates, results from state-vector simulations slightly deviate from results from our technique due to finite sampling effects. (b) Acceptance rate as a function of the physical error rate p . We observe that the numerical results coincide for both simulation techniques. A comparison of the runtime for both simulation techniques can be found in Fig. 4.11. Error bars correspond to one standard deviation. The number of shots employed for the stabilizer-based simulations was $N_{tot} \in [10^5, 10^7]$ and $N_{tot} \in [10^5, 10^6]$ for the state-vector simulations.

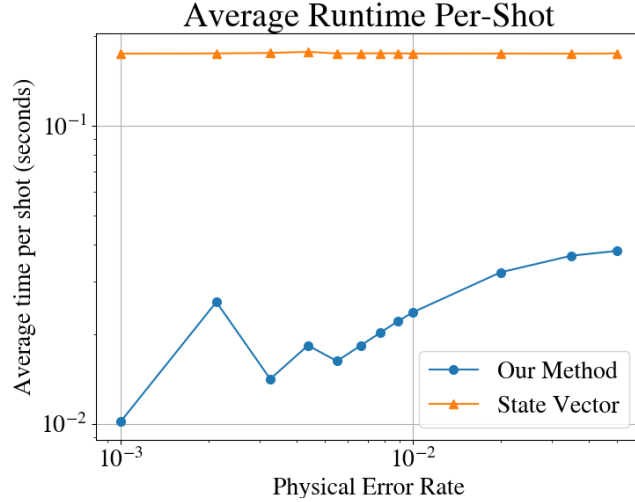


Figure 4.11: Average time per-simulation shot (in seconds) as a function of physical error rate p for the magic state $|\bar{H}\rangle$ preparation protocol on the $[[7, 1, 3]]$ Steane code. We observe an approximately $10\times$ improvement on the runtime of our technique (blue) compared to state-vector simulations (orange) for $p = 10^{-3}$.

under circuit-level noise; see Appendix B.4 for details. Since obtaining an analytic formula for the propagated Clifford error is tedious in general (for an error propagation algorithm, refer to [3]).

Second, in the simulation, on average only a small fraction of the simulation samples will have a nontrivial circuit-level error configuration. Let M be the number of error locations. The expected fraction of samples that will contain an error f is

$$f = 1 - (1 - p)^M \approx Mp, \quad (4.47)$$

for some small error probability p . For instance, if $M = 100$ and $p = 10^{-3}$, one would expect 10% of the samples to have non-trivial error configurations. The remaining samples need not require further processing.

Third, in `Stim` [96], propagating errors that occur while encoding a logical magic state (prior to measuring them) can be done using the `peek_pauli_flips()` function in the `FlipSimulator()` class. More precisely, for fidelity estimation [Section 4.6], one would plug in a set of stabilizer states corresponding to the stabilizer/Pauli rank decomposition of a magic state. For each such stabilizer state, error propagation can be performed with these functions, using the error model associated to the magic state [Appendix B.1].

Lastly, the main practical bottleneck of this approach, both in numerical simulations and hardware experiments involving magic states, is the sampling cost associated to the computation of Pauli expectation values necessary to estimate the fidelity. This is because these expectations have variance $O(1)$ since magic states are not eigenstates of logical Pauli operators. Indeed, the fidelity F of magic states can be estimated as $F = 1 - O(1/\sqrt{N_{\text{tot}}})$ for a total number of sampled shots N_{tot} , which is in stark contrast with the fidelity of Pauli eigenstates $F = 1 - O(1/N_{\text{tot}})$ [166]⁸. The phase-sensitive method can overcome this bottleneck in principle [Appendix B.5], but we leave the implementation of this idea for future work.

For numerical examples of simulations for code-switching, we refer to Chapter 2 for a distance 3 realization of Fig. 4.8.

⁸Recently, [2] proposed a method to overcome this constraint by giving a lower bound $F \geq 1 - O(1/N_{\text{tot}})$ with quadratic improvement in sampling complexity at the expense of storing *two copies* of the logical magic state and performing a logical Bell sampling; see also Ref. [123].

4.7.3 Complexity

We discuss the simulation complexity of our methods. Let n_{tot} be the total number of data and ancilla qubits the protocol acts on. We assume the protocol is defined by a measurement schedule consisting of r rounds of measurements of either logical PSC or stabilizer measurements. Stabilizer measurements are defined in terms of a parity check matrix H , whose maximum row and column weights are w_c and w_q , respectively. Finally, let M denote the number of locations on which a Pauli error can occur.

We make the following simplifying assumptions. First, we focus on the standard protocol for measurements [Section 4.5.1]. Second, we bound the number of tensor factors appearing in the logical PSC [Definition 2] with n_{tot} . A tighter bound on the complexity may be obtained by noting that (i) the number of tensor factors of the logical PSC is strictly smaller than n_{tot} and (ii) the gate complexity of the propagated Clifford error in fault-tolerant protocols is lower [Corollary 2]. We do not discuss such details here.

Let us now discuss the time complexity of the two methods, the phase-insensitive method based on the Pauli rank decomposition [Section 4.6] and the phase-sensitive method based on the stabilizer rank decomposition [Appendix B.5]. For both methods, each sample in a Monte Carlo simulation can be obtained by propagating a randomly sampled circuit-level error configuration to an end-of-circuit Clifford error. A conservative bound on the time complexity of obtaining this Clifford error is $O(Mr^3w_q^2n_{\text{tot}}^2)$ [3]. Furthermore, each such propagated error consists of at most $O(Mr^2w_qn_{\text{tot}})$ one- and two-qubit Clifford gates [Corollary 1].

One approach to obtain the Clifford error is by sequentially pushing sampled circuit-level errors through the protocol circuit from left-to-right to obtain an end-of-circuit Clifford error. A second approach, which we assume here, is to *individually* propagate circuit-level errors at each of the M error locations to a corresponding end-of-circuit Clifford error. These Clifford errors are then combined (in an appropriate order) to obtain the full end-of-circuit Clifford error. For either approach, this error can then be expressed as either a combined Clifford tableau (in the phase-insensitive method) or

as a sequence of one- and two-qubit gates (in the phase-sensitive method).

Subsequently, we describe the complexity of obtaining Monte Carlo samples for each of the two simulation methods. Note, these complexities do not include the one-time cost for constructing a look-up table that takes in as input an error location and a circuit-level error at that location and returns an end-of-circuit propagated Clifford error. In principle, such a look-up table can be constructed on a case-by-case basis using propagation rules as defined in Fig. 4.7.

Phase-insensitive method: For the Pauli rank-based method [Section 4.6], it is convenient to store each of the propagated errors in the standard stabilizer tableau representation [142]. Combining these for the M error locations would incur an additional $O(Mn_{\text{tot}}^3)$ time cost. This is the complexity needed for each sample.

Note that for this method, there are additional parameters needed to specify the complexity. Let p be the Pauli rank of the k -qubit logical magic state. To compute the fidelity of the noisy logical magic state, we require computing p Pauli expectation values, each of which requires simulating $O(p2^k)$ Clifford circuits (comprised of the encoding circuit, the end-of-circuit Clifford error, and final measurements) on stabilizer state inputs. Therefore, to estimate the fidelity up to an additive error ϵ , it suffices to have $O(p^2 2^k / \epsilon^2)$ samples. Thus the overall time cost is $O(p^2 2^k M n_{\text{tot}}^3 / \epsilon^2)$.

Phase-sensitive method: For the stabilizer rank-based method [Appendix B.5], it is convenient to store each of the propagated errors as a sequence of one- and two-qubit Clifford gates. The number of gates in the combined end-of-circuit Clifford error is $O(Mr^2 w_q n_{\text{tot}})$. Moreover, updating the stabilizer rank decomposition for each of these gates takes time at most $O(n_{\text{tot}}^2)$ [145]. Thus the complexity needed for each sample is $O(Mr^2 w_q n_{\text{tot}}^3)$.

Let q be the stabilizer rank of the logical magic state. To estimate the logical error rate up to an additive precision of ϵ , it suffices to have $O(1/\epsilon)$ samples [Appendix B.5]. For each such sample, the needed computation boils down to (i) updating q stabilizer states using the aforementioned method and (ii) computing the overlap with q stabilizer states. It is straightforward to see that the former costs $O(qMr^2 w_q n_{\text{tot}}^3)$. For the latter,

note that each overlap can be computed in $O(n_{\text{tot}}^3)$ time [145, Lemma 3, 4]. Thus, the overall time cost becomes $O(q^2 n_{\text{tot}}^3)$. In the $q = O(1)$ regime, the overall time complexity is $O(Mr^2 w_q n_{\text{tot}}^3 / \epsilon)$.

Comparison: These two methods have differing complexities and are incomparable at the moment. Nonetheless, the key point is that these methods have time and space complexity polynomial in the parameters that define the MSP protocol (except for the exponential dependence on k for the phase insensitive case). This is in stark contrast with expensive state-vector simulation, whose cost scales exponentially with n_{tot} .

Finally, the additive error of the fidelity also determines the overhead complexity in each case, which in practice represents a fundamental limitation for the simulations. Concretely, one may consider the task of estimating the logical error rate p_L up to (say) one standard deviation. For this task, the phase-sensitive method requires $O(1/p_L)$ independent samples whereas the phase-insensitive method requires $O(1/p_L^2)$ independent samples.

4.8 Conclusion

In this chapter, we introduce a new method for simulating logical MSP protocols under circuit-level noise. Our method is applicable to a broad range of protocols, including cultivation-style methods [68, 70, 71, 101, 136–138, 152], magic state distillation at the logical level [18, 52–61] and code-switching [1, 69, 82, 83, 112]. Thus, our work provides a flexible, accurate, and efficient method to benchmark these protocols.

We expect our method to enable the following studies, which we leave for future work. First, we may be able to address an open question concerning magic state cultivation [71]: the relationship between the fidelity of the prepared magic state and that of a closely related stabilizer state. Because there was no known method to simulate these protocols efficiently at large code distances, the ratio between the two at small code distance ($d = 3$) was used to deduce the magic state fidelity at higher distances. It may be possible to rigorously test the validity of this assumption using

our method.

In order to do so, we will need to develop a software toolkit capable of executing large-scale simulations of MSP protocols. One practical complication resides in the implementation of a general purpose efficient error propagation algorithm. For instance, the Clifford error cannot naively be stored in its tableau representation since propagation rules through non-Clifford gates are cumbersome to implement without an explicit circuit representation. Another approach consists of storing the Clifford error as an ordered list of gates, where propagation rules can be defined and applied layer by layer.

To efficiently obtain many samples of propagated errors, one can pre-compute propagated errors for each error location in a protocol circuit and store them in a table as Clifford tableaus. This one-time cost, although initially expensive, will not contribute to the per-shot runtime complexity as propagated errors for each sampled error configuration can be quickly constructed via a few cheap accesses to the pre-computed table. However, the implementation of such a software toolkit is beyond the scope of this article and its development is left for future work.

Second, we may be able to gain an analytic understanding of circuit-level Pauli noise in the presence of non-Clifford gates. The most striking effect of these gates is that a single-qubit Pauli error can propagate to an *entangling Clifford error*; see Fig. 4.4 for an example. Inspecting the form of the propagated errors may be helpful to further optimize quantum error correction protocols involving non-Clifford gates. In particular, it is important to understand the effectiveness of flag gadgets in the presence of these entangling Clifford errors [65–67].

One intriguing possibility is that one may be able to decode errors better by taking the error propagation rule into account. In the presence of an entangling Clifford error, measurement of a syndrome qubit induces a projective measurement on a subset of data qubits in some known basis. For instance, if there is a CZ error between a data qubit and a syndrome qubit, measuring the syndrome qubit in the X -basis induces a Z -basis measurement of the data qubit, wherein the post-measurement state of the data qubit is completely determined by the X -basis measurement. This extra information may be

useful for the decoder. We leave such studies for future work.

We also leave the following open questions for future work. One question is whether our method can be generalized to alternative protocols. For instance, it is possible to apply a non-Clifford gate by viewing a three-dimensional protocol involving a transversal non-Clifford gate as a two-dimensional protocol [157, 167–169] evolving in time (under some additional conditions). In these methods, the syndrome measurements cannot be deferred to the end, making our current simulation technique inadequate. We also note that these protocols can be viewed as fault-tolerant gates of recently studied Clifford stabilizer codes [157, 168], which are in fact generated by PSCs. Can the special properties of PSCs [Section 4.4] let us extend the stabilizer formalism to such Clifford stabilizers? Another family of protocols one may consider is a cultivation-style protocol involving Cliffords that do not square to a Pauli [137]. It is unclear if a central insight of this chapter — propagation of circuit-level Pauli noise to a Clifford — is valid in such protocols.

Lastly, we remark that our method is useful only for methods that prepare a small amount of magic. How to efficiently simulate magic state preparation protocols that can produce a large amount of magic [170–173] remains an interesting open question.

Chapter 5

Real-time adaptation of quantum noise channel estimates

In this chapter, we study the characterization of noise channels associated with quantum gates in a quantum computer and introduce a method to update its estimates in real-time. Notoriously, estimates of noise channels for quantum gates are required for most error mitigation techniques and are desirable for informing quantum error correction decoders. These estimates can be obtained by resource-intensive off-line characterization techniques, but can become stale due to device drift and fluctuations. We propose a method to address this issue by performing real-time adaptation of noise channel estimates during the execution of a quantum algorithmic circuit using extended flag gadgets, mid-circuit measurements and Bayesian inference. We carry out analytical calculations and numerical simulations employing a Dirichlet prior distribution for the error rates in a Pauli channel to demonstrate and evaluate the technique, which can be seen as a protocol for real-time calibration of high-level gate error information.

5.1 Introduction

Precise understanding of noise in quantum computers is essential for the continued maturation of quantum computing technology and for extracting algorithmic utility from these devices. In the near-term, error mitigation techniques, such as probabilistic

error cancellation (PEC) and Richardson extrapolation [174], which aim to extend the computational utility of noisy quantum computers [175], benefit from precise characterization of device noise. Looking into the future, knowledge of device noise and its variation in time and space will be critical for efficient error decoding and correction in error-corrected and fault-tolerant devices.

Although precise error characterization at the gate-level is possible using tools such as gate set tomography (GST) [22] and Pauli channel estimation [23], these techniques are time-consuming and are typically run infrequently. As a result, the descriptions of noise that they deliver might become inaccurate due to device and control drift during the execution of an algorithm. In fact, it has recently been noted that maintaining the accuracy of characterized noise models is challenging in the presence of device fluctuations such as those caused by uncontrolled two-level systems in superconducting devices, and that this limits the effectiveness of PEC [176, 177].

In this chapter, we propose a method to adapt noise channel estimates in *real-time*, during the execution of an algorithm. The technique relies on intermediate measurements using *extended flag gadgets* [24, 25], which provide information about gate errors while being non-intrusive and not interrupting algorithm execution. The idea of adapting noise channel estimates for more accurate PEC was also pursued by Dasgupta and Humble [177], however their technique relied on inference of noise parameter changes from a measurement of all qubits at the output of a circuit and so is not designed to non-intrusively adapt the noise channel estimates during execution of an algorithm. In addition, Gao *et al.* have proposed the idea of using information from extended flag gadgets to collect coarse-grained error information about a quantum processor in real time [178]. While we discuss our real-time adaptation technique in the context of near-term devices and PEC, we note that the same principles could be used to track changes in device noise in early fault-tolerant, error-corrected devices and inform decoding algorithms. Finally, we note that our method could be viewed as a real-time calibration tool, where the calibration is not of device or control parameters, but of the description of the quantum channel induced by gate noise.

The rest of this chapter is organized as follows. Section 5.2 provides some background material: Section 5.2.1 describes the error model, and Section 5.2.2 introduces flag gadgets. Section 5.3 presents our main findings regarding noise channel adaptation using flag gadgets. This is further subdivided: Section 5.3.1, formulates Bayesian inference rules based on flag gadget measurements. Section 5.3.2, describes the Dirichlet distribution used as the prior for the Bayesian inference. Section 5.3.3, analyzes the special case when the number of flag gadget layers is maximal. Section 5.3.4, provides exact update rules for generic flag gadgets, and Section 5.3.4 discusses an approximation to such exact inference rules. Section 5.3.5, studies the realistic scenario when noise is introduced by the flag gadgets. Finally, Section 5.4 is a discussion of the results, possible extensions, and conclusion. Appendix C.1 and C.2 provide additional information about flag gadgets and the approximate update rule. Appendix C.3 provides information about the numerical methods.

5.2 Background material

5.2.1 Error model

To account for the presence of errors in a given quantum circuit, we model the implementation of every noisy gate acting on a quantum state ρ as an ideal gate U with action $\rho_U = U\rho U^\dagger$, followed by an error channel Λ ,

$$\Lambda(U\rho U^\dagger) = \Lambda(\rho_U) . \quad (5.1)$$

The error channel Λ can be generically represented as a completely-positive trace-preserving (CPTP) map, acting on ρ_U as [179]

$$\Lambda(\rho_U) = \sum_i E_i \rho_U E_i^\dagger, \quad \sum_i E_i^\dagger E_i = 1 , \quad (5.2)$$

5.2 Background material

with Kraus operators E_i , labeled by a natural number $i \in [1, 4^{n_q}]$ for a n_q -qubit channel. In practice, we do not need to deal with such a generic error model. Indeed, error mitigation techniques such as PEC and Richardson extrapolation are less effective in the presence of such general error models. Instead, one typically uses randomized compiling [180] to convert the error channel into a purely stochastic Pauli channel,

$$\tilde{\Lambda}(\rho_U) = \sum_i \lambda_i P_i \rho_U P_i^\dagger, \quad \sum_i \lambda_i = 1, \quad (5.3)$$

with real coefficients $0 \leq \lambda_i \leq 1$ (again labeled by a natural number $i \in [1, 4^{n_q}]$) and Pauli matrices P_i belonging to the n_q -qubit Pauli group (up to a phase) $\mathcal{P}_{n_q} = \{I, X, Y, Z\}^{\otimes n_q}$, defined as the tensor product of single-qubit Pauli matrices I, X, Y, Z . Throughout this chapter, our main objective will be to update in real-time the estimated values of the Pauli coefficients λ_i for every noisy gate.

The mechanics of the Pauli twirling operation that underlies randomized compiling consist of applying elements of the Pauli group and their respective adjoint, before and after the error channel in place [181–183]

$$\frac{1}{|\mathcal{P}_{n_q}|} \sum_{P_i \in \mathcal{P}_{n_q}} P_i^\dagger \Lambda(P_i \rho_U P_i^\dagger) P_i = \tilde{\Lambda}(\rho_U), \quad (5.4)$$

where $|\mathcal{P}_{n_q}| = 4^{n_q}$ is the cardinality of the Pauli group. Since we cannot apply the error channel by itself, but only the full noisy gate, the actual operational twirling procedure applies a Pauli gate $P_i^\dagger$ after the gate, and an ideal gate conjugated Pauli before the gate, $\tilde{P}_i = U^\dagger P_i U$:

$$\begin{aligned} \frac{1}{|\mathcal{P}_{n_q}|} \sum_{P_i \in \mathcal{P}_{n_q}} P_i^\dagger \Lambda(U \tilde{P}_i \rho U^\dagger) P_i &= \tilde{\Lambda}(U \rho U^\dagger) \\ &= \tilde{\Lambda}(\rho_U). \end{aligned} \quad (5.5)$$

Notice that $\tilde{P}_i$ is a Pauli gate in case that U is a Clifford gate [179, 184]. In randomized compiling these extra Pauli gates are compiled into the circuit such that the overall circuit depth does not increase [180].

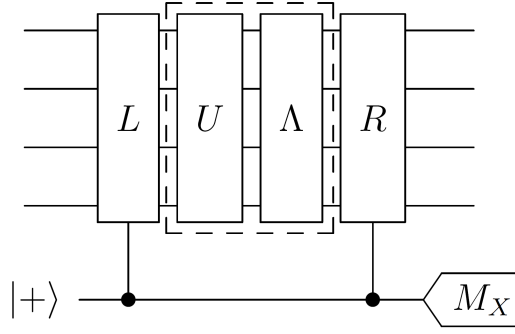


Figure 5.1: Flag gadget acting on a noisy gate (dashed region: represented as a noiseless gate U followed by a noise channel Λ). The gadget consist of an ancilla qubit prepared on the $|+\rangle$ state, followed by two controlled gates with unitaries left(L)/right(R), respectively, as well as a final measurement on the X -basis.

5.2.2 Flag gadgets

The general purpose of this section is to revisit a method to extract information from the noise channel Λ associated with a noisy gate, without disturbing the action of the gate. To accomplish this task, we utilize *flag gadgets* [24, 25, 66, 102, 151, 178, 185, 186], which were originally introduced to flag/detect higher-weight errors introduced by stabilizer circuit measurements in quantum error correcting codes [66, 102, 151]. The flag gadgets, see Fig. 5.1, consist of an auxiliary ancilla prepared in the state $|+\rangle$, along with two controlled gates labeled by the unitaries that act on the data qubits before (L) and after (R) an operation. Finally, the ancilla is measured in the X -basis.

Given a noiseless unitary gate U , if the condition

$$RUL = U, \quad (5.6)$$

holds, the gate U can be pushed through the left controlled gate in such a way that the gadget is effectively acting on the noise channel Λ , see Fig. 5.2. For practical ease, we will choose R to be a Pauli matrix, $R \in \mathcal{P}_{n_q}$. It is clear from Fig. 5.2 that if the noise is trivial, i.e., $\Lambda = I$, the action of the flag gadget is also trivial in the state ρ . Therefore, in a generic noisy scenario, we expect to answer a fundamental question: *what information do the flag gadget measurements provide about the error channels?*

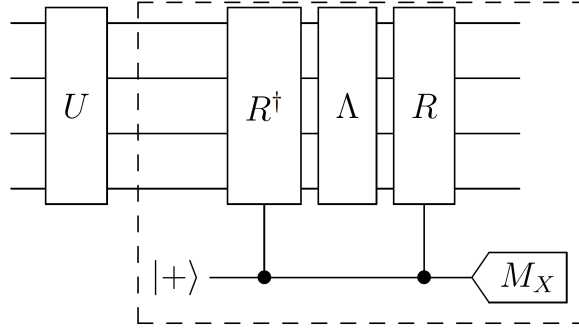


Figure 5.2: Flag gadget equivalent to Fig. 5.1, due to the relation (5.6). In case the error channel is also a Pauli channel $\tilde{\Lambda}$ (5.3), the dashed region acts as an effective Pauli channel $\tilde{\Lambda}_\pm(\rho_U; \vec{\lambda})$ (5.13), where the dependence on the measurement outcome $m_X = \pm 1$ is emphasized.

Initially, we will consider the ancilla preparation/measurement as well as the action of the controlled unitaries to be noiseless. We will discuss the impact of noisy flag gadgets in Section 5.3.5.

Upon introducing the extra ancilla in the plus state, the whole system is represented by the quantum state $\rho \otimes |+\rangle\langle+|$. Afterwards, the action of the flag gadget in Fig. 5.1 on the initial state ρ , yields a post-measurement state $\rho_{\text{post}}^\pm$ dependent on the measurement outcome $m_X = \pm 1$. In particular, if the error channel Λ is described by a CPTP map (5.2), the post-measurement state is [25]

$$\rho_{\text{post}}^\pm = \frac{\sum_i E_i^\pm \rho_U E_i^{\pm\dagger}}{\text{Tr}(\sum_i E_i^\pm \rho_U E_i^{\pm\dagger})}, \quad (5.7)$$

where $\rho_U = U\rho U^\dagger$ and $E_i^\pm$ is defined as

$$E_i^\pm = \frac{E_i \pm R E_i R^\dagger}{2}. \quad (5.8)$$

The probability of obtaining $\rho_{\text{post}}^\pm$ is, respectively,

$$p(m_X = \pm 1) = \text{Tr} \left(\sum_i E_i^\pm \rho_U E_i^{\pm\dagger} \right). \quad (5.9)$$

The effect of $E_i^\pm$ (5.8) becomes more evident when expanding the Kraus operators E_i

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in terms of Pauli matrices P_j

$$E_i = \sum_j \Gamma_{ij} P_j, \quad (5.10)$$

where Γ_{ij} are complex coefficients. In case that the measurement is given by $m_X = +1$, the new operators are such that their Pauli components commute with R

$$E_i^+ = \sum_{j/[R, P_j]=0} \Gamma_{ij} P_j. \quad (5.11)$$

Similarly, when $m_X = -1$ only those components that anti-commute with R survive

$$E_i^- = \sum_{j/\{R, P_j\}=0} \Gamma_{ij} P_j. \quad (5.12)$$

We will focus on the case where the error channel Λ is a Pauli channel (5.3), with $E_i = \sqrt{\lambda_i} P_i$. In such a case, an interpretation of (5.7) entails that the action of the flag gadget on the noisy gate (Fig. 5.1) is equivalent to the action of the noiseless gate U followed by a modified Pauli channel $\tilde{\Lambda}_\pm$ (Fig. 5.2) with Kraus operators $E_i = \sqrt{\frac{\lambda_i}{\mathcal{N}}} P_i$,

$$\tilde{\Lambda}_\pm(\rho_U; \vec{\lambda}) = \frac{1}{\mathcal{N}} \sum_{i \in [g]} \lambda_i P_i \rho_U P_i^\dagger, \quad (5.13)$$

with a normalization factor given by (5.9),

$$\mathcal{N} = \sum_{i \in [g]} \lambda_i. \quad (5.14)$$

The set $[g]$ is defined such that it contains all the integers from the set $i \in [1, 4^{n_q}]$ satisfying

$$[g] = \{i : [P_i, R]_b = 0, b = m_X\}, \quad (5.15)$$

where we have introduced the convention for the commutator ($b = +1$) and anti-commutator ($b = -1$),

$$[X, Y]_b = XY - bYX. \quad (5.16)$$

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This result is a consequence of the cyclic property of the trace $\text{Tr}(AB) = \text{Tr}(BA)$, that $E_i^{\pm\dagger} E_i^{\pm} = \lambda_i I$ for a Pauli channel and that $\text{Tr}(\rho_U) = 1$ since U is unitary. Notably, the flag gadget construction of Fig. 5.1 can be further generalized by adding multiple layers acting on the same noisy unitary [25]. In Fig. 5.3 we display an example of a 3-layered flag gadget acting on a n_q -qubit noisy unitary.

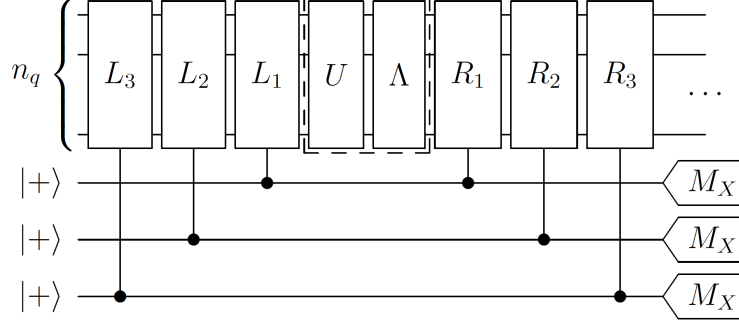


Figure 5.3: Example of a multi-layered flag gadget acting on a noisy n_q -qubit unitary (highlighted in the dashed region). In this case, there are $l = 3$ layers. Again, we require $R_i U L_i = U$.

Henceforth, we focus on the particular case where the error channel Λ is a Pauli channel and l -layered gadgets are utilized. The results (5.13) and (5.14) remain valid as long as the set $[g]$ (5.15) is redefined as the intersection of sets

$$[g] = \bigcap_{q=1}^l \{i : [P_i, R_q]_{b_q} = 0, b_q = m_X^{(q)}\}. \quad (5.17)$$

Thus, P_i either must commute or anti-commute with the respective Pauli R_q (depending of the measurement outcome of each gadget) to appear in the sum of (5.13) and (5.14). In order to unclutter the notation, we decided to omit the l dependence in the set notation $[g]$.

Note that for a l -layered gadget acting on a n_q -qubit noisy unitary, the maximum number of non-zero components of (5.13) and (5.14) is 2^{2n_q-l} . This is because originally there are $4^{n_q} = 2^{2n_q}$ Pauli terms, and every layer $q = 1, \dots, l$, removes half of them at a time. Finally, this result also implies that the maximal number of layers is given by $l_{\max} = 2n_q$, in which case the set $[g]$ contains a single element.

5.3 Adaptation of noise channel estimates

5.3.1 Bayesian inference

In the previous section we saw how flag gadget measurements post-select out portions of a Pauli error channel inconsistent with the measurement results. Now we describe how this information can be used to update in real-time the estimates of the noise channel for a gate. We employ a Bayesian approach and accordingly treat the available characterization of the noise channel associated to a gate (available through off-line characterization) as a prior distribution over Pauli error rates. Namely, the preliminary knowledge of a Pauli channel $\tilde{\Lambda}$ associated to a noisy unitary gate can be encoded in a prior probability distribution $P(\vec{\lambda}; \vec{\alpha})$, dependent on some variables $\vec{\lambda} = (\lambda_1, \dots, \lambda_K)$ and hyperparameters $\vec{\alpha} = (\alpha_1, \dots, \alpha_{K'})$. The expected values of the Pauli error rates under this prior distribution, $\{\langle \lambda_i \rangle_{P(\vec{\lambda}; \vec{\alpha})}\}$, specify the expected value $\mathbb{E}\{\cdot\}$ of the Pauli channel $\tilde{\Lambda}$ as

$$\begin{aligned} \mathbb{E}\{\tilde{\Lambda}(\rho_U; \vec{\lambda})\} &= \int d\lambda P(\vec{\lambda}; \vec{\alpha}) \tilde{\Lambda}(\rho_U; \vec{\lambda}) \\ &= \sum_i \langle \lambda_i \rangle_{P(\vec{\lambda}; \vec{\alpha})} P_i \rho_U P_i^\dagger. \end{aligned} \tag{5.18}$$

This description naturally allows the incorporation of characterization uncertainties in the form of a non-singular prior distribution over the Pauli error rates. *Bayes' rule* provides a procedure to incorporate the extra information acquired from the flag gadget measurement outcomes m_X and update our description of the error channel. Namely, Bayes' rule gives a formula for the posterior probability $P(\vec{\lambda}|m_X)$ after incorporation of the measurement outcomes m_X ,

$$P(\vec{\lambda}|m_X) = \frac{P(m_X|\vec{\lambda})P(\vec{\lambda}; \vec{\alpha})}{P(m_X)}. \tag{5.19}$$

Here, the likelihood $P(m_X|\vec{\lambda})$ gives the conditional probability of obtaining a measurement outcome m_X from the given prior distribution. The marginal probability $P(m_X)$, gives the unconditional probability of measuring m_X .

5.3 Adaptation of noise channel estimates

The likelihood is the quantum-mechanical probability of obtaining the post-measurement state $\rho_{\text{post}}^\pm$ (5.9), respectively,

$$P(m_X|\vec{\lambda}) = p(m_X) = \sum_{i \in [g]} \lambda_i, \quad (5.20)$$

which is by definition equal to the normalization factor of (5.14). The marginal probability is then,

$$\begin{aligned} P(m_X) &= \int d\lambda P(m_X|\vec{\lambda}) P(\vec{\lambda}; \vec{\alpha}) \\ &= \sum_{i \in [g]} \langle \lambda_i \rangle_{P(\vec{\lambda}; \vec{\alpha})}. \end{aligned} \quad (5.21)$$

Thus, the Bayes update rule is

$$P(\vec{\lambda}|m_X) = \left(\frac{\sum_{i \in [g]} \lambda_i}{\sum_{i \in [g]} \langle \lambda_i \rangle_{P(\vec{\lambda}; \vec{\alpha})}} \right) P(\vec{\lambda}; \vec{\alpha}). \quad (5.22)$$

The equation (5.22) provides an update rule for the expected values upon measuring m_X ,

$$\langle \lambda_j \rangle_{P(\vec{\lambda}; \vec{\alpha})} \longrightarrow \langle \lambda_j \rangle_{P(\vec{\lambda}|m_X)}. \quad (5.23)$$

A useful scenario for the application of the update rule (5.23) requires the repetition of the flag gadget measurements. Hence, we focus on the particular case where a given noisy unitary V acts repeatedly on the same subset of qubits. In addition, we also assume that the error channel $\tilde{\Lambda}$ does not drift with time (assumption that is valid if the time it takes to apply the full sequence of flag gadgets is much smaller than the characteristic drift time). Under these assumptions, we can apply a sequence of l -layered gadgets n consecutive times as in Fig 5.4.

We treat the posterior of the k -th step as the prior of the $(k + 1)$ -th step, for

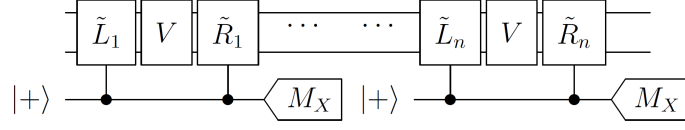


Figure 5.4: Repeated action of a noisy gate V n -consecutive times. For each application of the noisy gate V , a set of l -layered flag gadgets is measured (the tildes indicate that more than a single layer could be measured per step).

$k = 1, \dots, n$. Hence, we can write the recursive relation

$$P^{(k)}(\vec{\lambda}) = \frac{(\sum_{i_k \in [g_k]} \lambda_{i_k})}{(\sum_{i_k \in [g_k]} \langle \lambda_{i_k} \rangle_{P^{(k-1)}})} P^{(k-1)}(\vec{\lambda}). \quad (5.24)$$

Here $\langle \cdot \rangle_{P^{(k-1)}}$ indicates that the expected values are computed with respect to the prior distribution $P^{(k-1)}(\vec{\lambda})$, where we suppressed the dependence on the hyperparameters $\vec{\alpha}$ for notational simplicity. The initial distribution $P^{(0)}(\vec{\lambda})$ corresponds to the prior distribution $P(\vec{\lambda}; \vec{\alpha})$. In addition, the set $[g_k]$ stands for the set $[g]$ (5.17) obtained by using a l -layered gadget at the k -th step (thus, we only emphasize the step number and not the number of layers with this notation).

Using (5.24), we can compute the expected values after k -steps as

$$\langle \lambda_j \rangle_{P^{(k)}} = \frac{(\sum_{i_k \in [g_k]} \langle \lambda_j \lambda_{i_k} \rangle_{P^{(k-1)}})}{(\sum_{i_k \in [g_k]} \langle \lambda_{i_k} \rangle_{P^{(k-1)}})}. \quad (5.25)$$

The numerator of (5.25) can be rewritten by recalling the definition of covariance,

$$\begin{aligned} \langle \lambda_j \lambda_{i_k} \rangle_{P^{(k-1)}} &= \langle \lambda_j \rangle_{P^{(k-1)}} \langle \lambda_{i_k} \rangle_{P^{(k-1)}} \\ &\quad + \text{Cov}(\lambda_j, \lambda_{i_k})_{P^{(k-1)}}. \end{aligned} \quad (5.26)$$

Therefore the recursive update rule can be recast as

$$\begin{aligned} \langle \lambda_j \rangle_{P^{(k)}} &= \langle \lambda_j \rangle_{P^{(k-1)}} \\ &\quad + \frac{(\sum_{i_k \in [g_k]} \text{Cov}(\lambda_j, \lambda_{i_k})_{P^{(k-1)}})}{(\sum_{i_k \in [g_k]} \langle \lambda_{i_k} \rangle_{P^{(k-1)}})}. \end{aligned} \quad (5.27)$$

Intuitively (5.27) shows that if λ_j is correlated with λ_{i_k} the expected value increases,

whereas if it is anti-correlated, the expected value decreases. For example, in the next subsection we specialize to the Dirichlet distribution as the prior, where we compute the covariance and means explicitly (*e.g.*, (5.36) and (5.37)), and note that λ_j is correlated with λ_{i_k} when $j \in [g_k]$ and anti-correlated when $j \notin [g_k]$.

Finally, equation (5.24) can also be applied n -consecutive times starting from the original prior distribution $P^{(0)}(\vec{\lambda}) \equiv P(\vec{\lambda}; \vec{\alpha})$. This gives the probability distribution at the n -th step in terms of the probability distribution at the zero-th step

$$P^{(n)}(\vec{\lambda}) = \frac{\prod_{k=1}^n \left(\sum_{i_k \in [g_k]} \lambda_{i_k} \right)}{\prod_{k=1}^n \left(\sum_{i_k \in [g_k]} \langle \lambda_{i_k} \rangle_{P^{(k-1)}} \right)} P^{(0)}(\vec{\lambda}). \quad (5.28)$$

Furthermore, using (5.28) we can write down a generic update rule in terms of higher moments of the original prior distribution

$$\langle \lambda_j \rangle_{P^{(n)}} = \frac{\sum_{i_n \in [g_n]} \cdots \sum_{i_1 \in [g_1]} \langle \lambda_j \lambda_{i_n} \cdots \lambda_{i_1} \rangle_{P^{(0)}}}{\sum_{i_n \in [g_n]} \cdots \sum_{i_1 \in [g_1]} \langle \lambda_{i_n} \cdots \lambda_{i_1} \rangle_{P^{(0)}}}. \quad (5.29)$$

We explore this route further in Section 5.3.4.

5.3.2 Dirichlet distribution

The treatment so far has been for arbitrary prior distributions over the Pauli error rates, λ_i . Now we specialize to a particularly useful prior distribution. First, we note that a sensible prior distribution must accommodate certain characteristics. It has to be a multi-variable continuous probability distribution over bounded $\lambda_i \in [0, 1]$, and ideally should also incorporate the normalization constraint $\sum_i \lambda_i = 1$. A natural candidate that satisfies all these features is the Dirichlet distribution [187].

The Dirichlet distribution depends on $K \geq 2$ variables $\vec{\lambda} = (\lambda_1, \dots, \lambda_K)$ and positive real parameters $\vec{\alpha} = (\alpha_1, \dots, \alpha_K)$. It is explicitly defined as

$$D(\vec{\lambda}; \vec{\alpha}) = \frac{1}{B(\vec{\alpha})} \prod_{i=1}^K \lambda_i^{\alpha_i - 1}, \quad \sum_{i=1}^K \lambda_i = 1. \quad (5.30)$$

Note that there are only $K - 1$ independent variables. The denominator is given

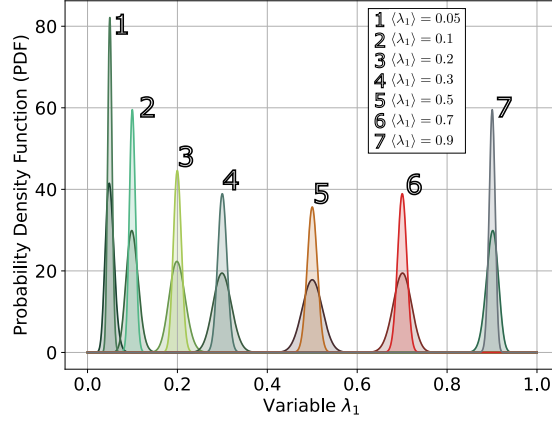


Figure 5.5: Numerical examples of the probability density function (PDF) for 14 different Dirichlet distributions with $K = 2$ variables (Beta distributions). For each of the different seven peaks the coefficient (α_1, α_2) were obtained from different values of $\langle \lambda_1 \rangle$ and α_0 . In particular, for a given peak number, the taller PDF corresponds to $\alpha_0 = 2000$ and the shorter to $\alpha_0 = 500$. Consistent with (5.33), larger values of α_0 give rise to a narrower distribution.

by the generalized Beta function, which is defined as

$$B(\vec{\alpha}) = \frac{\Gamma(\alpha_1) \cdots \Gamma(\alpha_K)}{\Gamma(\alpha_1 + \cdots + \alpha_K)}, \quad (5.31)$$

where $\Gamma(\cdot)$ is the Gamma function. When $K = 2$ the Dirichlet distribution becomes the Beta distribution. For a Pauli channel acting on n_q -qubits (5.3), $K = 4^{n_q}$. In Fig. 5.5, we show some plots of the Dirichlet distribution for the special case $K = 2$. The formula for the expected values is

$$\langle \lambda_i \rangle_{D(\vec{\lambda}; \vec{\alpha})} = \frac{\alpha_i}{\alpha_0}, \quad (5.32)$$

and for the variance

$$\text{Var}(\lambda_j)_{D(\vec{\lambda}; \vec{\alpha})} = \frac{\langle \lambda_j \rangle_{D(\vec{\lambda}; \vec{\alpha})} (1 - \langle \lambda_j \rangle_{D(\vec{\lambda}; \vec{\alpha})})}{\alpha_0 + 1}. \quad (5.33)$$

Here the sum over α_j is denoted as

$$\alpha_0 = \sum_{j=1}^K \alpha_j. \quad (5.34)$$

The Dirichlet distribution can be completely determined by specifying the set of expected values $\{\langle \lambda_i \rangle_{D(\vec{\lambda}; \vec{\alpha})}\}$ in conjunction with α_0 . This also implies that the variance of every λ_i are non-trivially related since

$$\frac{\text{Var}(\lambda_j)_{D(\vec{\lambda}; \vec{\alpha})}}{\text{Var}(\lambda_i)_{D(\vec{\lambda}; \vec{\alpha})}} = \frac{\langle \lambda_j \rangle_{D(\vec{\lambda}; \vec{\alpha})}(1 - \langle \lambda_j \rangle_{D(\vec{\lambda}; \vec{\alpha})})}{\langle \lambda_i \rangle_{D(\vec{\lambda}; \vec{\alpha})}(1 - \langle \lambda_i \rangle_{D(\vec{\lambda}; \vec{\alpha})})}. \quad (5.35)$$

An interesting property of the Dirichlet distribution is that the covariance has a closed form expression

$$\begin{aligned} \text{Cov}(\lambda_i, \lambda_j)_{D(\vec{\lambda}; \vec{\alpha})} &= \delta_{i,j} \frac{\langle \lambda_j \rangle_{D(\vec{\lambda}; \vec{\alpha})}}{\alpha_0 + 1} \\ &\quad - \frac{\langle \lambda_i \rangle_{D(\vec{\lambda}; \vec{\alpha})} \langle \lambda_j \rangle_{D(\vec{\lambda}; \vec{\alpha})}}{\alpha_0 + 1}, \end{aligned} \quad (5.36)$$

where $\delta_{i,j}$ is the Kronecker delta. Hence (5.36) allows us to extract an exact analytic update rule for $\langle \lambda_j \rangle_{P^{(1)}}$ using (5.27) when $k = 1$ and the prior is a Dirichlet distribution $P^{(0)}(\vec{\lambda}) = D(\vec{\lambda}; \vec{\alpha})$,

$$\langle \lambda_j \rangle_{P^{(1)}} = \frac{\alpha_0 \langle \lambda_j \rangle_{P^{(0)}}}{\alpha_0 + 1} + \frac{\delta(j, [g_1])}{\alpha_0 + 1} \frac{\langle \lambda_j \rangle_{P^{(0)}}}{\sum_{i_1 \in [g_1]} \langle \lambda_{i_1} \rangle_{P^{(0)}}}. \quad (5.37)$$

In (5.37) we utilized the generalized delta function defined as

$$\delta(j, [g_k]) = \begin{cases} 1 & \text{if } j \in [g_k] \\ 0 & \text{if } j \notin [g_k] \end{cases}. \quad (5.38)$$

In the following two subsections we will demonstrate flag gadget-based adaptation of noise channels when the prior distribution over Pauli error rates is Dirichlet.

5.3.3 Update rule: maximal number of layers

In this subsection we study the special case when the number of flag gadget layers is maximal $l = 2n_q$. As suggested by [25], the general n_q -qubit case entails utilizing for the right unitaries $R_1, \dots, R_{2n_q}$ all single qubit X and Z gates acting on every

5.3 Adaptation of noise channel estimates

data qubit. The left unitaries are then determined by the formula (5.6). We show an example of a 2-layered gadget for a single qubit unitary in Fig. 5.6, and of a 4-layered gadget for a CNOT gate in Appendix C.1.1.

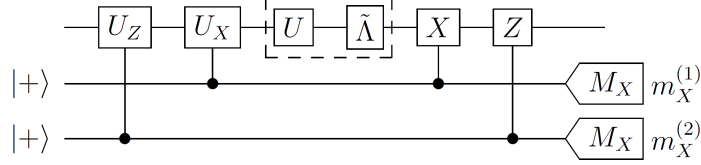


Figure 5.6: Single qubit noisy gate with a 2-layered gadget. The dashed region comprises of a noiseless gate U followed by a noise channel $\tilde{\Lambda}$. The unitaries are $U_P = UPU^\dagger$ for $P = X, Z$, which are also Pauli matrices when U is a Clifford gate.

We use the Dirichlet distribution (5.30) as the prior distribution

$$P^{(0)}(\vec{\lambda}) = D(\vec{\lambda}; \vec{\alpha}). \quad (5.39)$$

As observed earlier, using the maximal number of flag gadget layers, the post-selection and likelihood function singles out an individual λ_j in (5.24), because each layer eliminates half of the Pauli rates in the effective error channel (5.13). An example of this result can be seen in Table 5.1.

$m_X^{(1)}$	$m_X^{(2)}$	$P(m_X \vec{\lambda})$
+1	+1	λ_I
+1	-1	λ_X
-1	-1	λ_Y
-1	+1	λ_Z

Table 5.1: Likelihood probability of measuring m_X given a prior probability distribution $P(\vec{\lambda})$ for a 2-layered flag gadget acting on a single qubit unitary. The right column was constructed using (5.17), and indices $i \in [1, 4]$ where replaced by $i \in \{I, X, Y, Z\}$, respectively.

In case that λ_j is singled out by the measurement outcome m_X (i.e., $j \in [g]$ (5.17)) Bayes' equation (5.24) can be written as

$$P^{(1)}(\vec{\lambda}) = \frac{\lambda_j}{\langle \lambda_j \rangle_{D(\vec{\lambda}; \vec{\alpha})}} D(\vec{\lambda}; \vec{\alpha}) = D(\vec{\lambda}; \vec{\alpha}'). \quad (5.40)$$

As shown, $P^{(1)}(\vec{\lambda}) = D(\vec{\lambda}; \vec{\alpha}')$ is also a Dirichlet distribution for this particular case.

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Indeed, the exact update rule for the hyperparameters $\vec{\alpha}$ is

$$\alpha'_j = \alpha_j + 1 \quad , \quad \alpha'_i = \alpha_i \quad \text{for } i \neq j \, , \quad (5.41)$$

or equivalently,

$$\alpha'_i = \alpha_i + \delta(i, [g]) \, . \quad (5.42)$$

This remarkable result follows from the recursive property of the Gamma function $\Gamma(x+1) = x\Gamma(x)$ and the expression for the expected values (5.32). Indeed, if $\vec{e}_j$ represents a unit vector whose only non-zero component is in the j -th position, then

$$\begin{aligned} B(\vec{\alpha} + \vec{e}_j) &= \frac{\Gamma(\alpha_1) \cdots \Gamma(\alpha_j + 1) \cdots \Gamma(\alpha_K)}{\Gamma(\alpha_1 + \cdots + (\alpha_j + 1) + \cdots + \alpha_K)} \\ &= \frac{\alpha_j}{\alpha_0} \frac{\Gamma(\alpha_1) \cdots \Gamma(\alpha_j) \cdots \Gamma(\alpha_K)}{\Gamma(\alpha_1 + \cdots + \alpha_j + \cdots + \alpha_K)} \\ &= \langle \lambda_j \rangle_{D(\vec{\lambda}; \vec{\alpha})} B(\vec{\alpha}) \, . \end{aligned} \quad (5.43)$$

Given the exact analytic update rule for the Dirichlet distribution (5.41), we can also write down an exact analytic update rule for the expected values after n consecutive steps

$$\langle \lambda_j \rangle_{P^{(n)}} = \frac{\alpha_0}{\alpha_0 + n} \langle \lambda_j \rangle_{P^{(0)}} + \frac{1}{\alpha_0 + n} \sum_{t=1}^n \delta(j, [g_t]) \, , \quad (5.44)$$

Recall that the generalized delta function was defined in (5.38). Note that (5.44) corresponds to applying n consecutive times the equation (5.37) when the cardinality $|[g_i]| = 1$ for $i = 1, \dots, n$.

Furthermore, because the updated distribution is also a Dirichlet distribution, the variance after n steps is

$$\text{Var}(\lambda_j)_{P^{(n)}} = \frac{\langle \lambda_j \rangle_{P^{(n)}} (1 - \langle \lambda_j \rangle_{P^{(n)}})}{\alpha_0 + n + 1} \, . \quad (5.45)$$

A numerical simulation utilizing the update rule (5.44) for a 4-layered gadget acting on a CNOT gate is shown in Fig. 5.7. As this figure shows, the error rates are updated to reflect the new error channel.

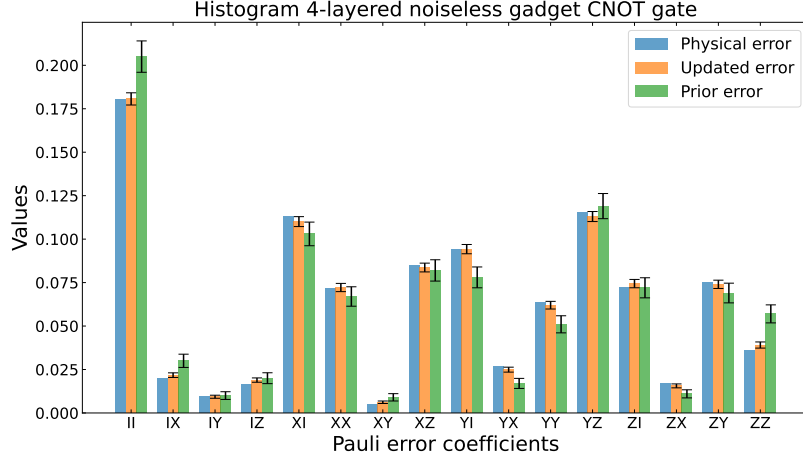


Figure 5.7: Histogram of the Pauli error rate estimates associated to a CNOT gate using noiseless 4-layered gadgets. The ‘prior error’ and the ‘updated error’ columns display the expected values under the prior distribution $\langle \lambda_i \rangle_{P^{(0)}}$, and the updated distribution $\langle \lambda_i \rangle_{P^{(n)}}$ (5.44), respectively. The ‘physical error’ column represents the error rates $\langle \lambda_i \rangle_{P_{\text{phy}}}$ of the real Pauli channel $\hat{A}$ associated to the CNOT gate. To simulate device drift, the ‘physical error’ values slightly deviate from the ‘prior error’ estimates, hence by utilizing the flag gadgets we aim to learn their differences in real-time. The numerical simulations were done considering the set up of Fig. 5.4 starting from the $|00\rangle$ state, taking $n = 10000$ consecutive updates and $\alpha_0 = 2000$, and using the stabilizer circuit simulator package stim [96]. The error bars represent one standard deviation obtained from the square root of (5.45). Details of the 4-layered flag gadgets for a CNOT gate are described in Appendix C.1.1.

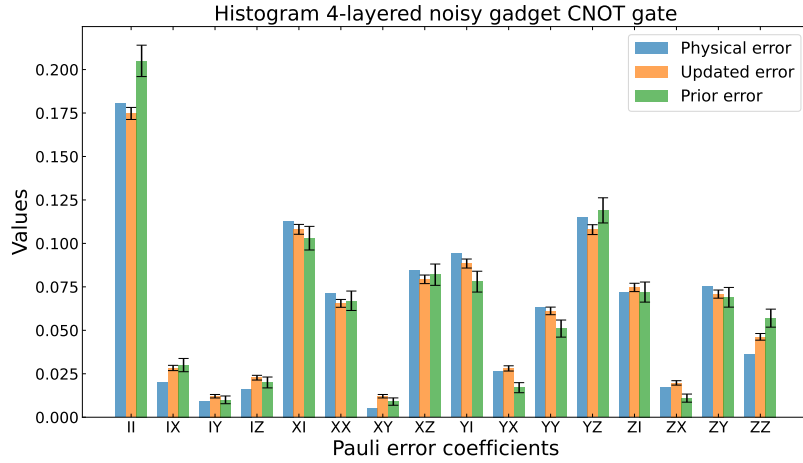


Figure 5.8: Histogram of the Pauli error estimates associated to a CNOT gate using noisy 4-layered gadgets. The noise introduced by the flag gadgets was modeled using a uniform depolarizing error model with strength $p = 0.01$ (described in Section 5.3.5). Otherwise, the simulations were done as in Fig. 5.7.

5.3.4 Generalized update rule

In this subsection we study the generic update rule case in which the number of layers is not necessarily maximal. In terms of practical implementation, this is the most relevant

case. Recall that at the end of the day, the gadgets do also introduce additional noise, hence reducing at maximum the total number of implemented gadgets is crucial.

Following the lines of the generic expression for the expected values obtained after n iterations of the l -layered gadgets (5.29), it turns out that the expected values can be written in close form. This is because high-moments of the Dirichlet distribution are determined in terms of the generalized Beta function (5.31), with a formula given by [187],

$$\langle \lambda_{i_k} \dots \lambda_{i_1} \rangle_{P^{(0)}} = \frac{B(\vec{\alpha} + \vec{e}_{i_1} + \dots + \vec{e}_{i_k})}{B(\vec{\alpha})}. \quad (5.46)$$

Note that the result (5.46) recovers the single variable case proven in (5.43),

$$\langle \lambda_j \rangle_{P^{(0)}} = \frac{B(\vec{\alpha} + \vec{e}_j)}{B(\vec{\alpha})}. \quad (5.47)$$

However, the number of terms to be summed in (5.29) is $O(|[g_k]|^n)$, where $|[g_k]|$ is the cardinality of the set $[g_k]$. This situation suggests that the computation is numerically intractable in its full form. To better understand this issue, let us analyze the two possible cases: i) the cardinality is $|[g_k]| = 1$, which corresponds to the maximal number of gadgets studied in Section 5.3.3. In this case, the distribution remains a Dirichlet distribution throughout every iteration; ii) the cardinality is $|[g_k]| > 1$. In such an event, after $n \geq 1$ iterations, the distribution becomes a convex combination of Dirichlet distributions. To illustrate this point, suppose that the first measurement outcome m_X selects $[g_1] = \{i, j\}$ with $i \neq j$, the posterior distribution is then

$$\begin{aligned} P(\vec{\lambda}|m_X) &= \frac{\lambda_i + \lambda_j}{\langle \lambda_i \rangle_{D(\vec{\lambda}; \vec{\alpha})} + \langle \lambda_j \rangle_{D(\vec{\lambda}; \vec{\alpha})}} D(\vec{\lambda}; \vec{\alpha}) \\ &= \frac{\langle \lambda_i \rangle_{D(\vec{\lambda}; \vec{\alpha})}}{\langle \lambda_i \rangle_{D(\vec{\lambda}; \vec{\alpha})} + \langle \lambda_j \rangle_{D(\vec{\lambda}; \vec{\alpha})}} D(\vec{\lambda}; \vec{\alpha} + \vec{e}_i) \\ &\quad + \frac{\langle \lambda_j \rangle_{D(\vec{\lambda}; \vec{\alpha})}}{\langle \lambda_i \rangle_{D(\vec{\lambda}; \vec{\alpha})} + \langle \lambda_j \rangle_{D(\vec{\lambda}; \vec{\alpha})}} D(\vec{\lambda}; \vec{\alpha} + \vec{e}_j). \end{aligned} \quad (5.48)$$

Thus, generically the number of terms describing the probability distribution also grows exponentially in the number of iterations as $O(|[g_k]|^n)$.

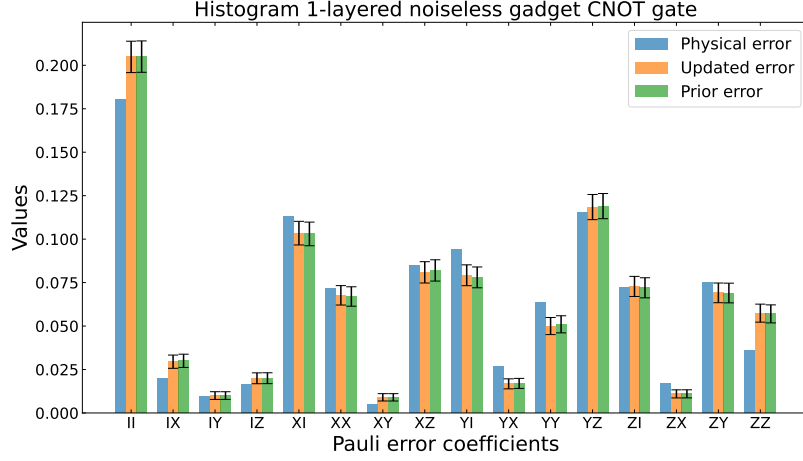


Figure 5.9: Histogram of the Pauli error estimates associated to a CNOT gate using noiseless 1-layered gadgets. The ‘prior error’ and the ‘updated error’ columns display the expected values under the prior distribution $\langle \lambda_i \rangle_{P^{(0)}}$ and the updated distribution $\langle \lambda_i \rangle_{P^{(n)}}$, respectively. The ‘physical error’ column represents the error rates $\langle \lambda_i \rangle_{P_{\text{phy}}}$ of the real Pauli channel $\tilde{\Lambda}$ associated to the CNOT gate. To simulate device drift, the ‘physical error’ values slightly deviates from the ‘prior error’ estimates, hence by utilizing the flag gadgets we aim to learn their differences in real-time. The ‘updated error’ columns were computed using the approximation (5.49), considering the set up of Fig. 5.4 starting from the $|00\rangle$ state, taking $n = 1000$ repetitions and $\alpha_0 = 2000$. In addition, the numerical simulations were done using the stabilizer circuit simulator package stim [96]. The 1-layered flag gadgets were chosen uniformly at random from the 2-qubit Pauli group excluding the identity $\mathcal{P}_2/\{I \otimes I\}$ (see Appendix C.1.2 for further details).

Approximate update rule

After a series of n consecutive flag gadget measurements, computing the expected values by numerically brute forcing the update rule (5.29), using the closed form result (5.46), is out of reach even for $n \gtrsim 10$. Thus, we opted to study an approximation to the exact update rule by considering an expansion in large α_0 , the only tunable parameter in our setup besides n and the prior Pauli estimates. The rationale behind this choice is that the variance of a Dirichlet distribution is order $\text{Var}(\lambda_i) \lesssim 10^{-4}$ when $\alpha_0 \sim 2000$. Larger values of α_0 assign more confidence to the prior distribution and require many shots n to reliably update the expected values. On the other hand, smaller values of α_0 assign less confidence to the prior distribution and the update rule is not robust enough – for instance, the Bayesian update can be overly aggressive and modify error rates, even in the situation when the physical error model $\tilde{\Lambda}$ is similar to the prior estimate (small drift). Furthermore, we will show that the expansion in powers of α_0^{-1} showcases a peculiar structure that is hidden in the general formula (5.29).

5.3 Adaptation of noise channel estimates

The expression for the expected values after n shots up to linear order in large α_0 is given by (see Appendix C.2 for a proof),

$$\begin{aligned} \langle \lambda_j \rangle_{P^{(n)}} &= \frac{\alpha_0}{\alpha_0 + n} \langle \lambda_j \rangle_{P^{(0)}} \\ &+ \frac{1}{\alpha_0 + n} \sum_{t=1}^n \frac{X_1(t) + \alpha_0^{-1} X_2(t) + \Omega(\alpha_0^{-2} n^3)}{1 + \alpha_0^{-1} Y_2 + \Omega(\alpha_0^{-2} n^3)}, \end{aligned} \quad (5.49)$$

where the quantities $X_1(t)$, $X_2(t)$ and Y_2 are

$$X_1(t) = \langle \lambda_j \rangle \frac{\delta(j, [g_t])}{(\sum_{i_t} \langle \lambda_{i_t} \rangle)}, \quad (5.50)$$

$$\begin{aligned} X_2(t) &= \langle \lambda_j \rangle \frac{\delta(j, [g_t])}{(\sum_{i_t} \langle \lambda_{i_t} \rangle)} \sum_{k=1, k \neq t}^n \left(\frac{\delta(j, [g_k])}{(\sum_{i_k} \langle \lambda_{i_k} \rangle)} \right. \\ &\quad \left. + \sum_{q=1, q \neq t}^{k-1} \frac{(\sum_{i \in [g_k] \cap [g_q]} \langle \lambda_i \rangle)}{(\sum_{i_k} \langle \lambda_{i_k} \rangle)(\sum_{i_q} \langle \lambda_{i_q} \rangle)} \right), \end{aligned} \quad (5.51)$$

$$Y_2 = \langle \lambda_j \rangle \sum_{k=1}^n \sum_{q=1}^{k-1} \frac{(\sum_{i \in [g_k] \cap [g_q]} \langle \lambda_i \rangle)}{(\sum_{i_k} \langle \lambda_{i_k} \rangle)(\sum_{i_q} \langle \lambda_{i_q} \rangle)}. \quad (5.52)$$

The expected values in (5.50), (5.51) and (5.52) should be understood as $\langle \lambda_j \rangle \equiv \langle \lambda_j \rangle_{P^{(0)}}$; also, a sum over i_k denotes a sum over $i_k \in [g_k]$. Notice that further terms in (5.49) scale with higher powers of $\alpha_0 n$, as emphasized by the Big- Ω notation. Thus, the expansion is only valid as long as $n < \alpha_0$ because it becomes strongly coupled when $n \gtrsim \alpha_0$. The expected values (5.49) are guaranteed to be normalized since

$$\sum_j \sum_{t=1}^n X_1(t) = n \quad , \quad \sum_j \sum_{t=1}^n X_2(t) = n Y_2. \quad (5.53)$$

There are two important takeaways from (5.49). First, the expansion suggests that the exact update rule (5.29) cannot be recursive. This is due to the existence of correlations between different iterations, manifested in the presence of terms that depend on $[g_k] \cap [g_q]$ with $k \neq q$ and $k, q = 1, \dots, n$. The root of these correlations can be traced-back to the derivation of the approximation, particularly, when expanding high-moments of the Dirichlet distribution (5.46) in powers of α_0 (see Eqn. (C.4) in the Appendix).

5.3 Adaptation of noise channel estimates

More generally, we expect higher-orders of α_0^{-p} to exhibit correlations between $p + 1$ different iterations.

Second, the expansion (5.49) truncated to the zero-th order in α_0^{-1} displays a tight connection with the maximal layered case (5.44) and the l -layered single-shot $n = 1$ case (5.37). Concretely, those results emerge as particular cases of the zero-th order expansion, which has the following expression,

$$\begin{aligned} \langle \lambda_j \rangle_{P^{(n)}} &= \frac{\alpha_0}{\alpha_0 + n} \langle \lambda_j \rangle_{P^{(0)}} \\ &+ \frac{\langle \lambda_j \rangle_{P^{(0)}}}{\alpha_0 + n} \sum_{t=1}^n \frac{\delta(j, [g_t])}{(\sum_{i_t \in [g_t]} \langle \lambda_{i_t} \rangle_{P^{(0)}})} . \end{aligned} \quad (5.54)$$

The result (5.54) is indeed recursive since

$$\begin{aligned} \langle \lambda_j \rangle_{P^{(n)}} &= \frac{\alpha_0 + n - 1}{\alpha_0 + n} \langle \lambda_j \rangle_{P^{(n-1)}} \\ &+ \frac{\langle \lambda_j \rangle_{P^{(0)}}}{\alpha_0 + n} \frac{\delta(j, [g_n])}{(\sum_{i_n \in [g_n]} \langle \lambda_{i_n} \rangle_{P^{(0)}})} . \end{aligned} \quad (5.55)$$

A complementary interpretation of (5.54) is that the updated probability distribution $P^{(n)}(\vec{\lambda})$ is also a Dirichlet distribution, whose coefficients $\vec{\alpha}$ can be computed from $\{\langle \lambda_i \rangle_{P^{(n)}}\}$ and the effective parameter $\alpha_0^{\text{eff}} = \alpha_0 + n$. Using the same language as in (5.40), if at a given iteration the set $[g]$ is obtained from the measurement outcome m_X , the update rule that transforms the prior Dirichlet distribution $D(\vec{\lambda}, \vec{\alpha})$ into the updated Dirichlet distribution $D(\vec{\lambda}, \vec{\alpha}')$, is a generalization of (5.42) when $||[g]|| > 1$,

$$\alpha'_i = \alpha_i + \delta(i, [g]) \frac{\langle \lambda_i \rangle_{D(\vec{\lambda}, \vec{\alpha})}}{(\sum_{j \in [g]} \langle \lambda_j \rangle_{D(\vec{\lambda}, \vec{\alpha})})} . \quad (5.56)$$

Finally, a numerical simulation of the first order expansion (5.49) for the most relevant practical case, with $l = 1$ layers, can be found in Fig. 5.9. Unfortunately, the performance of the noise channel adaptation is not good in this case. There are two issues at play. Firstly, due to the computational intractability of the exact update rule the approximate update rule must be utilized, and this leads to inaccuracies. Secondly, a single gadget does not provide enough information to isolate the error rates and thus

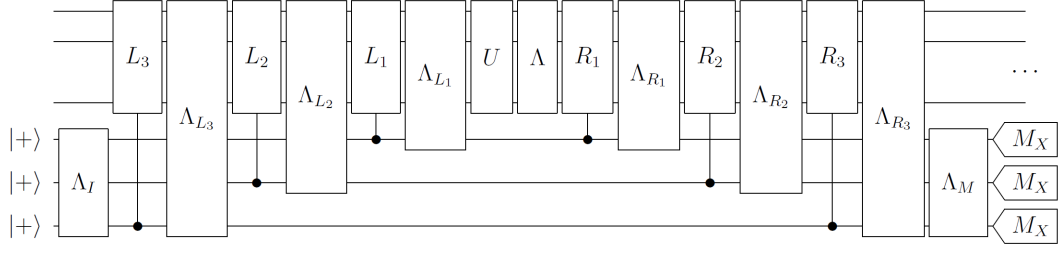


Figure 5.10: Example of a multi-layered flag gadget acting on a noisy unitary gate including quantum error channels for every noisy component. The quantum channels represent noise due to: the unitary gate U (Λ), state initialization (Λ_I), measurement (Λ_M), and the controlled unitaries ($\Lambda_{L_i}, \Lambda_{R_i}$ for $i = 1, \dots, l$). In this example, there are $l = 3$ layers.

the Bayesian updates are not effective. We conclude that the number of gadgets should be as close to the maximal $2n_q$ number as possible to enable effective noise adaptation.

5.3.5 Impact of noisy gadgets

To model the impact of noise introduced by the flag gadgets, we assume that every part of them is faulty: including state preparation, gate implementation and measurements, see Fig. 5.10. The precise definition of the error channels used in the numerical simulations is described with details in Appendix C.3.

As a practical example, in Fig. 5.8 we show a numerical simulation of 4-layered noisy gadgets acting on a CNOT gate. The result of Fig. 5.8 has to be contrasted with Fig. 5.7, where the flag gadgets are assumed to be noiseless. We can observe that both histograms give similar updated error channels for a low physical error rate.

To quantify the effect of the noise introduced by the flag gadgets, we utilize the total variation distance (TVD) d_{TVD} as a figure of merit:

$$d_{\text{TVD}} = \frac{1}{2} \sum_{i=1}^{4^{n_q}} \left| \langle \lambda_i \rangle_{P^{(n)}} - \langle \lambda_i \rangle_{P_{\text{phy}}} \right|, \quad (5.57)$$

which compares the updated Pauli error rates after n steps $\{\langle \lambda_j \rangle_{P^{(n)}}\}$ against the actual physical error rates $\{\langle \lambda_j \rangle_{P_{\text{phy}}}\}$. A numerical simulation of the TVD as a function of n , for several noise strength values p , can be found in Fig. 5.11. Given the set of physical error rates employed in the numerical simulations, we observe that when $p \gtrsim 0.02$ the TVD does not decay for large n . Moreover, after sufficient repetitions the TVD becomes

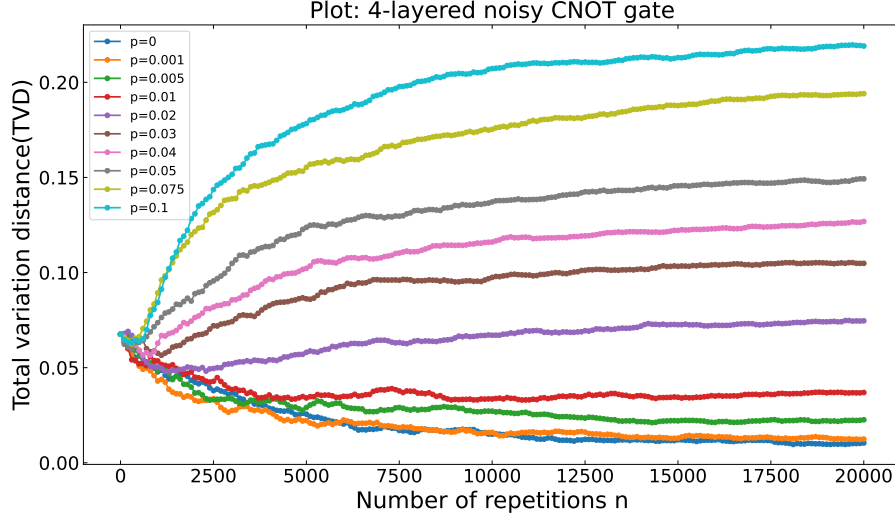


Figure 5.11: Total variation distance (TVD) (5.57) between Pauli error rates updates $\langle \lambda_j \rangle_{P(n)}$ (5.44) and physical error rates $\langle \lambda_j \rangle_{P_{\text{phy}}}$ (see Fig. 5.7) as a function of the number of repetitions n for 4-layered flag gadgets acting on a CNOT gate. The numerical simulations were done considering the set up of Fig. 5.4 starting from the $|00\rangle$ state, taking $n \in [1, 20000]$ repetitions with $\alpha_0 = 2000$, and using the stabilizer circuit simulator package stim [96]. The noisy flag gadgets were modeled using a uniform depolarizing error model of strength p (see Section 5.3.5).

bigger than the distance with respect to the prior Pauli estimates. This observation suggests that the Bayesian inference is not robust to noise in the flag gadgets above a certain threshold.

It is possible that the Bayesian update rule can be modified to incorporate the noise due to flag gadgets if the latter is well characterized. Here we show how this can be done for *measurement noise*. For example, consider a probability of X -type measurement error of p . In such a case, the likelihood probability in the Bayesian analysis (Eqn. (5.20)) should be amended as

$$\begin{aligned}
 P(m_X | \vec{\lambda}) &= P(m_X | \vec{\lambda}; 0\text{-errors}) \tilde{P}(m_X; 0\text{-errors}) \\
 &+ \sum_{k=1}^l P(m_X | \vec{\lambda}; k\text{-errors}) \tilde{P}(m_X; k\text{-errors}),
 \end{aligned} \tag{5.58}$$

where $\tilde{P}(m_X; k\text{-errors})$ indicates the probability of having k measurement errors and $P(m_X | \vec{\lambda}; k\text{-errors})$ indicates the likelihood probability with k measurement errors.

In case that every measurement error occurs with probability p , then the likelihood

probability for the *maximal number of layers* case ($l = 2n_q$) is

$$P(m_X | \vec{\lambda}) = (1-p)^{2n_q} \lambda_i + \sum_{k=1}^{2n_q} p^k (1-p)^{2n_q-k} \left(\sum_{j/\text{wt}(P_i, P_j)=k} \lambda_j \right). \quad (5.59)$$

Here $\binom{2n_q}{k}$ is the binomial coefficient, and $\text{wt}(P_i, P_j)$ is the Hamming distance between two Pauli matrices P_i and P_j . The later one is defined as the number of different entries in the binary representation of P_i^1 and P_j . Recall that the binary representation of a Pauli matrix Q acting on n_q qubits is given by the $2n_q$ dimensional string $(c_1, \dots, c_{n_q}, d_1, \dots, d_{n_q})$ such that

$$Q \sim \bigotimes_{s=1}^{n_q} X_s^{c_s} Z_s^{d_s} \quad , \quad c_s, d_s \in \{0, 1\}, \quad (5.60)$$

where we have ignored the global phase. Note that given P_i , there are exactly $\binom{2n_q}{k}$ matrices P_j such that $\text{wt}(P_i, P_j) = k$. The proof of formula (5.59) has two parts: i) since single qubit measurement errors occur with probability p , the probability of not measuring any error is just $(1-p)^{2n_q}$. In addition, the factor λ_i is associated with the Pauli matrix P_i singled out by the noiseless measurement outcome m_X , i.e., with $i \in [g]$; ii) if k error occurs, they will appear with probability $p^k (1-p)^{2n_q-k}$. The coefficients λ_j that are singled out have Hamming distance $\text{wt}(P_i, P_j) = k$ because of the structure of the flag gadgets for the maximal layered case. This is because the right unitaries $R_1, \dots, R_{2n_q}$ are single qubit X and Z gates acting on every data qubit. The commutation/anti-commutation relations of a given Pauli Q (5.60) with every single qubit gate $X_s(Z_s)$ acting on the s -th qubit with $s = 1, \dots, n_q$ are

$$[Q, X_s]_{b_q} = 0 \iff d_s = \sin\left(\frac{b_q + 3}{4}\pi\right), \quad (5.61)$$

$$[Q, Z_s]_{b_q} = 0 \iff c_s = \sin\left(\frac{b_q + 3}{4}\pi\right). \quad (5.62)$$

¹The Pauli matrix P_i stands for the matrix singled out by the measurement outcome m_X of the maximal layered flag gadget in a noiseless scenario, i.e., $i \in [g]$ (see Section 5.3.3).

Recall that $b_q = \pm 1$ (see (5.16)) is given by the measurement outcome of each layer $b_q = m_X^{(q)}$, with $q = 1, \dots, 2n_q$ (5.17). Hence, given an initial matrix P_i , all the commutators/anti-commutators with single qubit gates $X_s(Z_s)$ that are equal to zero are known. In case that exactly k errors occur, only k of them will be different with respect to their original value (in other words, only k generalized commutators will flip the value b_q of $[P_i, X_s]_{b_q}$) and $2n_q - k$ will be unaltered. Since Pauli matrices either commute or anti-commute, equations (5.61) and (5.62) then suggest that this new condition could be achieved by only changing k different elements of the binary representation of the Pauli P_i . This indeed corresponds to the aforementioned Hamming distance condition for P_j .

In contrast, the modified likelihood probability for the *single-layered* case ($l = 1$) has a simpler form

$$P(m_X | \vec{\lambda}) = (1 - p) \left(\sum_{i \in [g]} \lambda_i \right) + p \left(1 - \sum_{i \in [g]} \lambda_i \right). \quad (5.63)$$

The proof of (5.63) follows a similar logic as the proof of (5.59). In either case, both expressions (5.59) and (5.63) contain more than a single λ_i in their respective sums. Hence, as argued in Section 5.3.4, after several iterations of the flag gadgets, the probability distribution will be a convex combination of Dirichlet distributions that grows exponentially, so in practice some sort of approximation has to be implemented. We postpone this kind of analysis for future work.

To conclude this section, we would like to show explicit formulas for the update rules in the specific case of noisy single-layered flag gadgets. After a single iteration, Bayes' equation becomes

$$P_{\text{noisy}}^{(1)} = \frac{p + (1 - 2p) \left(\sum_{i_1 \in [g_1]} \lambda_{i_1} \right)}{p + (1 - 2p) \left(\sum_{i_1 \in [g_1]} \langle \lambda_{i_1} \rangle_{P^{(0)}} \right)} P^{(0)}. \quad (5.64)$$

5.4 Conclusion

Thus, the update rule for the expected values are

$$\begin{aligned} \langle \lambda_j \rangle_{P^{(1)}}^{\text{noisy}} = & \frac{p}{p + (1 - 2p) \left(\sum_{i_1 \in [g_1]} \langle \lambda_{i_1} \rangle_{P^{(0)}} \right)} \langle \lambda_j \rangle_{P^{(0)}} \\ & + \frac{(1 - 2p) \left(\sum_{i_1 \in [g_1]} \langle \lambda_{i_1} \rangle_{P^{(0)}} \right)}{p + (1 - 2p) \left(\sum_{i_1 \in [g_1]} \langle \lambda_{i_1} \rangle_{P^{(0)}} \right)} \langle \lambda_j \rangle_{P^{(1)}}, \end{aligned} \quad (5.65)$$

where $\langle \lambda_j \rangle_{P^{(1)}}$ is defined as in (5.37). Intuitively, for $p > 0$, the first terms slows down the updating of the error rates, since the measurement results cannot be fully trusted due to measurement errors.

5.4 Conclusion

We have developed and analyzed a technique for adapting the estimates of noise channels associated to gates on a quantum computer. This is a task that is critical for the success of modern error mitigation techniques because time-dependent fluctuations of device parameters (drift) makes estimates of noise channels stale within the execution time of quantum algorithms. The technique uses *extended flag gadgets* to gather information about gate noise without interrupting the execution of the underlying algorithmic circuit. We show how the information gathered from the flag gadget measurements can be used within a Bayesian inference framework to update parameters associated to a noise channel.

Through numerical simulations we showed that the technique is very effective in the regime where a maximum number of extended flag gadgets ($2n_q$ for a gate operating on n_q qubits) is used. This adds at least $4n_q$ additional controlled gates to ancilla qubits, and thus it is desirable to also study the performance when fewer extended flag gadgets are used. However, our numerical studies show that the technique rapidly becomes less effective as the number of flag gadgets is decreased, essentially due to a mismatch between the small amount of information available from measurements (1 bit per flag gadget) and the large number of parameters that must be updated. In addition, our numerical studies show that noise on the gates implementing the extended flag gadgets

5.4 Conclusion

corrupts the information gain and slows down the convergence of the noise channel adaptation process. As a result, the technique we develop here is most useful in the low noise regime where one can afford to implement the maximum number of flag gadgets and the impact of noise on their implementation is minimal.

Part II: Entanglement Entropy in Quantum Field Theory

Chapter 6

Entanglement entropy of a Rarita-Schwinger field in a sphere

In this chapter, we begin to study aspects of relativistic Quantum Field Theories through the lens of quantum information. In concrete, we study the universal logarithmic coefficient of the entanglement entropy (EE) in a sphere for free fermionic field theories in a $d = 4$ Minkowski spacetime. As a warm-up, we revisit the free massless spin-1/2 field case by employing a dimensional reduction to the $d = 2$ half-line and a subsequent numerical real-time computation on a lattice. Surprisingly, the area coefficient diverges for a radial discretization but is finite for a geometric regularization induced by the mutual information. The resultant universal logarithmic coefficient $-11/90$ is consistent with the literature. For the free massless spin-3/2 field, the Rarita-Schwinger field, we also perform a dimensional reduction to the half-line. The reduced Hamiltonian coincides with the spin-1/2 one, except for the omission of the lowest total angular momentum modes. This gives a universal logarithmic coefficient of $-71/90$. Finally, we discuss the physical interpretation of the universal logarithmic coefficient for free higher spin field theories without a stress-energy tensor.

6.1 Introduction

The entanglement of vacuum fluctuations is an ubiquitous property of relativistic quantum fields, as implied by the Reeh-Schlieder theorem [188]. Moreover, in recent years, it has proven to be relevant to the study of quantum field theory and quantum gravity [189, 190]. Specifically, given a vacuum state and a von Neumann algebra of observable operators localized inside a region, the entanglement entropy (EE) can be used to provide a measure of entanglement between such region and its complement. For spherical regions, the assignation of an algebra in the continuum is unique [191]. Further, in any conformal field theory (CFT), the structure of the corresponding EE for a sphere of radius R embedded in a $d = 4$ Minkowski spacetime takes the form

$$S(R) = c_2 \frac{R^2}{\epsilon^2} + c_{\log} \log \left(\frac{R}{\epsilon} \right) + c_0, \quad (6.1)$$

where ϵ represents any given short-distance cutoff introduced to regulate the UV divergences of the EE. The area coefficient c_2 is regularization dependent and might even diverge for a given scheme [192]. Also, the constant coefficient c_0 is cutoff dependent. On the other hand, the logarithmic coefficient $c_{\log}$ is a universal quantity of the theory because it is well defined in the continuum limit. Remarkably, this universal coefficient has been used to provide an entropic proof of the irreversibility A-theorem [43, 193], so it can be regarded as an effective measure of the degrees of freedom in the underlying theory at a given energy scale. Irreversibility theorems associated to the subleading coefficients have also been established [6, 43, 194, 195]. Indeed, the logarithmic coefficient is proportional to the type-A trace anomaly, which can be extracted from the coefficient of the expectation value of the trace of the stress-energy tensor proportional to the Euler density in curved space-time [196]. This has been proven using holography [197], as well as for general CFTs with a well-defined stress-energy tensor using a conformal map to de Sitter spacetime [198].

The logarithmic coefficients $c_{\log}(h)$ for all physical massless fields with spin $h \leq 1$ were computed from the type A trace-anomaly using euclidean methods [199, 200],

yielding

$$c_{\log}(0) = -\frac{1}{90}, \quad c_{\log}(1/2) = -\frac{11}{90}, \quad c_{\log}(1) = -\frac{31}{45}. \quad (6.2)$$

These coefficients have also been computed by other means both analytically [51, 201–203] and numerically [48, 49]. For the cases of Klein-Gordon scalar and Dirac fermion fields all computations coincide. However, for the free Maxwell field, explicit field theoretic calculations performed in [49], as well as thermodynamic computations in de Sitter spacetime [51], reveal a different result

$$\tilde{c}_{\log}(1) = -\frac{16}{45}. \quad (6.3)$$

The reason behind this mismatch is that the result for the entropy depends on the details of the operators inserted at the boundary of the entangling region, together with the possible non-local correlations induced by them. This ambiguity appears in all theories that are not complete, in the sense that they exhibit non-local sectors where the presence of these operators at the boundary can modify the expected anomaly result [204]. For example, in the Maxwell case, the difference between these two computations is that (6.3) corresponds to a free Maxwell theory, while (6.2) corresponds to an effective Maxwell theory in the IR where interactions produced by heavy electric and magnetic charges appearing in the UV completion were integrated out. This coupling to charges in the UV can also be interpreted as the physical origin of the “edge modes” proposed in [202, 205–207] for the IR theory.

For theories with spin $h \geq 3/2$ there seems to be a more severe problem, as the Weinberg-Witten theorem [208] forbids the existence of a well-defined stress-energy tensor. This makes the notion of trace anomaly unclear from the field theory point of view [200]. However, in such cases, the logarithmic coefficient can still be computed without invoking the trace anomaly. Such calculations have been performed for the spin 2 case in [50, 209]. Even more, it was conjectured [50, 210] and proved using the replica trick [209] that the logarithmic coefficients for any field of integer spin h are

given by

$$c_{\log}^{\text{bos}}(h) = -g(h) \frac{1 + 15h^2}{90}, \quad g(h) = \begin{cases} 1 & h = 0 \\ 2 & h > 0 \end{cases}. \quad (6.4)$$

The result for half-integer spin h fields was also proposed by [210]

$$c_{\log}^{\text{fer}}(h) = -\frac{7 + 60h^2}{180}. \quad (6.5)$$

By studying the universal logarithmic coefficients in the EE for free higher spin theories, we aim to gain more insight regarding its physical interpretation. Following this line, we begin by performing the explicit real-time computation of the logarithmic coefficient associated with a massless spin-3/2 field described by the free Rarita-Schwinger field [211–213]. We do so by working with the approach developed in [48–50, 214]. The procedure consists of using a harmonic mode decomposition on the transverse sphere S^2 , and a subsequent dimensional reduction that produces a $d = 2$ effective radial Hamiltonian. The former is made of a tower of modes labeled by the total angular momentum eigenvalues j . The EE of each mode can be computed numerically on a lattice and the final result follows from a careful addition over modes. Surprisingly, for spin 1/2 fields, this calculation has not been done in the context of an EE computation. We do provide such computation. For spin 3/2 fields, we prove that the effective radial Hamiltonian obtained matches with the spin 1/2 result without the lowest total angular momentum mode $j = 1/2$. We will demonstrate that this result guarantees that (6.5) holds for $h = 3/2$.

The structure of the remainder of the chapter is: in Section 6.2, we dimensionally reduce a massless Dirac field in $d = 4$ in a sphere using spinor spherical harmonics. We use this result to compute numerically the EE in a sphere. The radial discretization [214] gives a divergent area coefficient, so the logarithmic coefficient is obtained from a regularized EE defined in terms of the mutual information [215]. In Section 6.3, we review the free Rarita-Schwinger theory in $d = 4$. We mainly work with the gauge invariant phase space generated by the field strengths that can be defined from the usual

gauge-dependent vector-spinor fields. Subsequently, in Section 6.4, we decompose its massless Hamiltonian using spinor-vector spherical harmonics. We employ the same ideas used in the spin $1/2$ case to conclude that the logarithmic coefficient is $-71/90$. Finally, Section 6.5 is devoted to a discussion regarding the existence of ambiguities in the logarithmic coefficient of free higher spin fields, with special focus on the RG flow interpretation of such a quantity. In Appendix D.1, we provide a summary of useful properties of spinor and spinor-vector spherical harmonics; in Appendix D.2, we review the real-time numerical method necessary for the simulations and provide an analytic proof of the divergence of the sum over angular momentum modes when computing the EE with a radial discretization for fermionic fields in $d = 4$; in Appendix D.3, we show that the correlators of gauge invariant operators display conformal symmetry, by identifying the field strength as a conformal primary and explicitly computing its two-point function. In addition, we provide a review of the embedding space formalism, and give the explicit expression for the six-dimensional terms that produce the two-point function of a gauge invariant spin $3/2$ conformal primary field in four dimensions.

6.2 Entanglement entropy of a Dirac field in a sphere

In this section, we revisit the entanglement entropy of a massless Dirac field in a sphere. We start by decomposing the Dirac Hamiltonian in $d = 4$ in a spherical wave basis composed of spinor spherical harmonics and by integrating over the angular variables. This procedure dimensionally reduces the problem to a tower of $d = 2$ fermions with a radial potential quadratic in the fields whose entanglement entropy can be computed numerically on a finite line. We discover that the area term in the entanglement entropy obtained by summing over the entropy of each mode diverges for the radial regularization. Notwithstanding, using the regularized entanglement entropy defined via the mutual information, the calculated logarithmic and area terms are in accordance with the literature.

6.2.1 Decomposition in spherical harmonics

The massless Dirac Hamiltonian in $(3 + 1)$ spacetime dimensions is given by¹

$$H = \int d^3x \psi^\dagger(\vec{x})(\vec{\alpha} \cdot \vec{p})\psi(\vec{x}), \quad (6.6)$$

where $(\vec{\alpha})^a = \gamma^0 \gamma^a$ is defined in terms of gamma matrices and $\vec{p} = -i\vec{\nabla}$ is the momentum operator. As is well known, choosing the Weyl representation of the gamma matrices

$$\gamma^\mu = \begin{pmatrix} 0 & \sigma_R^\mu \\ \sigma_L^\mu & 0 \end{pmatrix}, \quad \sigma_L^\mu \equiv (\mathbb{I}_2, -\sigma^i), \quad \sigma_R^\mu \equiv (\mathbb{I}_2, \sigma^i), \quad (6.7)$$

decouples the Hamiltonian (6.6) as

$$H = H_L + H_R, \quad H_{\frac{L}{R}} = \mp \int d^3x \psi_{\frac{L}{R}}^\dagger(\vec{x})(\vec{\sigma} \cdot \vec{p})\psi_{\frac{L}{R}}(\vec{x}), \quad (6.8)$$

with ψ_L and ψ_R being two-components Weyl spinors that represent left and right-handed fermions, respectively. These can be obtained from the original spinor $\psi(\vec{x})$ by acting with with chirality projection operators defined in terms of $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3$ as

$$\frac{1 - \gamma^5}{2}\psi(\vec{x}) = \begin{pmatrix} \psi_L(\vec{x}) \\ 0 \end{pmatrix}, \quad \frac{1 + \gamma^5}{2}\psi(\vec{x}) = \begin{pmatrix} 0 \\ \psi_R(\vec{x}) \end{pmatrix}. \quad (6.9)$$

The canonical phase space of the theory is spanned by the Weyl spinors ψ_L and ψ_R as canonical coordinates together with their corresponding conjugates $\psi_L^\dagger$ and $\psi_R^\dagger$ as canonical momenta or viceversa. The corresponding canonical anticommutation relations at equal times are given by

$$\{(\psi_{\frac{L}{R}}(\vec{x}))_i, (\psi_{\frac{L}{R}}^\dagger(\vec{x}'))_j\} = \delta_{ij}\delta^{(3)}(\vec{x} - \vec{x}'), \quad (6.10)$$

¹We use Lorentz spacetime indices $\mu, \nu, \dots = 0, \dots, 3$ and signature $\eta_{\mu\nu} = (+, -, -, -)$, Lorentz spatial indices $a, b, \dots = 1, 2, 3$ and spinorial indices $i, j, \dots = 1, \dots, 4$. In addition, time coordinate t dependence is omitted as we are interested in computing entanglement entropies over constant time slices.

where the spinorial indices run in the subset $i, j = 1, 2$ for the Weyl spinors.

Taking into account the rotational symmetry of the problem at hand, it is useful to perform a dimensional reduction of the chiral Dirac Hamiltonian over the sphere. For simplicity, we perform this over the left-handed Hamiltonian, but such procedure can be likewise applied for the right-handed one. To begin with, we expand the spinor ψ_L in the spherical wave basis given by

$$\psi_L(\vec{x}) = \sum_{\kappa\mu} \left(\frac{P_{\kappa\mu}(r)}{r} \right) \Omega_{\kappa\mu}(\theta, \varphi), \quad \psi_L^\dagger(\vec{x}) = \sum_{\kappa\mu} \left(\frac{P_{\kappa\mu}^*(r)}{r} \right) \Omega_{\kappa\mu}^\dagger(\theta, \varphi), \quad (6.11)$$

where $\Omega_{\kappa\mu}(\theta, \varphi)$ are the spinor spherical harmonics defined in [216] via the scalar spherical harmonics Y_{lm} as

$$\Omega_{\kappa\mu}(\theta, \varphi) = \begin{pmatrix} \text{sgn}(-\kappa) \sqrt{\frac{\kappa + \frac{1}{2} - \mu}{2\kappa + 1}} Y_{l, \mu - 1/2}(\theta, \varphi) \\ \sqrt{\frac{\kappa + \frac{1}{2} + \mu}{2\kappa + 1}} Y_{l, \mu + 1/2}(\theta, \varphi) \end{pmatrix}. \quad (6.12)$$

The label κ is related to the orbital angular momentum l by $\kappa = |l + \frac{1}{2}| - \frac{1}{2}$ and the total angular momentum $j = |\kappa| - \frac{1}{2}$ taking the discretized values $\kappa = \pm 1, \pm 2, \dots$ with projections $\mu = -|\kappa| + \frac{1}{2}, -|\kappa| + \frac{3}{2}, \dots, |\kappa| - \frac{1}{2}$. For a brief review of useful properties of spinor spherical harmonics, see Appendix D.1.1.

Replacing (6.11) into the left-handed Hamiltonian (6.8) gives

$$H_L = -i \sum_{\kappa'\mu'\kappa\mu} \int d^3x \left[\left(\frac{P_{\kappa'\mu'}^*}{r} \right) \Omega_{\kappa'\mu'}^\dagger \right] \left(\partial_r + \frac{\kappa + 1}{r} \right) \left[\left(\frac{P_{\kappa\mu}}{r} \right) \Omega_{-\kappa\mu} \right]. \quad (6.13)$$

Further, the orthonormality of the spinor spherical harmonics enables us to integrate out the angular dependence. Thus, the $(3 + 1)$ dimensional Hamiltonian is reduced to an effective tower of $(1 + 1)$ dimensional Hamiltonians in the half-line labeled by (κ, μ) . The corresponding symmetrized real version of (6.13) is

$$H_L^{\text{sym}} = -\frac{i}{2} \sum_{\kappa\mu} \int_0^\infty dr \left[P_{-\kappa\mu}^* P_{\kappa\mu}' - P_{\kappa\mu}^{*'} P_{-\kappa\mu} + \frac{\kappa}{r} (P_{-\kappa\mu}^* P_{\kappa\mu} - P_{\kappa\mu}^* P_{-\kappa\mu}) \right], \quad (6.14)$$

6.2 Entanglement entropy of a Dirac field in a sphere

where we have used the notation $'$ to denote radial derivatives acting over radial functions (for example, $P'_{\kappa\mu}(r) = \partial_r P_{\kappa\mu}(r)$). We will use this notation throughout the paper.

The statistics for $(1+1)$ dimensional complex fields $P_{\kappa\mu}$ can be recovered using the projections of the original spinor fields over the spinor spherical harmonics as

$$P_{\kappa\mu}(r) = r \int_{S^2} d\Omega \psi_L(\vec{x}) \Omega_{\kappa\mu}^\dagger(\theta, \varphi), \quad P_{\kappa\mu}^*(r) = r \int_{S^2} d\Omega \psi_L^\dagger(\vec{x}) \Omega_{\kappa\mu}(\theta, \varphi). \quad (6.15)$$

Then, from (6.10), we get the equal time anticommutation relations

$$\{(P_{\kappa'\mu'}(r'))_i, (P_{\kappa\mu}^\dagger(r))_j\} = \delta_{ij} \delta_{\kappa\kappa'} \delta_{\mu\mu'} \delta(r - r'). \quad (6.16)$$

However, we can reinterpret the $(1+1)$ dimensional fields $P_{\kappa\mu}$. To understand how $P_{\kappa\mu}$ couples with $P_{-\kappa\mu}$, one can rewrite H_L^{sym} as a sum over positive modes $\kappa > 0$. This leads to a theory described by a $(1+1)$ dimensional two-component spinor field $\Psi_{\kappa\mu}$ whose Hamiltonian is

$$H_L^{\text{sym}} = \sum_{\kappa=1}^{\infty} \sum_{\mu} \int_0^{\infty} dr \Psi_{\kappa\mu}^\dagger(r) \left(\alpha_r \overset{\leftrightarrow}{p}_r + \frac{\kappa}{r} \beta_r \right) \Psi_{\kappa\mu}(r), \quad \Psi_{\kappa\mu}(r) = \begin{pmatrix} P_{-\kappa\mu}(r) \\ P_{\kappa\mu}(r) \end{pmatrix}. \quad (6.17)$$

The induced radial representation gives $\alpha_r = \sigma^1$ and $\beta_r = \sigma^2$, where $\overset{\leftrightarrow}{p}_r = -\frac{i}{2}(\vec{\partial}_r - \vec{\partial}_r)$ is the symmetrized momentum operator on the radial direction. The sum over κ can be thought of as a sum over all modes with definite angular momenta $j = \frac{1}{2}, \frac{3}{2}, \dots$, recalling that $j = |\kappa| - \frac{1}{2}$. Also, from (6.16) the spinor field $\Psi_{\kappa\mu}$ obeys the equal time canonical anticommutation relations

$$\{(\Psi_{\kappa'\mu'}(r'))_i, (\Psi_{\kappa\mu}^\dagger(r))_j\} = \delta_{ij} \delta_{\kappa\kappa'} \delta_{\mu\mu'} \delta(r - r'). \quad (6.18)$$

To sum up, we have obtained a tower of Dirac fields in the half-line with a position-dependent quadratic term $\frac{\kappa}{r}$ that appear as a consequence of the Kaluza-Klein reduction on the transverse sphere S^2 .

The Hamiltonian (6.17) together with (6.18) represent the main results of this subsection. They will prove useful when performing a numerical computation of the entanglement entropy in Section 6.2.2, as well as when comparing with the analogue mode decomposition for the Rarita-Schwinger field in Section 6.4.3. The effective radial equations for the Dirac field have been obtained via different methods and for arbitrary dimensions in the literature, for instance by [217]² Further study regarding the modular Hamiltonians of these (1+1) fermionic modes and their contribution to the universal coefficients of the EE in general dimensions, as performed for scalars in [203], appeared later in [218].

6.2.2 Entanglement entropy and logarithmic coefficient

This subsection is devoted to the study of the EE associated to a spherical region of radius R for a free massless Dirac fermion in $d = 4$ space-time dimensions. We will follow a similar procedure as for the scalar field in [214]. Therefore, we are particularly interested in the EE associated with the tower of two-dimensional Dirac fermions with a radial potential in the half-line. Given that the Hamiltonian (6.17) is expressed as a sum over different modes (κ, μ) , the resulting expression for the EE $S(R)$ of Dirac fermions on the sphere holds after summing over each of them

$$S(R) = S_L(R) + S_R(R) = 2 \sum_{\kappa=1}^{\infty} \sum_{\mu} S_{\kappa}(R) = 2 \sum_{\kappa=1}^{\infty} (2\kappa) S_{\kappa}(R). \quad (6.19)$$

The first factor of two is due to the left/right chiralities in (6.8), and the factor 2κ accounts for the multiplicity of μ -projections for a given κ , because the EE $S_{\kappa}(R)$ associated to each of the modes in (6.17) is μ -independent³. Note that the sum (6.19) is a formal expression, since this bare series may not be convergent for some choices of regularization. We will argue in what follows that this is the case for the radial

²The matching with (6.17) follows first from a unitary map of the spinor field and a subsequent axial rotation. The transformed field satisfies the equations of motion like those in [217].

³The fact that the contributions $S_{\kappa}(R)$ are independent of μ follows from the expression (6.17), given that for a given κ all the modes have the same Hamiltonian. In other words, for a fixed κ , all the modes have the same dynamics, as well the same algebra (6.18), yielding the same entanglement entropy.

discretization introduced for a scalar field in [214], when applied to a fermion field.

For quadratic Hamiltonians such as (6.17), the vacuum is a Gaussian state. This implies that Wick's theorem holds, and all non-zero multipoint correlators can be obtained from the two-point function. In the light of this, the EE $S_\kappa(R)$ can be computed numerically by the real-time method introduced in [40, 219]. The idea is to consider the Hamiltonian on the lattice, with a total of M lattice sites, as well as the correlator $C_{mn} = \langle \psi_m^\dagger \psi_n \rangle$, where ψ_n stands for the lattice discretization of $\Psi_{\kappa\mu}(r)$. Hence, considering a spherical region of radius $R = N + \frac{1}{2}$, the EE $S_\kappa(N, M)$ depends exclusively on the eigenvalues of C_{mn} when restricted to $m, n = 1, \dots, N$. A holistic explanation of this standard procedure is found in Appendix D.2.1.

The contributions from modes with large angular momentum κ are relevant for the convergence of the sum (6.19). The entropies $S_\kappa(N, M)$ are independent of the infrared cutoff M for $\kappa \gg M$ and behave as

$$4\kappa S_\kappa(N, M) \sim 8\xi(N) \left(\frac{\log(\kappa)}{\kappa} \right) + 4\xi(N) [1 - \log(\xi(N))] \left(\frac{1}{\kappa} \right) + \dots, \quad (6.20)$$

where $\xi(N)$ is given by

$$\xi(N) = \frac{N^2(N+1)^2}{4(2N+1)^2}. \quad (6.21)$$

For an analytic derivation of this asymptotic behavior, see Appendix D.2.2, and for a numerical verification, refer to the left plot of Fig. 6.1. As a consequence of (6.20), the sum introduced in (6.19) diverges for an arbitrary cutoff M . This behavior is in stark contrast to what happens with a scalar field in $d = 4$, where the radial discretization of the EE is convergent. This is so because the leading term of the entropy of each mode decays as $\sim \frac{\log(l)}{l^3}$ for large angular momentum l [214]. The physical interpretation of this phenomena is that for a Dirac field, the radial discretization is not sufficient for inducing a finite area coefficient c_2 in (6.1). This situation is not unfamiliar, as a similar scenario occurs for scalar fields in $d > 4$ [192].

The area coefficient c_2 is regularization dependent, so this issue can be overcome by choosing another regulator. Conveniently, the mutual information gives a geometrical

6.2 Entanglement entropy of a Dirac field in a sphere

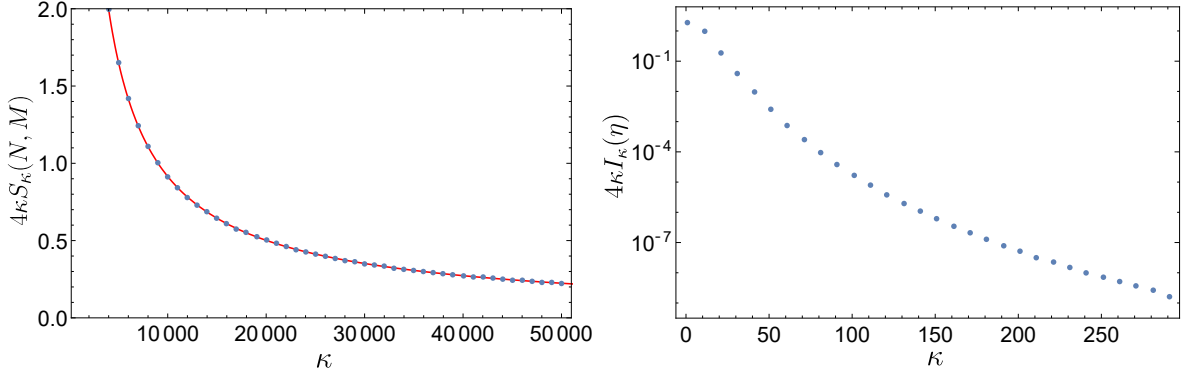


Figure 6.1: Left plot: Entanglement entropy for a massless Dirac field in $d = 4$ as a function of angular momentum κ for large κ . The dotted points indicate the lattice simulation data and the red continuous line indicates the fit function $f(\kappa) = a \frac{\log(\kappa)}{\kappa} + b \frac{1}{\kappa}$. The fitted values $a = 1274.94$ and $b = -2595.83$ match with relative error of 0.005% and 0.03%, respectively, with the coefficients of (6.20). The numerical simulation was done with $M = 100$ physical sites and considered a spherical region of fixed radius $R = N + \frac{1}{2} = 50.5$. Right plot: Mutual information in logarithmic scale, for a massless Dirac field in $d = 4$, as a function of angular momentum κ for fixed η . In stark contrast with the entanglement entropy (in radial regularization), the mutual information is exponentially suppressed for large κ . The simulation was done for fixed $\eta = 9.5$ and $M = 100$ physical sites.

prescription for computing a regularized EE [49, 215]. This construction relies on the mutual information of a spherical region A of radius R_A and a region B defined as the complement of a sphere of radius R_B , with $R_B > R_A$, that contains the region A (see Fig. 6.2). The mutual information is defined as usual

$$I(A, B) = S(A) + S(B) - S(A \cup B). \quad (6.22)$$

Purity of the vacuum state implies that the entropy of a region coincides with the entropy of its complement. This means that $S(B)$ can be computed as the entropy of a sphere of radius R_B and $S(A \cup B)$ as the entropy of an annular region defined between R_A and R_B . We can introduce a geometric regularization by expressing the radii in terms of two new variables R and ϵ such that $R_A = R - \epsilon/2$ and $R_B = R + \epsilon/2$. This motivates the following definition

$$\eta \equiv \frac{R}{\epsilon} = \frac{R_A + R_B}{2(R_B - R_A)}. \quad (6.23)$$

In this vein, for $\eta \gg 1$ the mutual information gives a prescription for the regularized

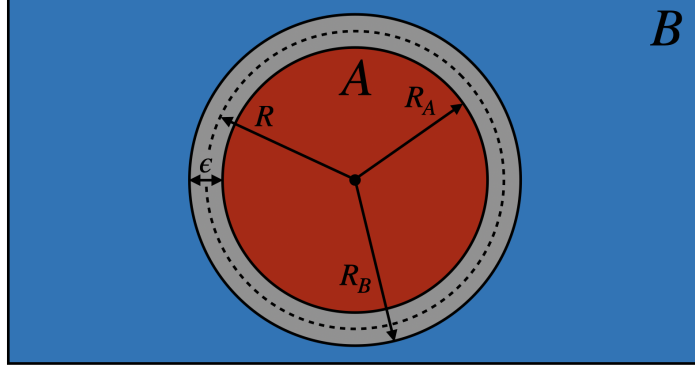


Figure 6.2: Set-up used to compute the mutual information $I(A, B)$. The region A is a sphere of radius R_A and B is the complementary region of a sphere of radius R_B that contains A . Both radii can also be parameterized in terms of new variables ϵ and R as $R_A = R - \epsilon/2$ and $R_B = R + \epsilon/2$.

EE in the form of

$$S_{\text{reg}}(\eta) = \frac{I(\eta)}{2} = s_2 \eta^2 + c_{\log} \log(\eta), \quad \eta \gg 1. \quad (6.24)$$

In Fig. 6.3, we show numerical simulations in the range $8 < \eta < 20$. In opposition to the slowly decaying behavior of the EE as a function of κ , we observed an exponentially suppressed decay for large κ for the mutual information⁴ (see right plot of Fig. 6.1). This is because the mutual information is less sensitive to ultraviolet contributions than the EE. For the maximum lattice size considered $M_{\text{max}} = 200$, we noted that it was sufficient to sum up to $\kappa_{\text{max}} = 250$ in (6.19). The extraction of a numerical value for s_2 and $c_{\log}$ requires the elimination of the dependence on the infrared cutoff M . Therefore, by fitting (6.24) for lattices with size $M = 100, 125, 150, 175, 200$, the fitted coefficients were extrapolated to the continuum by using the functions

$$s_2(M) = s_2^\infty + \frac{a}{M^2}, \quad c_{\log}(M) = c_{\log}^\infty + \frac{b}{M^2}. \quad (6.25)$$

The resulting s_2^∞ and $c_{\log}^\infty$, interpreted as the continuum limit results, are

$$s_2^\infty = 0.14145., \quad c_{\log}^\infty = -0.12285. \quad (6.26)$$

⁴This same behavior was also numerically observed for the Maxwell field in [49].

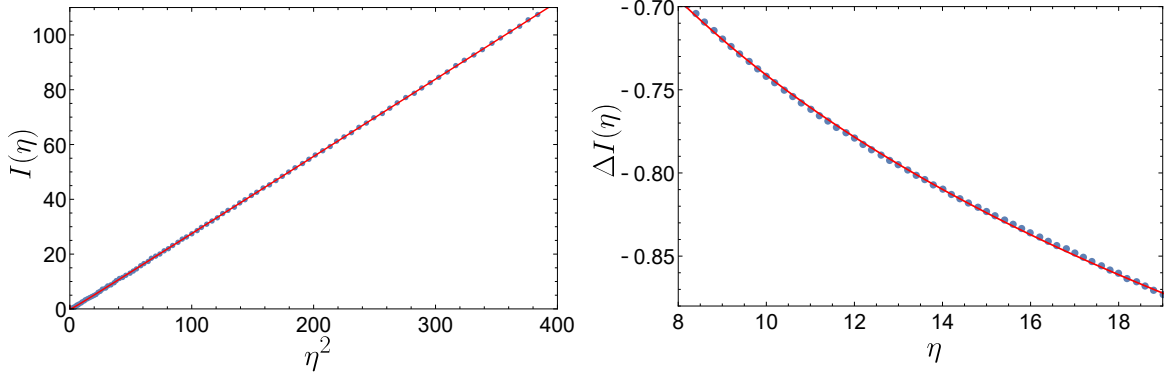


Figure 6.3: Left plot: Mutual information $I(\eta)$ for a Dirac field as a function of η^2 for several values of R_1, R_2 , with $M = 200$ physical sites. The dotted points indicate the lattice simulation data and the continuous red line indicates the fitting function $f(\eta) = 2c_2^{\text{fit}}\eta^2 + 2c_{\log}^{\text{fit}}\log(\eta) + c_0^{\text{fit}}$. Right plot: Mutual information with the area term subtracted, $\Delta I(\eta) = I(\eta) - 2c_2^{\text{fit}}\eta^2$, as a function of η . The fit exhibits a subleading logarithmic contribution that goes like $\Delta I(\eta) = 2c_{\log}^{\text{fit}}\log(\eta) + c_0^{\text{fit}}$.

The logarithmic coefficient matches with the expected value $c_{\log}(1/2) = -\frac{11}{90} = -0.1\bar{2}$ with 0.5% of relative error. The area term also coincides with an approximation present in the literature⁵ with 4.6% of relative error.

6.3 Free Rarita-Schwinger theory

The objective of this section is to study the Rarita-Schwinger field [211–213] as a free quantum field theory describing massless spin 3/2 degrees of freedom in $d = 4$ spacetime dimensions. The free massless field theory is well defined at the classical and quantum level (see [212] and references therein). In this vein, we start by reviewing the canonical quantization considering a vector-spinor gauge field⁶. Then, we show how such procedure is implemented over the gauge invariant phase space spanned by spinor two-form field strength defined from the original gauge field. This is known to only include the spin 3/2 degrees of freedom [222, 223].

⁵The area coefficient of the regularized EE can be obtained as $s_2 = 4\pi(2\kappa_4) = 0.13521\dots$ where $\kappa_4 = 0.00538\dots$ represents the area coefficient of the EE associated to a region between two parallel plates [40, 49].

⁶The vector-spinor gauge field does not transform under an irreducible representation of the four-dimensional Lorentz group, and a priori describes propagating spin 3/2 degrees of freedom together with spin 1/2 ones (see for instance [212, 213] and [220, 221] for a more recent discussion).

6.3.1 Canonical formulation

A theory with propagating spin 3/2 fermions can be described by a vector-valued spinor field $\psi_\nu(x)$ with $\nu = 0, 1, 2, 3$ in $d = 4$. The dynamics of such fields can be given by the Rarita-Schwinger Lagrangian [212, 213]. The latter, in the strict massless limit, is written as [224, 225]

$$\mathcal{L} = \frac{i}{2} \epsilon_{\nu\rho\sigma\lambda} \bar{\psi}^\nu \gamma^5 \gamma^\rho \partial^\sigma \psi^\lambda, \quad (6.27)$$

where $\epsilon_{\nu\rho\sigma\lambda}$ is the 4-dimensional Levi-Civita tensor, γ^ρ and $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3$ are the usual gamma matrices and $\bar{\psi}_\mu = i\psi_\mu^\dagger \gamma^0$. In analogy with spin 1/2 fermions, we can choose the Weyl representation such that the Lagrangian decouples into two independent sectors

$$\mathcal{L} = \mathcal{L}_L + \mathcal{L}_R, \quad \mathcal{L}_{\frac{L}{R}} = \frac{1}{2} \epsilon_{abc} \left(\psi_{\frac{L}{R}}^{a\dagger} \sigma^b \dot{\psi}_{\frac{L}{R}}^c \pm \psi_{\frac{L}{R}}^{a\dagger} \partial^b \psi_{\frac{L}{R}}^c + \psi_{\frac{L}{R}}^{0\dagger} \sigma^a \partial^b \psi_{\frac{L}{R}}^c - \psi_{\frac{L}{R}}^{a\dagger} \sigma^b \partial^c \psi_{\frac{L}{R}}^0 \right), \quad (6.28)$$

where the Weyl spinors ψ_L^μ and ψ_R^μ are defined using the chiral projectors as in (6.9), and ϵ_{abc} represents the 3-dimensional Levi-Civita tensor.

From here, we will only deal with the theory of left-handed fermions. However, the following procedure can also be straightforwardly generalized to right-handed fermions too. First, the timelike component ψ_L^0 of the field only appears in the last two terms of (6.28) as a Lagrange multiplier. On the other hand, the space-like components ψ_L^a of the field appear as dynamical variables associated with the canonical momenta

$$\pi_a^L = \frac{\partial \mathcal{L}}{\partial \dot{\psi}_L^a} = \frac{1}{2} \epsilon_{abc} \psi_L^{b\dagger} \sigma^c. \quad (6.29)$$

At a quantum level, these anticommute with the canonical coordinates at equal times, giving

$$\{(\psi_L^a(\vec{x}))_i, (\pi_L^b(\vec{x}'))_j\} = -i\delta^{ab}\delta_{ij}\delta^{(3)}(\vec{x} - \vec{x}'). \quad (6.30)$$

Conveniently, we can use $\psi_L^{a\dagger} = i\pi_L^a - \epsilon^{abc}\pi_b^L\sigma_c$, to obtain a more useful expression in terms of the conjugated field

$$\{(\psi_L^a(\vec{x}))_i, (\psi_L^{b\dagger}(\vec{x}'))_j\} = (\sigma^b\sigma^a)_{ij}\delta^{(3)}(\vec{x} - \vec{x}'). \quad (6.31)$$

6.3 Free Rarita-Schwinger theory

In this setup, we can compute the Hamiltonian, via a Legendre transformation, to be

$$\mathcal{H}_L = \pi_a^L \dot{\psi}_L^a - \mathcal{L}_L = -\frac{1}{2} \epsilon_{abc} \left(\psi_L^{a\dagger} \partial^b \psi_L^c + \psi_L^{0\dagger} \sigma^a \partial^b \psi_L^c - \psi_L^{a\dagger} \sigma^b \partial^c \psi_L^0 \right). \quad (6.32)$$

Then, we are allowed to derive the constraints from the equations of motion of the timelike component of the fields. These yield the Gauss-law-like constraints

$$2 \partial_a \pi_L^a = \epsilon_{abc} \sigma^a \partial^b \psi_L^{c\dagger} = 0, \quad 2 \partial_a \pi_L^{a\dagger} = \epsilon_{abc} \sigma^a \partial^b \psi_L^c = 0. \quad (6.33)$$

In the massless theory, there is a gauge symmetry that can be described in terms of an arbitrary local spinor function $\chi(x)$ as $\psi^\nu(x) \rightarrow \psi^\nu(x) + \partial^\nu \chi(x)$. Therefore, acting over the left-handed spinor as the chiral projection of this symmetry

$$\psi_L^\nu(x) \rightarrow \psi_L^\nu(x) + \partial^\nu \chi_L(x). \quad (6.34)$$

This implies that neither the dynamical fermion field $\psi_L^a(x)$ nor any of its bilinears can be considered observables. We will deal with this issue in the following section.

6.3.2 Gauge invariant phase space

The formulation of the Rarita-Schwinger theory in terms of phase space gauge invariant variables, makes the computation of the EE easier to understand, as it can be formulated in terms of algebras of local observables attached to regions consisting solely of spin 3/2 degrees of freedom. To begin, we consider the gauge-invariant operators spanned from the spinor field strength associated with the vector-spinor field [212, 222, 223]. Specifically, this is a spinor 2-form given by

$$F_{\mu\nu} = \partial_\mu \psi_\nu - \partial_\nu \psi_\mu. \quad (6.35)$$

6.3 Free Rarita-Schwinger theory

The dynamics obtained from (6.27), can be recovered in terms of the spinor field strength as

$$\gamma^\mu F_{\mu\nu} = 0, \quad \partial^\mu F_{\mu\nu} = 0. \quad (6.36)$$

These conditions secure that field strength F belongs to the representation $(3/2, 0) \oplus (0, 3/2)$ of the Lorentz group [222]. Moreover, the irreducibility condition $\gamma^\mu \gamma^\nu F_{\mu\nu} = 0$, follows trivially from (6.36). Physically the irreducibility condition eliminates the spin $1/2$ degrees of freedom that transform in the representation $(1/2, 0) \oplus (0, 1/2)$ [226]. Therefore, F is a gauge invariant operator that describes the propagation of free massless particles of spin $3/2$ ⁷.

Although the spinor field strength F is a generator of the gauge invariant phase space, we can also use the Levi-Civita tensor to produce new tensors. That is, one should also include the dual spinor 2-form given by

$$F_{\mu\nu}^* = \frac{1}{2} \epsilon_{\mu\nu\sigma\rho} F^{\sigma\rho}. \quad (6.37)$$

However, it is clear that both spinor 2-form fields F and F^* span the same phase space. More precisely, considering the equations of motion $\gamma^\mu F_{\mu\nu} = 0$, we can explicitly check that

$$F_{\mu\nu} + i\gamma^5 F_{\mu\nu}^* = 0. \quad (6.38)$$

Indeed, the description in terms of F and F^* are interchangeable since both obey the same equations of motion as well as divergenceless conditions. Namely,

$$\gamma^\mu F_{\mu\nu}^* = 0, \quad \partial^\mu F_{\mu\nu}^* = 0. \quad (6.39)$$

The irreducible representations $(3/2, 0)$ and $(0, 3/2)$ are described by the self-dual and anti-self dual parts of the field strength, respectively. These are defined to have eigen-

⁷It would be interesting to understand how this description overlaps with a recent discussion about the propagating spin-3/2 and spin-1/2 degrees of freedom [220, 221] in terms of local algebras of observables.

6.4 Entanglement entropy of a Rarita-Schwinger field in a sphere

values $\pm i$ with respect to the Hodge star operator $*$ in Minkowski spacetime

$$*(F_{\mu\nu} \pm iF_{\mu\nu}^*) = (\mp i)(F_{\mu\nu} \pm iF_{\mu\nu}^*). \quad (6.40)$$

In this way, the equation (6.38) becomes clear as it dictates that the self/anti-self dual forms are related to the left and right-handed parts of the vector-spinor field strength

$$\frac{1}{2}(F_{\mu\nu} + iF_{\mu\nu}^*) = \left(\frac{1 - \gamma^5}{2}\right) F_{\mu\nu} = \begin{pmatrix} F_{\mu\nu}^L(\vec{x}) \\ 0 \end{pmatrix}, \quad F_{\mu\nu}^L = \partial_\mu \psi_\nu^L - \partial_\nu \psi_\mu^L, \quad (6.41)$$

$$\frac{1}{2}(F_{\mu\nu} - iF_{\mu\nu}^*) = \left(\frac{1 + \gamma^5}{2}\right) F_{\mu\nu} = \begin{pmatrix} 0 \\ F_{\mu\nu}^R(\vec{x}) \end{pmatrix}, \quad F_{\mu\nu}^R = \partial_\mu \psi_\nu^R - \partial_\nu \psi_\mu^R. \quad (6.42)$$

Also, in the Weyl representation of the gamma matrices (6.7), the equations of motion and divergenceless conditions are

$$\sigma_L^\mu F_{\mu\nu}^L = 0, \quad \partial^\mu F_{\mu\nu}^L = 0, \quad \sigma_R^\mu F_{\mu\nu}^R = 0, \quad \partial^\mu F_{\mu\nu}^R = 0. \quad (6.43)$$

In addition, from the canonical anticommutation relations (6.31) we can ascertain that the components of F_{ab}^L and $F_{ab}^{L\dagger}$ do not anticommute

$$\{(F_{ab}^L(\vec{x}))^i, (F_{cd}^{L\dagger}(\vec{x}'))^j\} = [\sigma_g \sigma_f]^{ij} \delta_{ab}^{ef} \delta_{cd}^{gh} \partial_e \partial_g \delta^{(3)}(\vec{x} - \vec{x}'), \quad \delta_{ab}^{cd} = \delta_a^c \delta_b^d - \delta_a^d \delta_b^c. \quad (6.44)$$

The remaining relations involving F_{0a}^L follow from (6.43). The right-handed field strength (6.42) obeys analogous anticommutation relations.

6.4 Entanglement entropy of a Rarita-Schwinger field in a sphere

In this section, we study the EE of a free massless Rarita-Schwinger field in a sphere. Mimicking the procedure outlined in Section 6.2.1, the Hamiltonian is decomposed in

a spherical wave basis of vector-spinor spherical harmonics. By integrating over the angular variables, this course of action dimensionally reduces the problem to a Dirac Hamiltonian without the $j = \frac{1}{2}$ mode. This identification offers a method for evaluating the EE. Although the decomposition is performed over the gauge-dependent vector-spinor field, we explicitly provide a gauge fixing condition that describes the field in terms of gauge invariant operators localized in the sphere. This condition also secures that the EE result corresponds solely to propagating spin $3/2$ degrees of freedom. We provide the logarithmic coefficient that appears in the EE and suggests a further generalization to higher free half-integer spin fields.

6.4.1 Decomposition in spherical harmonics

To perform the mode decomposition for the Rarita-Schwinger Hamiltonian, we need to introduce the notion of vector-spinor spherical harmonics. These can be defined by extending the definition of the spinor spherical harmonics (6.12) using vector spherical harmonics instead of scalar spherical harmonics. More specifically, we can write

$$\vec{\Omega}_{\kappa\mu}^s(\theta, \varphi) = \begin{pmatrix} \text{sgn}(-\kappa) \sqrt{\frac{\kappa + \frac{1}{2} - \mu}{2\kappa + 1}} \vec{Y}_{l, \mu - 1/2}^s(\theta, \varphi) \\ \sqrt{\frac{\kappa + \frac{1}{2} + \mu}{2\kappa + 1}} \vec{Y}_{l, \mu + 1/2}^s(\theta, \varphi) \end{pmatrix}, \quad s = r, e, m, \quad (6.45)$$

where the index $s = r, m, e$ is not a Lorentz spatial index, instead it indicates the type of vector spherical harmonic, denoted as: radial $\vec{Y}_{lm}^r$, electric $\vec{Y}_{lm}^e$, and magnetic $\vec{Y}_{lm}^m$ vector spherical harmonics. These vector spherical harmonics are vectors themselves that can be used to expand vector-valued functions (see [49] for an example in the context of entanglement entropy calculations). More specifically, they can be obtained

from the usual spherical harmonics as

$$\vec{Y}_{lm}^r(\theta, \varphi) = Y_{lm}(\theta, \varphi) \hat{r}, \quad l \geq 0 \quad -l \leq m \leq l \quad (6.46)$$

$$\vec{Y}_{lm}^e(\theta, \varphi) = \frac{r \vec{\nabla} Y_{lm}(\theta, \varphi)}{\sqrt{l(l+1)}}, \quad l \geq 1 \quad -l \leq m \leq l \quad (6.47)$$

$$\vec{Y}_{lm}^m(\theta, \varphi) = \frac{\vec{r} \times \vec{\nabla} Y_{lm}(\theta, \varphi)}{\sqrt{l(l+1)}}, \quad l \geq 1 \quad -l \leq m \leq l. \quad (6.48)$$

Note that in (6.45) the $\kappa = -1$ mode corresponds to the $l = 0$ mode, thus $\vec{\Omega}_{-1\mu}^e$ and $\vec{\Omega}_{-1\mu}^m$ are not well defined. Further properties of vector-spinor spherical harmonics, such as orthonormality, extend from the properties of vector spherical harmonics. See Appendix D.1.2 for a summary of useful expressions.

To proceed, we expand the dynamical variables $\vec{\psi}_L$ using vector-spinor spherical harmonics and the Lagrange multipliers ψ_L^0 using spinor spherical harmonics,

$$\vec{\psi}_L(\vec{x}) = \sum_{s \kappa \mu} \left(\frac{P_{\kappa\mu}^s(r)}{r} \right) \vec{\Omega}_{\kappa\mu}^s(\theta, \varphi), \quad \psi_L^0(\vec{x}) = \sum_{\kappa \mu} \left(\frac{P_{\kappa\mu}^0(r)}{r} \right) \Omega_{\kappa\mu}(\theta, \varphi). \quad (6.49)$$

We now replace the expansion (6.49) in the Rarita-Schwinger Hamiltonian coming from the density (6.32), which in vector notation reads

$$H_L = -\frac{1}{2} \int d^3x \left[\vec{\psi}_L^\dagger \cdot (\vec{\nabla} \times \vec{\psi}_L) + \psi_L^{0\dagger} (\vec{\sigma} \cdot (\vec{\nabla} \times \vec{\psi}_L)) - ((\vec{\nabla} \times \vec{\psi}_L^\dagger) \cdot \vec{\sigma}) \psi_L^0 \right]. \quad (6.50)$$

The resulting Hamiltonian for $\kappa = -1$ is trivially zero since the electric and magnetic modes are not defined. The Hamiltonian recovered by summing over the remaining

cases yields⁸

$$\begin{aligned}
 H_L = & -\frac{1}{2} \sum_{\kappa \neq -1} \sum_{\mu} \int_0^{\infty} dr \left\{ \left[P_{\kappa\mu}^{e*} P_{\kappa\mu}^m - P_{\kappa\mu}^{m*} P_{\kappa\mu}^e + \frac{\sqrt{\kappa(\kappa+1)}}{r} (P_{\kappa\mu}^{r*} P_{\kappa\mu}^m + P_{\kappa\mu}^{m*} P_{\kappa\mu}^r) \right] + \right. \\
 & + \sqrt{\frac{\kappa+1}{\kappa}} P_{\kappa\mu}^{0*} \left[\sqrt{\frac{\kappa-1}{\kappa+1}} \left(P_{-\kappa\mu}^m - \frac{\kappa}{r} P_{-\kappa\mu}^m \right) - i \left(P_{\kappa\mu}^e - \frac{\sqrt{\kappa(\kappa+1)}}{r} P_{\kappa\mu}^r \right) \right] + \\
 & \left. + \sqrt{\frac{\kappa+1}{\kappa}} \left[\sqrt{\frac{\kappa-1}{\kappa+1}} \left(P_{-\kappa\mu}^{m*} - \frac{\kappa}{r} P_{-\kappa\mu}^{m*} \right) + i \left(P_{\kappa\mu}^{e*} - \frac{\sqrt{\kappa(\kappa+1)}}{r} P_{\kappa\mu}^{r*} \right) \right] P_{\kappa\mu}^0 \right\} ,
 \end{aligned}$$

where we have considered the action of the differential operators in (6.50) acting on $\vec{\psi}_L$ as

$$\vec{\nabla} \times \vec{\psi}_L = \frac{1}{r} \sum_{\kappa\mu} \left[-\frac{\sqrt{\kappa(\kappa+1)}}{r} P_{\kappa\mu}^m \vec{\Omega}_{\kappa\mu}^r - P_{\kappa\mu}^m \vec{\Omega}_{\kappa\mu}^e + \left(P_{\kappa\mu}^e - \frac{\sqrt{\kappa(\kappa+1)}}{r} P_{\kappa\mu}^r \right) \vec{\Omega}_{\kappa\mu}^m \right] , \quad (6.51)$$

as well as the scalar product with the Pauli matrices

$$\vec{\sigma} \cdot (\vec{\nabla} \times \vec{\psi}_L) = \frac{1}{r} \sum_{\kappa\mu} \sqrt{\frac{\kappa+1}{\kappa}} \left[\left(P_{\kappa\mu}^m + \frac{\kappa}{r} P_{\kappa\mu}^m \right) \Omega_{-\kappa\mu} - i \left(P_{\kappa\mu}^e - \frac{\sqrt{\kappa(\kappa+1)}}{r} P_{\kappa\mu}^r \right) \Omega_{\kappa\mu} \right] . \quad (6.52)$$

In this context, the constraints for each mode are enforced by the equations of motion of the $d = 2$ dimensional multipliers $P_{\kappa\mu}^0$ and $P_{\kappa\mu}^{0*}$. From (6.51), we compute the constraint

$$P_{\kappa\mu}^e - \frac{\sqrt{\kappa(\kappa+1)}}{r} P_{\kappa\mu}^r = -i \sqrt{\frac{\kappa-1}{\kappa+1}} \left(P_{-\kappa\mu}^m - \frac{\kappa}{r} P_{-\kappa\mu}^m \right) . \quad (6.53)$$

Replacing this in the Hamiltonian (6.51) we get a tower of $d = 2$ dimensional Hamiltonians that only depend on the magnetic components of the original spinor

$$H_L = \frac{i}{2} \sum_{\kappa \neq \pm 1, \mu} \int_0^{\infty} dr \sqrt{\frac{\kappa-1}{\kappa+1}} \left[P_{-\kappa\mu}^{m*} P_{\kappa\mu}^m - P_{\kappa\mu}^{m*} P_{-\kappa\mu}^m + \frac{\kappa}{r} (P_{\kappa\mu}^{m*} P_{-\kappa\mu}^m - P_{-\kappa\mu}^{m*} P_{\kappa\mu}^m) \right] . \quad (6.54)$$

Each of the Hamiltonians is similar to the $d = 2$ dimensional Dirac field Hamiltonians obtained in (6.14). However, they are not exactly the same because of the presence of the κ -dependent global prefactor. The latter assures that the Hamiltonian for $\kappa = 1$ is

⁸We remind the reader that we use the notation $'$ to denote radial derivatives ∂_r acting over functions that depend on the radial coordinate r .

zero, so it can be explicitly removed from the sum.

To continue we compute the equal time anticommutator of the magnetic modes $P_{\kappa\mu}^m$

$$\{P_{\kappa\mu}^m(r), P_{\kappa'\mu'}^{*m}(r')\} = \left(\frac{\kappa-1}{\kappa}\right) \delta_{\kappa\kappa'} \delta_{\mu\mu'} \delta(r-r'), \quad (6.55)$$

which motivates the following rescaling

$$P_{\kappa\mu}^m = \sqrt{\frac{\kappa-1}{\kappa}} R_{\kappa\mu}^m, \quad P_{\kappa\mu}^{*m} = \sqrt{\frac{\kappa-1}{\kappa}} R_{\kappa\mu}^{*m}, \quad (6.56)$$

so that the new redefined fields satisfy the canonical anticommutation relations (6.16) at equal times. The rescaled Hamiltonian reads

$$H_L = -\frac{i}{2} \sum_{\kappa \neq \pm 1, \mu} \int_0^\infty dr \left(1 - \frac{1}{\kappa}\right) \left[R_{-\kappa\mu}^{m*} R_{\kappa\mu}^m - R_{\kappa\mu}^{m*} R_{-\kappa\mu}^m + \frac{\kappa}{r} (R_{-\kappa\mu}^{m*} R_{\kappa\mu}^m - R_{\kappa\mu}^{m*} R_{-\kappa\mu}^m) \right], \quad (6.57)$$

where we have also integrated by parts the radial derivatives. The first contribution in (6.57) is just the reduced Dirac Hamiltonian (6.14) without the $\kappa = \pm 1$ modes. The second contribution is suppressed by a factor κ^{-1} that changes the parity of the terms, so by summing over κ it becomes a boundary term that can be discarded. Finally, writing the expression in terms of $\kappa > 1$, the theory reduces to

$$H_L = \sum_{\kappa=2}^\infty \sum_{\mu} \int_0^\infty dr \tilde{\Psi}_{\kappa\mu}^\dagger(r) \left(\alpha_r \overset{\leftrightarrow}{p}_r + \frac{\kappa}{r} \beta_r \right) \tilde{\Psi}_{\kappa\mu}(r), \quad \tilde{\Psi}_{\kappa\mu}(r) = \begin{pmatrix} R_{-\kappa\mu}(r) \\ R_{\kappa\mu}(r) \end{pmatrix}, \quad (6.58)$$

with the equal time anticommutation relations

$$\left\{ (\tilde{\Psi}_{\kappa'\mu'}(r'))_i, (\tilde{\Psi}_{\kappa\mu}^\dagger(r))_j \right\} = \delta_{ij} \delta_{\kappa\kappa'} \delta_{\mu\mu'} \delta(r-r'). \quad (6.59)$$

In conclusion, using a mode decomposition in spherical harmonics we proved that the left Rarita-Schwinger Hamiltonian (6.58) can be written as the left Dirac Hamiltonian (6.17) excluding the $j = \frac{1}{2}$ contribution. In both cases the fields obey the same canonical anticommutation relations at equal times (6.59) and (6.18). This is the main result

of this subsection and will prove crucial for computing the universal coefficient of the EE for a Rarita-Schwinger field in Section 6.4.3.

6.4.2 Gauge fixing

To compute the EE of any given region one must assign a von Neumann algebra of observables to such region. In the Rarita-Schwinger theory, the gauge-invariant phase space is generated by the field strength (6.35). Therefore, to obtain the sphere EE from (6.58) we should describe how the gauge-dependant spinor field can be recovered from combinations of these gauge invariant operators localized on the sphere.

Note that the Rarita-Schwinger Hamiltonian can be reduced to a tower of Dirac Hamiltonians for any gauge choice. However, not all these choices allow us to write down the dynamical spinor $\vec{\psi}_L$. To be specific, the left-hand action of the gauge symmetry is given by (6.34) as $\delta\vec{\psi}_L = \vec{\nabla}\chi_L$, so it is reasonable to expand out χ_L in the spinorial harmonics basis as

$$\chi_L(\vec{x}) = \sum_{\kappa\mu} \left(\frac{\chi_{\kappa\mu}(r)}{r} \right) \Omega_{\kappa\mu}(\theta, \varphi). \quad (6.60)$$

From here we can see that the electric component of $\vec{\psi}_L$ can be easily set to zero since

$$\delta\vec{\psi}_L = \sum_{\kappa\mu} \left[\left(\chi'_{\kappa\mu} - \frac{\chi_{\kappa\mu}}{r} \right) \vec{\Omega}_{\kappa\mu}^r + \frac{\sqrt{\kappa(\kappa+1)}}{r^2} \chi_{\kappa\mu} \vec{\Omega}_{\kappa\mu}^e \right]. \quad (6.61)$$

Thus, by considering $P_{\kappa\mu}^e(r) = 0$ for all κ and μ the spatial part of equation (6.49) reduces to

$$\vec{\psi}_L(\vec{x}) = \sum_{\kappa\mu} \left[\left(\frac{P_{\kappa\mu}^r(r)}{r} \right) \vec{\Omega}_{\kappa\mu}^r(\theta, \varphi) + \left(\frac{P_{\kappa\mu}^m(r)}{r} \right) \vec{\Omega}_{\kappa\mu}^m(\theta, \varphi) \right]. \quad (6.62)$$

The same procedure can be employed for $\psi_L^\dagger$ and the right-handed fields ψ_R and $\psi_R^\dagger$.

On the other hand, the electric projection of the field strength can be written, for

spatial Lorentz indices $a, b = 1, 2, 3$, is

$$F_{ea}^L = \int d\Omega [\Omega^{\dagger e}_{\kappa\mu}]^b [F^L]_{ab} = - \sum_{\kappa'\mu'} \int d\Omega \left([\Omega^{\dagger e}_{\kappa\mu}]^b \partial_b [\psi_{\kappa'\mu'}^L]_a - [\Omega^{\dagger e}_{\kappa\mu}]^b \partial_a [\psi_{\kappa'\mu'}^L]_b \right), \quad (6.63)$$

where the gauge choice (6.62) allows to eliminate all the derivatives of the spinor field present in the second term by means of

$$\begin{aligned} \int d\Omega [\Omega^{\dagger e}_{\kappa\mu}]^b \partial_a [\psi_{\kappa'\mu'}^L]_b &= \int d\Omega \left(\partial_a ([\Omega^{\dagger e}_{\kappa\mu}]^b [\psi_{\kappa'\mu'}^L]_b) - (\partial_a [\Omega^{\dagger e}_{\kappa\mu}]^b) [\psi_{\kappa'\mu'}^L]_b \right) \\ &= - \int d\Omega (\partial_a [\Omega^{\dagger e}_{\kappa\mu}]^b) [\psi_{\kappa'\mu'}^L]_b. \end{aligned} \quad (6.64)$$

Therefore, the electric projection of the field strength can be obtained from the spinor field obeying the gauge condition (6.62) as

$$F_{ea}^L = - \sum_{\kappa'\mu'} \int d\Omega \left([\Omega^{\dagger e}_{\kappa\mu}]^b \partial_b [\psi_{\kappa'\mu'}^L]_a + (\partial_a [\Omega^{\dagger e}_{\kappa\mu}]^b) [\psi_{\kappa'\mu'}^L]_b \right). \quad (6.65)$$

Although this relation is highly non-local, it only involves integrals and derivatives in the angular variables of the sphere at a fixed radius. Namely, it can be used to obtain an expression for the gauge-fixed spinor in terms of the field strength that does not involve radial integrals that go outside the spherical region of interest.

In addition, the identification of ψ_L with F_L given by (6.62) implies that they generate the same algebras with the same particle content. Thus this geometric gauge choice allows to describe pure spin 3/2 algebras, without propagating spin 1/2 degrees of freedom⁹, that can be assigned to spherical regions.

⁹In the literature the propagating spin 1/2 degrees of freedom are usually eliminated by the gauge choice $\gamma^\mu \psi_\mu = 0$. For this calculation, this choice is not convenient as it does not correspond to a clear geometric prescription.

6.4.3 Entanglement entropy and logarithmic coefficient

In conclusion, the EE of a massless Rarita-Schwinger field in $d = 4$ in a spherical region is equivalent to the EE of a massless Dirac field excluding the contributions coming from the total angular momentum $j = \frac{1}{2}$ mode, i.e. with $\kappa = 1$. The dynamics of such modes are described by the left-handed Hamiltonian

$$H_L^{\kappa=1} = \sum_{\mu=\pm\frac{1}{2}} \int_0^\infty dr \Psi_{1\mu}^\dagger(r) \left(\alpha_r \overleftrightarrow{p}_r + \frac{1}{r} \beta_r \right) \Psi_{1\mu}(r). \quad (6.66)$$

These consist of a Dirac field on the $d = 2$ half-line $r > 0$ with a $1/r$ mass term. To compute the EE on a finite segment $r \in (0, R)$, we can neglect the effects induced by the mass term because the UV divergent contributions come from high energy fluctuations near the entangling surface at $r = R$. In fact, its EE matches with the result for a free Dirac fermion in the half line [227]

$$S_{\text{half-line}} = \frac{1}{6} \log \left(\frac{R}{\epsilon} \right), \quad (6.67)$$

for a UV cutoff ϵ . We have explicitly verified this behavior numerically. Therefore, the logarithmic coefficient for a massless Rarita-Schwinger field in $d = 4$ is given by

$$c_{\log}(3/2) = 2 \left(-\frac{11}{180} - 2 \left(\frac{1}{6} \right) \right) = -\frac{71}{90}, \quad (6.68)$$

where $\frac{11}{180}$ is the chiral fermion contribution computed in Section 6.2.2. The first factor of two takes into account both left/right chiralities, and the latter factor of two corresponds to the contribution from both modes with $\mu = \pm\frac{1}{2}$ whose entropy is given by (6.67). Note that we have assumed that the EE for the Rarita-Schwinger field has the structure (6.1) of a CFT. This is because the theory exhibits conformal symmetry, as it can be explicitly inferred from the correlators of the gauge invariant field strength (refer to Appendix D.3 for a complete discussion).

We have numerically checked these results by applying the methods described in Section 6.2.2, using the Hamiltonian (6.58). Indeed, the regularized entanglement

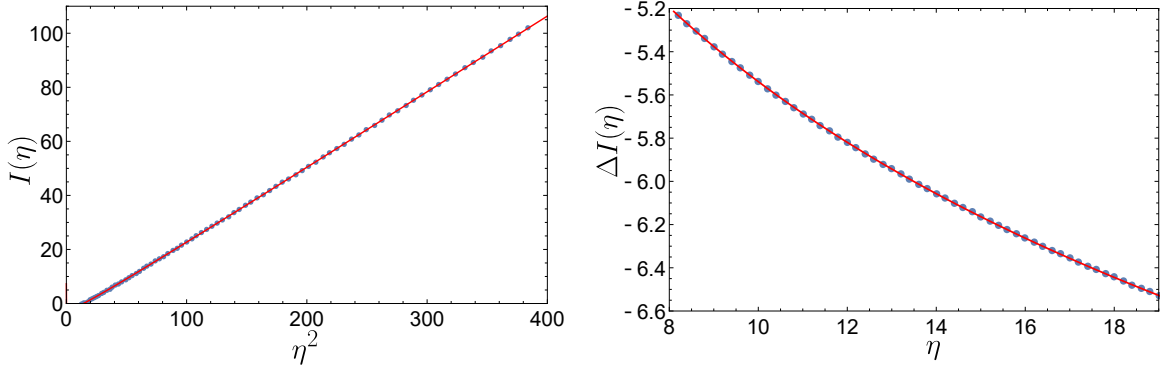


Figure 6.4: Left plot: Mutual information $I(\eta)$ for a Rarita-Schwinger field as a function of η^2 , with $M = 200$ physical sites. The fitting function is $f(\eta) = 2c_2^{\text{fit}}\eta^2 + 2c_{\log}^{\text{fit}}\log(\eta) + c_0^{\text{fit}}$. Right plot: Mutual information with the area term subtracted, $\Delta I(\eta) = I(\eta) - 2c_2^{\text{fit}}\eta^2$, as a function of η . This exhibits the subleading logarithmic term appearing in the Rarita-Schwinger case $\Delta I(\eta) = 2c_{\log}^{\text{fit}}\log(\eta) + c_0^{\text{fit}}$.

entropy can be expanded as (6.24) and then numerically simulated, as shown in Fig. 6.4. The fitted coefficients in the continuum limit are

$$s_2^\infty(3/2) = 0.14145, \quad c_{\log}^\infty(3/2) = -0.79102, \quad (6.69)$$

which entail a 0.3% of relative error in comparison with the expected logarithmic coefficient $c_{\log}(3/2) = -71/90 = -0.788889$ (6.68). Again, the area term also coincides with the parallel plates approximation present in the literature [40, 49] with 4.6% of relative error. Note that the area term is not changed by subtracting the $\kappa = \pm 1$ modes as these have a purely logarithmic contribution of the form (6.67).

In light of these results, we can move forward to produce an extra argument for the conjecture presented in [210]. Proceeding as in [50], it is straightforward to think about a generalization for arbitrary free half-integer spin fields. Proposing that in a theory of half-integer spin h the modes with momentum $\kappa < h - \frac{1}{2}$ cannot be excited we obtain

$$c_{\log}^{\text{fer}}(h) = 2 \left(-\frac{11}{180} - \frac{1}{6} \sum_{\kappa=0}^{h-1/2} (2\kappa) \right) = -\frac{7 + 60h^2}{180}. \quad (6.70)$$

where the factor $1/6$ takes into account the logarithmic contributions coming from the low angular momentum modes that behave as (6.67). Although this coincides with the proposal of [210], actual proof is still lacking in the literature. One possibility

could be to adapt the arguments in [209] for fermionic fields, or to perform a mode decomposition using more general tensor-spinor spherical harmonics.

6.5 Conclusion

We have computed the EE for a spherical region for a free massless spin $3/2$ field. The result coincides with the EE associated with a spin $1/2$ field without the lowest angular momentum mode. In this case, the real-time approach clarifies that the entropy computed corresponds to that of the algebra of gauge invariant operators localized inside the sphere spanned by the spinor field strength. Thus, the computed entropy relates to pure spin $3/2$ fields.

An issue we have avoided so far is the existence of ambiguities reaching the logarithmic coefficients (6.68) and (6.70). Both results have been obtained from the regularized EE, as they follow from the calculation performed in Section 6.2. Hence, the coefficients coincide with the universal terms appearing in the mutual information (6.22). The mutual information for separated regions is free of any ambiguities in the continuum limit [204, 228]. Consequently, the aforementioned coefficients are well-defined quantities in the continuum field theory when interpreted as the universal coefficients of the mutual information.

The logarithmic coefficients (6.68) and (6.70) are subject to ambiguities when interpreted in terms of the EE (6.1). This can be made evident when computing the EE in the lattice. For every lattice theory, there are ambiguities regarding which operators are included in the boundary of a given region. These elections represent particular choices of algebras, which differ from each other because of the presence of specific centers. The elements of the corresponding center are labeled by the sectors of the theory and have an associated classical Shannon contribution to the EE that might change the universal coefficients [228]. These are known in the literature as "edge modes" contributions.

For instance, there used to be a well-known mismatch between the logarithmic

coefficient for a free Maxwell field obtained from the conformal anomaly (6.2), and the result obtained using the same real-time approach reported in the present chapter [49], or by studying thermodynamics in de Sitter spacetime [51], yielding (6.3). The edge modes contributions have been computed for the Maxwell field in [202, 205–207, 229] resolving the mismatch between the coefficients (6.2) and (6.3). Further, the gravitational edge modes contribution for the linearized spin 2 theory has been computed in [229] in the context of a similar spherical wave decomposition as presented in the chapter. Such a procedure should be applicable to the Rarita-Schwinger field considering the sectors emerging from the constraints (6.33).

In the continuum, general von Neumann algebras of observables do not contain a center, and the assignation of an algebra to spherical regions is expected to be unique. Nevertheless, the ambiguities due to the presence of sectors still persist, but they have a different physical origin [204]. In the continuum, this difference emerges because $c_{\log}$ behaves as an unprotected RG charge, in the sense that it depends on the UV completion of the theory [204]. To be more specific, in the Maxwell theory, the non-local IR correlations of some Wilson and t’Hooft loops can be eliminated by adding a UV coupling to the charges, provided that the characteristic mass scale is larger than the regulating distance. The change in the contribution of these non-local operators near the boundary of the entangling region can be considered as an RG flow justification of the results obtained by adding “edge modes” when computing the EE. This kind of mismatch in the logarithmic coefficient is expected to arise not only in the Maxwell field but also in every theory that is not complete, namely, that exhibits sectors.

The fact that ambiguities in the continuum are related to the UV completion of the theory complicates their interpretation for spin $h \geq 3/2$ fields. If we consider free higher spin theories as IR fixed points, several problems regarding possible RG flows arise. For instance, the free massless Rarita-Schwinger (minimally) coupled to an external electromagnetic field cannot be quantized while respecting all of the positivity constraints [225, 230]. Indeed, following [231, 232] one should expect that these theories do not have a QFT-like well-defined RG flow, as they exhibit non-local sectors

charged under the action of space-time symmetries. See [233, 234] and [235] for more explicit constructions of emergent IR generalized symmetries in the spin 2 and 3/2 cases, respectively.

These difficulties in the UV completion also obstruct a useful interpretation of the logarithmic coefficient. Theories with fields of spin $h \geq 3/2$ do not have a local gauge invariant stress-energy tensor, as it is prohibited by the Weinberg-Witten theorem [208]. The lack of stress-energy tensor makes the notion of the conformal anomaly in curved backgrounds uncertain from the field theory standpoint and is therefore not reached by the A-theorem proof in [236, 237]. On the other hand, the logarithmic term is still well-defined in the conformal field theory and even reached by the entropic A-theorem. In fact, the corresponding proof presented in [43] requires only Poincaré invariance and strong subadditivity as assumptions, both of which are fulfilled in any free higher-spin theory. Naively, this seems to imply that there still is an interpretation of the logarithmic coefficient as counting the degrees of freedom along RG flows with free higher spin theories as IR fixed points, assuming that such flows exist. However, as we have suggested, this seems improbable.

In this context, the remaining possibility is that the RG flow is trivial, and the theory is always free. In such a case, there is of course a logarithmic term in the EE, which coincides with the coefficient found in the mutual information, but does not flow. This indeed can be the interpretation of the coefficient for the free spin-3/2 field discussed in this chapter. Nevertheless, in this discussion, we are assuming the theory has to be UV completed in a QFT-like manner, so this argument does not necessarily have to hold for other types of UV completions. Perhaps the logarithmic coefficient computed here can be related to a non-trivial RG flow in such a context. This does seem a more reasonable approach, considering that the Rarita-Schwinger field appears in a wide variety of UV complete models of gravity (such as in supergravity models).

Chapter 7

Holographic entanglement entropy inequalities beyond strong subadditivity

In this chapter we continue to study aspects of Quantum Field Theories through the lens of quantum information. Remarkably, the vacuum entanglement entropy in quantum field theory provides nonperturbative information about renormalization group flows. Most studies so far have focused on the universal terms, related to the Weyl anomaly in even space-time dimensions, and the sphere free energy F in odd dimensions. In this chapter we study the entanglement entropy on a sphere of radius R in a large radius limit, for field theories with gravity duals. At large radius the entropy admits a geometric expansion in powers of R ; the leading term is the well-known area term, and we also consider the subleading contributions. These terms can be physical, they contain information about the full renormalization group flow, and they reproduce known monotonicity theorems in particular cases. We set up an efficient method for calculating them using the Hamilton-Jacobi equation for the holographic entanglement entropy. We first reproduce the known result for the area term, the coefficient multiplying R^{d-2} in the entanglement entropy. We then obtain the holographic result for the R^{d-4} term and establish its irreversibility. Finally, we derive the R^{d-6} coefficient

for holographic theories, and also establish its irreversibility. This result goes beyond what has been proved in quantum field theory based on strong subadditivity, and hints towards new methods for analyzing the monotonicity of the renormalization group in space-time dimensions bigger than four.

7.1 Introduction

Irreversibility theorems provide key insights into the nonperturbative structure of quantum field theories (QFTs). The first such theorem was proved by [238], and established the decrease of the central charge C in $d = 1 + 1$ dimensions along renormalization group flows. This theorem was rederived using quantum information tools in [41], and an extension of these methods allowed to establish the F-theorem in $d = 2 + 1$ dimensions [42]. In $d = 3 + 1$ dimensions, the A-theorem was proved by [236] using unitarity and the dilaton, and then in [43] based on strong subadditivity of the entanglement entropy.

This situation is somewhat puzzling. On the one hand, these proofs use quite different methods (euclidean, Lorentzian and information theoretic), and it is not clear how they are related. One would hope for some unifying understanding, but it has not emerged so far. Furthermore, none of the results extend to more than 3+1 space-time dimensions. A clue that these issues should have a positive resolution comes from QFTs with holographic duals. Indeed, for such theories, the null energy condition (NEC) allows to construct a running C-function and establish the irreversibility of holographic renormalization group (RG) flows [239–241]. The proposed C-function depends on the metric scale factor, and coincides with the universal A or F terms at fixed points. Further progress for understanding holographic RG flows in terms of the EE was made in [242, 243]; we will revisit their method in Appendix E.

Motivated by these questions, in the present chapter we will analyze the entanglement entropy for holographic RG flows with the goal of finding new inequalities. We use holography because we want to access $d > 4$ dimensions, and because we hope that

this may provide clues for future field theoretic approaches. We will go beyond previous irreversibility results by obtaining new inequalities for the geometric large radius terms of the holographic entanglement entropy. As we will discuss, these contain physical information about the renormalization group and about the effective gravitational action induced by integrating out the QFT degrees of freedom.

We consider Poincare invariant QFTs in d space-time dimensions. We assume that at short distances the theory is described by a conformal field theory; relevant perturbations trigger an RG flow, which we assume ends at an IR CFT (different from the UV one). We will analyze the EE associated to a spherical region of radius R . Near a fixed point, it admits an expansion

$$S(R) = \mu_{d-2}R^{d-2} + \mu_{d-4}R^{d-4} + \dots + \begin{cases} (-1)^{\frac{d}{2}-1}4A \log(R/\epsilon) , & d \text{ even} \\ (-1)^{\frac{d-1}{2}}F , & d \text{ odd} \end{cases} \quad (7.1)$$

A and F are the so-called universal terms (related to the Weyl anomaly in even space-time dimensions, and the sphere free energy in odd dimensions), and ϵ is a short distance cutoff. The R^{d-2k} terms arise from geometric quantities of the boundary of the entangling region [244], and they will be the main focus in our work.

The entropy and its μ coefficients diverge as the short distance cutoff $\epsilon \rightarrow 0$. However, we will be interested in comparing two different theories: the UV fixed point one, and the theory that undergoes the nontrivial RG flow. We will review below how this leads to a finite, cutoff-independent, entropy difference ΔS .

For an RG flow with a typical mass scale m , the UV CFT corresponds to $m = 0$. In this limit, the sphere EE has the form (7.1) with coefficients that we call $\mu_{d-2k}^{UV\ CFT}$. For $mR \gg 1$, the IR fixed point is approached, and the EE is also of the form (7.1) but with different coefficients μ_{d-2k}^{IR} .¹ We will be interested in the entropy difference

$$\Delta S(R) = S^{IR}(R) - S^{UV\ CFT}(R) = \Delta\mu_{d-2}R^{d-2} + \Delta\mu_{d-4}R^{d-4} + \dots , \quad (7.2)$$

¹Being an IR fixed point, the theory contains irrelevant deformations, and the typical mass scale m acts as a UV cutoff for the IR effective theory.

with

$$\Delta\mu_{d-2k} = \mu_{d-2k}^{IR} - \mu_{d-2k}^{UV\,CFT} . \quad (7.3)$$

As discussed in Sec. 7.3.3, this becomes independent of the cutoff and hence is a property of the continuum theory. The entropy difference appears naturally in information-theoretic approaches to irreversibility [43, 245–247].

The ΔA or ΔF are intrinsic to the fixed points, namely they are independent of the RG flow that connected the UV and IR CFTs. This is what “universal” means in this context. The other quantities $\Delta\mu_{d-2k}$ in the large mR expansion do depend on the RG trajectory, but can still be physical (i.e. finite in the continuum limit). The simplest example is $\Delta\mu_{d-2}$, the coefficient of the area term. It corresponds to the renormalization of $1/G_N$ when weakly coupling gravity to the QFT; equivalently, the flow of the area term in the EE coincides with the low energy QFT contribution to black hole entropy. Ref. [194] showed that

$$\Delta\mu_{d-2} = -\frac{\pi}{d(d-1)(d-2)} \int d^d x \, x^2 \langle \Theta(x) \Theta(0) \rangle , \quad (7.4)$$

where $\Theta(x)$ is the trace of the energy-momentum tensor. From here and reflection positivity or unitarity, it follows that

$$\Delta\mu_{d-2} \leq 0 , \quad d \geq 2 . \quad (7.5)$$

This result for $\Delta\mu_{d-2}$ is also interesting because it contains the C-theorem as a particular case. Indeed, in the limit $d \rightarrow 2$, $\Delta\mu_{d-2} R^{d-2} \rightarrow -\frac{1}{6}(c_{UV} - c_{IR}) \log(mR)$, and

$$c_{UV} - c_{IR} = 3\pi \int d^2 x \, x^2 \langle \Theta(x) \Theta(0) \rangle \geq 0 . \quad (7.6)$$

Eq. (7.6), established first in [248], is known as a sum-rule: the integrand in the right hand side depends on the RG trajectory, but its integral should only depend on the end-point central charges.

Further progress on understanding the coefficients in the expansion of the EE was

made in [43], which showed that

$$\Delta\mu_{d-4} \geq 0, \quad d \geq 4. \quad (7.7)$$

The A-theorem is obtained for $d \rightarrow 4$. Given these results, it is natural to conjecture that the higher order terms satisfy

$$(-1)^k \Delta\mu_{d-2k} \geq 0. \quad (7.8)$$

This would also imply the validity of A-theorems for all even d by setting $2k = d$. So far there is no proof of this conjecture.

Our goal in this chapter is to analyze the $\Delta\mu_{d-2k}$ in theories with gravity duals. With this aim, we consider asymptotically AdS geometries that represent holographic RG flows. We will find that the Hamilton-Jacobi equation for the holographic EE as a function of the radius R and a radial cutoff ϵ provides an efficient method for obtaining the μ_{d-2k} . The null energy condition will then allow us to establish new inequalities of the form (7.8). We will obtain holographic expressions for μ_{d-4} and μ_{d-6} , and will prove (7.8) for $k = 1, 2, 3$. The result for $k = 3$ is also conceptually important as it goes beyond current results based on strong subadditivity. It also gives further support for the conjecture (7.8) which, however, we will not be able to prove in general.

The remainder of the chapter is structured as follows. In Sec. 7.2 we describe the holographic setup. In Sec. 7.3 we derive the Hamilton-Jacobi (HJ) equation for the holographic EE, we discuss properties of the large radius expansion, and we compare this with the linearized holographic RG. Secs. 7.4 and 7.5 contain the main results – the expressions for $\mu_{d-2}, \mu_{d-4}, \mu_{d-6}$ and the associated inequalities. Finally, in Sec. 7.6 we present a conclusion and future directions. Additional explicit calculations that supplement the main text are given in the Appendix E, where in particular we explore an alternative method based on solving the minimal surface equation and matching UV and IR approximations.

7.2 Holographic setup

In this chapter we consider QFTs that are described by a UV CFT at very short distances, and a different IR CFT at long distances. The two fixed points are connected by an RG flow. For concreteness, we can think that this RG flow is triggered by perturbing the UV CFT by a single relevant deformation,

$$S = S_{\text{CFT,UV}} + \int d^d x g \mathcal{O}(x), \quad (7.9)$$

where $\mathcal{O}$ is a primary operator of dimension $\Delta < d$. The relevant coupling g defines a mass scale typical for the RG, $m \sim g^{1/(d-\Delta)}$. Multiple relevant operators can also be added, and this will not change our analysis. We will probe the properties of the RG flow using the entanglement entropy for a spherical region of radius R . We will focus on QFTs that admit gravity duals, where the EE is calculated by the Ryu-Takayanagi (RT) formula [38, 39, 249]. Let us briefly describe this next.

7.2.1 Gravity dual

The holographic dual is taken as Einstein-Hilbert gravity coupled to a scalar field ϕ dual to the relevant operator $\mathcal{O}$:

$$S = \frac{1}{16\pi G_N^{(d+1)}} \int d^{d+1}x \sqrt{-g} (R^{(d+1)} - g^{MN} \partial_M \phi \partial_N \phi - V(\phi)) - \frac{1}{8\pi G_N^{(d+1)}} \int d^d x \sqrt{\gamma} K. \quad (7.10)$$

Additional scalars are straightforward to include. In order to represent an arbitrary RG flow between two fixed points, the potential should have two critical points at ϕ_c such that $V(\phi_c) = -\frac{d(d-1)}{2\ell_c^2}$, where $c = \text{UV, IR}$ (see Figure 7.1). If $\phi = \phi_c$, the gravity solution is AdS_{d+1} with radius ℓ_c . We require that the matter sector satisfies the NEC. This energy condition has been used previously in the holographic proof of the irreversibility of the universal term in arbitrary dimensions [239–241]. Moreover it is the weakest of the most common local conditions [250].

The solution to the scalar wave equation in AdS has two decay modes near the

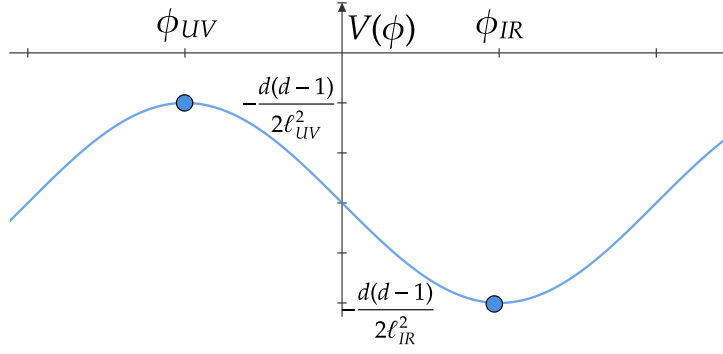


Figure 7.1: Schematic representation of the bulk potential that interpolates between the UV and IR fixed points for an arbitrary holographic RG flow. The conformal fixed points at ϕ_c have $V(\phi_c) = -\frac{d(d-1)}{2\ell_c^2}$ and are described by AdS_{d+1} geometries with radius ℓ_c ($c = \text{UV}, \text{IR}$).

asymptotic boundary: a source-type term, and the VEV-type term [37]. The relevant deformation (7.9) is dual to turning on a source in the asymptotic boundary. This perturbs ϕ away from ϕ_{UV} , which will then evolve radially towards ϕ_{IR} . The background that describes this (preserving Poincare symmetry in the boundary) can be parametrized as

$$ds^2 = \frac{\ell_{UV}^2}{z^2} \left(\frac{dz^2}{f(z)} - (dx^0)^2 + d\rho^2 + \rho^2 d\Omega_{d-2}^2 \right), \quad \phi = \phi(z). \quad (7.11)$$

To proceed, we will only need the following properties. First, note that when $f(z) = 1$ for all z , this geometry recovers the AdS_{d+1} spacetime with radius ℓ_{UV} . For arbitrary $f(z)$ we only require that $f(z) \rightarrow 1$ near the asymptotic boundary $z \rightarrow 0$. On the other hand, at large z , $f \rightarrow (\ell_{UV}/\ell_{IR})^2$. Also, the NEC for the matter sector translates on the equations of motions to the monotonicity requirement $f'(z) > 0$. So in summary, the main properties of the scale factor are

$$1 \leq f(z) \leq \left(\frac{\ell_{UV}}{\ell_{IR}} \right)^2, \quad f'(z) \geq 0, \quad (7.12)$$

with $f'(z) = 0$ for AdS_{d+1} spacetimes. See Appendix E.1 for more details.

7.2.2 Holographic Entanglement Entropy

For an entangling region Σ in a constant time slice, the holographic EE in asymptotically AdS spacetimes is given by the Ryu-Takayanagi prescription [38, 249]

$$S = \min \frac{\text{Area}(\sigma)}{4G_N^{(d+1)}}, \quad (7.13)$$

where σ is a codimension-2 hypersurface in the bulk, anchored on $\partial\Sigma$ and which minimizes the area; $G_N^{(d+1)}$ is the $(d+1)$ -dimensional Newton constant. This result was established in [39].

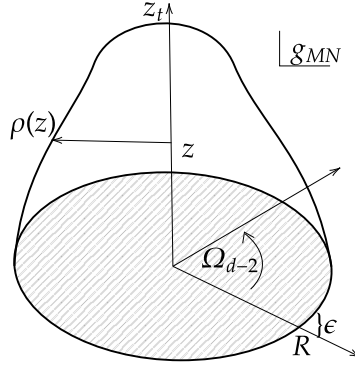


Figure 7.2: Representation of the minimal surface σ for a spherical region Σ of radius R anchored at $z = \epsilon$.

To calculate the area of the minimal surface σ we exploit the fact that the bulk metric (7.11) is diagonal and that the boundary is time independent and spherically symmetric. The minimal surface is a $(d-1)$ -hypersurface parametrized by $d-2$ angular variables Ω_i and a radial function $\rho(z)$. See Figure 7.2 for a schematic representation. Thus, S is given by

$$S = \gamma_d \int_{\epsilon}^{z_t} dz \frac{\rho(z)^{d-2}}{z^{d-1}} \sqrt{(\rho'(z))^2 + \frac{1}{f(z)}}, \quad \gamma_d \equiv \frac{\text{Vol}(S^{d-2}) \ell_{\text{UV}}^{d-1}}{4G_N^{(d+1)}} = \frac{2\pi^{\frac{d-1}{2}}}{\Gamma(\frac{d-1}{2})} \frac{\ell_{\text{UV}}^{d-1}}{4G_N^{(d+1)}}, \quad (7.14)$$

where ϵ is a geometric cutoff that regulates the entropy, and z_t is a bulk radial turning point.² The turning point z_t arises at $\rho = 0$ as a consequence of spherical symmetry.

²The radial cutoff ϵ , which preserves Poincare invariance, is dual to the TT deformation in the UV CFT [251].

7.2 Holographic setup

The profile described by $\rho(z)$ has the boundary condition

$$\rho(\epsilon) = R. \quad (7.15)$$

The turning point obeys

$$\rho(z_t) = 0, \quad \rho'(z_t) = -\infty. \quad (7.16)$$

Note also that when the size of the entangling region $R \rightarrow 0$, the minimal surface collapses to a point, and this gives zero area,

$$\lim_{R \rightarrow 0^+} S = 0. \quad (7.17)$$

We must evaluate S on the profile $\rho(z)$ that minimizes the area. This is the solution for $\rho(z)$ given by the Euler-Lagrange equation for (7.14),

$$\rho(z)z^{d-1}\sqrt{\rho'(z)^2 + \frac{1}{f(z)}}\partial_z\left(\frac{\rho'(z)}{z^{d-1}\sqrt{\rho'(z)^2 + \frac{1}{f(z)}}}\right) - \frac{(d-2)}{f(z)} = 0. \quad (7.18)$$

This is a non-linear second order ODE in z for $\rho(z)$. It cannot be solved in closed form for a general metric $f(z)$ except for $d = 2$.

At large R , (7.18) can be solved approximately in the UV and IR regions, and then both expressions can be matched in some overlapping regime [242, 243]. We will discuss this in Appendix E.2. But we will find it more convenient to apply the Hamilton-Jacobi method at large R , and we turn to this next.

7.3 Hamilton-Jacobi approach

The Hamilton-Jacobi method for a mechanical degree of freedom $q(t)$ gives an equation for its on-shell action S as a function of initial data $q(t_0) = q_0$,

$$-\frac{\partial S(q_0, t_0)}{\partial t_0} = H\left(q_0, p_0 = \frac{\partial S}{\partial q_0}, t_0\right), \quad (7.19)$$

with H the Hamiltonian. It appears naturally in holography with the radius playing the role of time, and the on-shell gravity action giving the large N partition function of the dual field theory. In this context, the HJ formulation is very convenient as it gives directly an equation for the on-shell action in terms of boundary data, without having to go through solving the bulk equations of motion. It has been applied extensively to the holographic RG, starting from [252], to Wilson loops [253] and to the entanglement entropy [254, 255], among others.

7.3.1 Derivation

We begin by briefly reviewing how to obtain (7.19) for the holographic entropy (7.14), explaining some subtle points specific to our case.

The solution to the equation of motion (7.18) gives a function $\rho(z; \epsilon, R)$ that depends explicitly on the boundary data ϵ and R . Similarly, the on-shell entropy is a function $S = S(\epsilon, R)$. In general, the derivatives $\partial_z \rho$ and $\partial_\epsilon \rho$ are different. However, at $z = \epsilon$, we have $\rho(z = \epsilon; \epsilon, R) = R$. Since R is independent of ϵ , the total derivative $d\rho/d\epsilon = 0$ at $z = \epsilon$, and hence

$$\left.\frac{\partial \rho}{\partial \epsilon}(z; \epsilon, R)\right|_{z=\epsilon} = -\left.\frac{\partial \rho}{\partial z}(z; \epsilon, R)\right|_{z=\epsilon}. \quad (7.20)$$

This relation is needed for the following derivation.

To proceed, we compute the variation $\partial_\epsilon S(\epsilon, R)$. This varies the endpoints as well as the integrand in (7.14), which on-shell depends on ϵ . There is no contribution from varying the endpoint z_t , because the integrand vanishes at $z = z_t$. On the other hand, varying the integrand, imposing the equation of motion and integrating by parts, gives

7.3 Hamilton-Jacobi approach

a purely boundary term. Using here (7.20) and combining with the contribution from the endpoint at $z = \epsilon$ obtains

$$\frac{\partial S}{\partial \epsilon} = -\frac{\gamma_d}{f(z)} \frac{\rho(z)^{d-2}}{z^{d-1}} \frac{1}{\sqrt{(\partial_z \rho)^2 + \frac{1}{f(z)}}} \Big|_{z=\epsilon}. \quad (7.21)$$

We recognize the right hand side as minus the Hamiltonian $H = L - \frac{\partial L}{\partial \rho'} \rho'$ at $z = \epsilon$.

To complete the derivation, we need the relation between the momentum conjugate to $\rho(z)$ and $\partial_R S$. A calculation very similar to the one just described gives

$$\frac{\partial S}{\partial R} = -\gamma_d \frac{\rho(z)^{d-2}}{z^{d-1}} \frac{\partial_z \rho}{\sqrt{(\partial_z \rho)^2 + \frac{1}{f(z)}}} \Big|_{z=\epsilon}. \quad (7.22)$$

Using this equation to write $\partial_z \rho$ in terms of $\partial_R S$ and replacing into (7.21), we arrive at

$$\frac{\partial S}{\partial \epsilon} = -\frac{1}{f(\epsilon)^{1/2}} \sqrt{\left(\gamma_d \frac{R^{d-2}}{\epsilon^{d-1}}\right)^2 - \left(\frac{\partial S}{\partial R}\right)^2}. \quad (7.23)$$

This is the desired HJ equation for the holographic entanglement entropy. It has to be solved in the domain $\epsilon \in (0, \infty)$, $R \in (0, \infty)$ and, recalling (7.17), the boundary condition is

$$S(\epsilon, R \rightarrow 0^+) = 0. \quad (7.24)$$

We will use it to solve directly for $S = S(\epsilon, R)$ without recourse to the equations of motion.

A conceptually important point is that, while originally ϵ was introduced as a very small and fixed geometric cutoff, in the HJ equation ϵ is varied in $0 < \epsilon < \infty$. This is very similar to what happens with the running Wilsonian cutoff, and is at the basis of the connection between the HJ equation and the holographic RG [252].

We will also use an equivalent form of (7.23),

$$f(\epsilon) \left(\frac{\partial S}{\partial \epsilon}\right)^2 + \left(\frac{\partial S}{\partial R}\right)^2 = \left(\gamma_d \frac{R^{d-2}}{\epsilon^{d-1}}\right)^2. \quad (7.25)$$

This is an eikonal equation, and it would be interesting to explore potential connections

with the bit thread formulation [256], something that we leave for future work.³

7.3.2 Exact solution for pure AdS

It is in general not possible to solve explicitly the HJ equation (7.23) for arbitrary $f(z)$, but we will shortly see that it can be easily solved in a large R expansion. Before turning to that, however, we will focus on the case of pure AdS_{d+1} , $f(z) = 1$ for all z , where an exact solution can be obtained.

We solve the equation by proposing that the entropy depends on the dimensionless combination $y(\epsilon, R) = \sqrt{\left(\frac{R}{\epsilon}\right)^2 + 1}$, $S(\epsilon, R) = S(y(\epsilon, R))$.⁴ For $R = 0$ there is no entanglement entropy in this new variable so the boundary condition (7.24) is written as

$$S_{\text{AdS}}(y = 1) = 0. \quad (7.26)$$

Now the new equation in one variable is integrable

$$\frac{dS_{\text{AdS}}}{dy} = \gamma_d (y^2 - 1)^{\frac{d-3}{2}}. \quad (7.27)$$

Using the condition (7.26) we get the final result

$$S_{\text{AdS}}(y) = \gamma_d \int_1^y d\tilde{y} (\tilde{y}^2 - 1)^{\frac{d-3}{2}}. \quad (7.28)$$

The result is the incomplete beta function⁵

$$\begin{aligned} S_{\text{AdS}}(y) &= \gamma_d \int_{1/y}^1 d\omega \, \omega^{1-d} (1 - \omega^2)^{\frac{d-3}{2}} \\ &= \frac{\gamma_d}{2} \left(-B \left(\frac{1}{1 + \left(\frac{R}{\epsilon}\right)^2}; \frac{2-d}{2}, \frac{d-1}{2} \right) + \frac{\Gamma(\frac{2-d}{2})\Gamma(\frac{d-1}{2})}{\sqrt{\pi}} \right). \end{aligned} \quad (7.29)$$

³A similar result for the gravitational action is interpreted as the WKB limit of the bulk Wheeler-de Witt equation [252, 257].

⁴This particular combination is actually z_t/ϵ and is motivated by the solution using the Euler-Lagrange equation in Appendix E.2, where it is clear that the surface that minimizes the area is a cut of a sphere of radius $\sqrt{R^2 + \epsilon^2}$.

⁵The incomplete beta function $B(x; a, b) = \int_0^x dt \, t^{a-1} (1-t)^{b-1}$ for $a, b > 0$ and $0 \leq x \leq 1$.

The expansion in powers of $\frac{\epsilon}{R}$ gives

$$\begin{aligned}
 -\frac{1}{2}B\left(\frac{1}{1+\left(\frac{R}{\epsilon}\right)^2}, \frac{2-d}{2}, \frac{d-1}{2}\right) &= \left(\frac{R}{\epsilon}\right)^{d-2} \left(\frac{1}{(d-2)} - \frac{1}{2(d-4)} \left(\frac{\epsilon}{R}\right)^2 + \dots \right. \\
 &\quad \left. + (-1)^{k+1} \frac{(2k-3)!!}{(2k-2)!!} \frac{1}{(d-2k)} \left(\frac{\epsilon}{R}\right)^{2(k-1)} + \dots \right).
 \end{aligned} \tag{7.30}$$

We recognize the structure (7.1), with

$$\mu_{d-2k}^{UV CFT}(\epsilon) = (-1)^{k+1} \frac{(2k-3)!!}{(2k-2)!!} \frac{1}{(d-2k)} \frac{1}{\epsilon^{d-2k}}. \tag{7.31}$$

In particular, the logarithmic universal term is recovered for even $d = 2k$ recalling that

$$\frac{\Gamma(\frac{2-d}{2})\Gamma(\frac{d-1}{2})}{2\sqrt{\pi}} = \left((-1)^k \frac{(2k-3)!!}{(2k-2)!!} \right) \frac{1}{(d-2k)} + \mathcal{O}\left((d-2k)\right), \tag{7.32}$$

and

$$\lim_{d \rightarrow 2k} \frac{x^{(d-2k)} - 1}{(d-2k)} = \log(x). \tag{7.33}$$

It is worth noting that these coefficients are different from the ones obtained in the original calculation [249] –except for the universal terms that are identical. This is due to a different radial cutoff: in [249], the integral starts at $z = \epsilon$, but the boundary condition is taken as $\rho(z=0) = R$. In our case, we instead impose $\rho(z=\epsilon) = R$. One could view ϵ simply as a regulator, always taking $\epsilon \rightarrow 0$, and then we have just two different regularization schemes. However, in the HJ approach it is important that we vary ϵ over all scales in order to solve the HJ equation. So it is not necessarily the smallest scale in the problem. In fact, the EE with the cutoff procedure of [249] does not satisfy the HJ equation (7.25). We instead prefer to view the introduction of the Dirichlet wall at $z = \epsilon$ as a physical deformation of the boundary theory, akin to the TT deformation [251].

7.3.3 Large R expansion

We will now use the HJ equation to solve for the entropy in the large R expansion. Let us first analyze some properties of this expansion.

The RG flow introduces some characteristic mass scale $m \sim g^{1/(d-\Delta)}$ (see (7.9)), which in the gravity side translates into the value of z for which $f(z)$ starts to differ appreciably from the UV value $f(0) = 1$. At long distances, the theory flows to an IR fixed point; in gravity language, $f(z \rightarrow \infty) \sim \ell_{UV}^2/\ell_{IR}^2$. This regime is probed by the EE with radius $R \gg 1/m$. As reviewed in Sec. 2.1, near a fixed point the EE admits a geometric expansion

$$\begin{aligned} S(\epsilon, R) &= \gamma_d (\mu_{d-2}(\epsilon) R^{d-2} + \mu_{d-4}(\epsilon) R^{d-4} + \mu_{d-6}(\epsilon) R^{d-6} + \dots) \\ &= \gamma_d \left(\sum_{k=1}^{\lfloor d/2 \rfloor} R^{d-2k} \mu_{d-2k}(\epsilon) + \dots \right). \end{aligned} \quad (7.34)$$

In the semiclassical bulk description, the leading contribution to the EE is proportional to γ_d , as in (7.14).⁶ To simplify the following formulas, we have made γ_d explicit here in front of the large R expansion. The coefficients μ_{d-2k} here then differ from their QFT counterparts (7.1) by this factor of γ_d .

The expansion is valid for positive integer powers of R . The terms that decay with R (the ‘...’ in the last line) generically have non-integer powers; these are related to the specific dimensions of the leading irrelevant operators that control the approach to the IR fixed point. We will not consider such terms in this chapter; Refs. [242, 243] studied them in holographic theories.

The entropy is dimensionless, so μ_{d-2k} has dimensions of $1/(\text{length})^{d-2k}$ to compensate. On dimensional grounds then, for a dimensionless function $\hat{\mu}_{d-2k}$

$$\mu_{d-2k} = \frac{1}{\epsilon^{d-2k}} \hat{\mu}_{d-2k}(g\epsilon^{d-\Delta}). \quad (7.35)$$

These expressions are not known in general; however, their parametric dependence may

⁶In dual QFT variables, $\gamma_d \sim C_T$, the coefficient in the stress tensor two-point function. For instance, in $\mathcal{N} = 4$ $SU(N)$ super Yang-Mills, $\gamma_d \sim N^2$.

be understood near a fixed point using conformal perturbation theory. In particular, near the UV fixed point $\epsilon \ll g^{1/(d-\Delta)}$ we expect, up to order one constants,

$$\mu_{d-2k} \sim \frac{1}{\epsilon^{d-2k}} + \frac{1}{\epsilon^{d-2k}} (g^2 \epsilon^{2(d-\Delta)}) + \dots + g^{\frac{d-2k}{d-\Delta}}, \text{ for } \epsilon \ll g^{1/(d-\Delta)}, \quad (7.36)$$

where we used that the leading perturbation arises at order $g^2 \langle \mathcal{O}\mathcal{O} \rangle$ [258].

The first term is an ultraviolet divergence coming from the UV CFT. The simplest example is the divergent area term, but such divergences also afflict other terms in the geometric large R expansion. The second term, on the other hand, is a consequence of the relevant perturbation. Recalling that $\Delta < d$, this term will diverge for $\epsilon \rightarrow 0$ in the window

$$\frac{d+2k}{2} < \Delta < d. \quad (7.37)$$

These divergences are familiar from renormalizable interactions in QFT. They may also be understood from the gravitational action induced by the QFT. We will instead restrict to

$$\Delta < \frac{d+2k}{2}, \quad (7.38)$$

so that there are no UV divergences associated to the relevant perturbation. While the μ 's are cutoff dependent, the difference $\Delta\mu_{d-2k}$ is finite as $\epsilon \rightarrow 0$,

$$\Delta\mu_{d-2k} \sim g^{\frac{d-2k}{d-\Delta}}. \quad (7.39)$$

Therefore, by comparing the large radius expansion of the UV fixed point and of the theory with nontrivial RG flow we obtain physical (cut-off independent) entropy coefficients $\Delta\mu_{d-2k}$. They are a property of the continuum theory.⁷ The inequalities below will refer to these coefficients.

Let us now obtain the differential equations for the coefficients μ_{d-2k} . For this, we

⁷Instead of restricting Δ as in (7.38) there is another possibility. It was found in [244] that the strong subadditivity formulas also work if one compares the EE $S(R)$ to the entropy of the CFT plus appropriate ‘counterterms’ whose role is to cancel the UV divergences. However, this procedure in the gravity dual gives rise to expressions whose sign is not fully determined by the NEC. So we will not pursue this approach here.

replace (7.34) into (7.23) and set to zero the coefficient multiplying each independent power R^{d-2k} . Denoting $\epsilon \rightarrow z$ here, this gives linear differential equations $\mu'_{d-2k}(z)$ in terms of lower μ 's. In particular, the first three are

$$\begin{aligned}\partial_z \mu_{d-2} &= -\frac{1}{z^{d-1} f(z)^{1/2}} \\ \partial_z \mu_{d-4} &= \frac{(d-2)^2}{2} \frac{z^{d-1}}{f(z)^{1/2}} \mu_{d-2}(z)^2 \\ \partial_z \mu_{d-6} &= \frac{(d-2)^4}{8} \frac{z^{3(d-1)}}{f(z)^{1/2}} \mu_{d-2}(z)^4 + (d-2)(d-4) \frac{z^{d-1}}{f(z)^{1/2}} \mu_{d-2}(z) \mu_{d-4}(z).\end{aligned}\tag{7.40}$$

Therefore, the HJ equation in the large R expansion gives first order equations that can be solved iteratively. The area coefficient μ_{d-2} is sourced by the inhomogeneous area term in the HJ equation, and the higher order coefficients are in turn sourced by a nontrivial μ_{d-2} . In Secs. 7.4 and 7.5 we will solve these equations and establish inequalities for the resulting solutions.

7.3.4 Linearized approximation

The Wilsonian RG can often be seen as an infinitesimal step in the exact RG [259–261] and holographic RG equations [252, 257, 262]. It is then interesting to consider a linearized version of the EE HJ equation in order to derive a flow interpretation. The connection with the RG was stressed in [254].

With this aim, let us consider the first step in the large radius expansion, writing

$$S(\epsilon, R) = \gamma_d \left(S_{area}(\epsilon, R) + \hat{S}(\epsilon, R) \right), \tag{7.41}$$

where S_{area} cancels the inhomogenous right hand term in (7.25),

$$S_{area}(\epsilon, R) = R^{d-2} \int_{\epsilon}^{\infty} \frac{dz}{z^{d-1} f(z)^{1/2}} = R^{d-2} \mu_{d-2}(\epsilon). \tag{7.42}$$

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The HJ equation for $\hat{S}$ then reads

$$-2\frac{R^{d-2}}{\epsilon^{d-1}}f(\epsilon)^{1/2}\partial_\epsilon\hat{S} + \frac{2(d-2)}{R}S_{area}\partial_R\hat{S} + f(\epsilon)(\partial_\epsilon\hat{S})^2 + (\partial_R\hat{S})^2 = -\frac{(d-2)^2}{R^2}S_{area}^2. \quad (7.43)$$

This is still the complete HJ equation now for $\hat{S}$; it contains both linear and quadratic terms, and shows that S_{area} acts like a source term for $\hat{S}$.

The idea now is to neglect the terms that are quadratic in derivatives of $\hat{S}$,

$$-2\frac{R^{d-2}}{\epsilon^{d-1}}f(\epsilon)^{1/2}\partial_\epsilon\hat{S} + \frac{2(d-2)}{R}S_{area}\partial_R\hat{S} \approx -\frac{(d-2)^2}{R^2}S_{area}^2. \quad (7.44)$$

We will check the validity of this approximation shortly. This equation may be interpreted as a geometric flow equation for the EE, relating the change in cutoff to the geometric deformation $\partial_R\hat{S}$ and the area term.

The linear differential equation can be solved by the method of characteristics. The general solution is

$$\begin{aligned} \hat{S}_{ren}(\epsilon, R) = & -\frac{(d-2)^2}{2} \int_\epsilon^\infty dv \frac{v^{d-1}\mu_{d-2}(v)^2}{f(v)^{1/2}} \left[R^2 + 2(d-2) \int_v^\epsilon du \frac{u^{d-1}}{f(u)^{1/2}} \mu_{d-2}(u) \right]^{\frac{d-4}{2}} \\ & + G \left(\sqrt{R^2 + 2(d-2) \int_{\epsilon_0}^\epsilon dv \frac{v^{d-1}}{f(v)^{1/2}} \mu_{d-2}(v)} \right), \end{aligned} \quad (7.45)$$

where $G(\eta)$ is some arbitrary function we should fix with boundary conditions, and ϵ_0 comes from a choice of integration constant in the method.

In order to assess the validity of the linearized approximation, we expand $\hat{S}$ at large R in terms of the μ_{d-2p} , and plug into (7.44). This gives ODEs term by term in the $1/R$ expansion; the first are

$$\begin{aligned} -2z\sqrt{f(z)}\mu'_{d-4}(z) + (d-2)^2z^d\mu_{d-2}(z)^2 &= 0 \\ -2z\sqrt{f(z)}\mu'_{d-6}(z) + 2(d-4)(d-2)z^d\mu_{d-2}(z)\mu_{d-4}(z) &= 0 \\ -2z\sqrt{f(z)}\mu'_{d-8}(z) + 2(d-6)(d-2)z^d\mu_{d-2}(z)\mu_{d-6}(z) &= 0. \end{aligned} \quad (7.46)$$

As opposed to the full nonlinear ODEs for the μ_{d-2p} , these keep only terms that are linear in $(\mu_{d-4}, \mu_{d-6}, \dots)$.

Relating (7.40) and (7.46), we find that μ_{d-4} is captured completely by the linearized approximation, while from the order μ_{d-6} the linearized approximation fails. The quadratic terms that are neglected (7.44) turn out to be comparable to (7.46) beginning at $O(R^{d-6})$, and for this reason the linearized approximation is not useful for such non-universal terms. The equations (7.40) are still linear differential equations in the unknowns, and hence resemble RG beta functions for the entropy coefficients. But getting these right requires taking into account more nonlinear terms beyond the leading area contribution.

7.3.5 Sphere free energy

The large R expansion (7.34) must be modified for odd space-time dimensions d and has to include a term $F(\epsilon)$,

$$S(\epsilon, R) = \gamma_d (\mu_{d-2}(\epsilon) R^{d-2} + \mu_{d-4}(\epsilon) R^{d-4} + \mu_{d-6}(\epsilon) R^{d-6} + \dots) + (-1)^{\frac{d-1}{2}} F(\epsilon). \quad (7.47)$$

Inserting this new expansion in the Hamilton-Jacobi equation (7.25) gives

$$F'(\epsilon) = 0, \quad (7.48)$$

therefore F is a constant. In a CFT this is the constant term of the free energy of a d dimensional euclidean sphere [198, 263].

The term F can be fully determined at fixed points in our holographic context from the expression (7.29) for the entropy when $f(z)$ is constant. More precisely,

$$S^{\text{UV}} \supset \gamma_d \frac{\Gamma(\frac{2-d}{2})\Gamma(\frac{d-1}{2})}{2\sqrt{\pi}}, \quad S^{\text{IR}} \supset \gamma_d \left(\frac{\ell_{\text{IR}}}{\ell_{\text{UV}}} \right)^{d-1} \frac{\Gamma(\frac{2-d}{2})\Gamma(\frac{d-1}{2})}{2\sqrt{\pi}}, \quad (7.49)$$

7.4 Analysis of the R^{d-2} and R^{d-4} terms

are the constant terms in the UV and IR expansions. This gives the inequality⁸

$$\Delta F = F^{\text{IR}} - F^{\text{UV}} = \frac{(-1)^{\frac{d-1}{2}} \pi^{\frac{d-2}{2}} \Gamma\left(\frac{2-d}{2}\right)}{4G_N^{(d+1)}} (\ell_{\text{IR}}^{d-1} - \ell_{\text{UV}}^{d-1}) \leq 0 \quad \forall d \text{ odd}, \quad (7.50)$$

because of $\ell_{\text{UV}} \geq \ell_{\text{IR}}$ as a consequence of the NEC (7.12) and the positivity of the prefactor for d odd. This F-theorem was obtained by [240, 241] in an holographic analysis for all d odd and by [42, 43] using QFT methods involving the SSA in $d = 3$. At the moment there is no QFT proof for F-theorems in $d > 3$ spacetime dimensions.

7.4 Analysis of the R^{d-2} and R^{d-4} terms

In this section we calculate the $\mu_{d-2}(z)$ and $\mu_{d-4}(z)$ terms in the large R expansion of the EE. The area term has been calculated for holographic theories in [195] using a different method based on stress-tensor correlators; we will reproduce their result. The holographic result for $\mu_{d-4}(z)$ has not appeared in the literature, as far as we are aware.

For each coefficient we give expressions in terms of a single integral involving $f(z)$ that allow to prove the inequalities $\Delta\mu_{d-2} \leq 0$ and $\Delta\mu_{d-4} \geq 0$ for $\Delta\mu_{d-2k} = \mu_{d-2k} - \mu_{d-2k}^{\text{UV CFT}}$ using the NEC (7.12). We will also rewrite these coefficients in a way that makes manifest the anomaly result when $d \rightarrow 2$ and $d \rightarrow 4$ respectively. This “anomaly oriented” procedure will also be useful for our analysis of $\Delta\mu_{d-6} \leq 0$ in Sec. 7.5.

7.4.1 $\Delta\mu_{d-2}(z)$

The equation for $\mu_{d-2}(z)$ is

$$\mu'_{d-2}(z) = -\frac{1}{z^{d-1} f(z)^{1/2}}. \quad (7.51)$$

⁸The holographic value for F matches with the universal term $a_d^* = \frac{\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \left(\frac{\ell}{\ell_P}\right)^{d-1}$ defined in [240, 241] via the identification $F = 2\pi a_d^*$, $\ell_P^{d-1} = 8\pi G_N^{(d+1)}$ and recalling that $\frac{(-1)^{\frac{d-1}{2}} \Gamma(1-\frac{d}{2})}{\pi} = \frac{1}{\Gamma(\frac{d}{2})}$ due to the Euler’s reflection formula.

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The integration constant should be independent of R , and z ; moreover for $z = \epsilon \rightarrow 0$, this must reproduce the UV CFT expansion $\mu_{d-2}^{UV\,CFT}(\epsilon) \sim \epsilon^{-(d-2)}$ (7.31). Therefore, this integrates to

$$\mu_{d-2}(z) = \int_z^\infty \frac{dv}{v^{d-1} f(v)^{1/2}} > 0. \quad (7.52)$$

Subtracting the contribution of pure AdS, $f(v) = 1$, gives the inequality for the area term

$$\Delta\mu_{d-2}(z) = \int_z^\infty \frac{dv}{v^{d-1} f(v)^{1/2}} - \int_z^\infty \frac{dv}{v^{d-1}} \leq 0, \quad (7.53)$$

because $f(z) \geq 1$ for all z . The decrease of the area term coefficient along RG flows has been proved in QFT in [194, 246]. The holographic calculation using stress-tensor correlators was carried out in [195]. Our HJ method is extremely simple and gives the same result.⁹

In the limit $d \rightarrow 2$, (7.53) should reproduce the holographic C-theorem, and so it should only depend on UV and IR CFT quantities and not on the full RG flow. To exhibit this, we integrate by parts the $1/v^{d-1}$ factor,

$$\mu_{d-2}(z) = \frac{1}{d-2} \frac{1}{z^{d-2} f(z)^{1/2}} - \frac{1}{2} \frac{1}{d-2} g_{d-2}(z), \quad (7.54)$$

where we define

$$g_{d-2}(z) \equiv \int_z^\infty \frac{dv}{v^{d-2}} \frac{f'(v)}{f(v)^{3/2}} \geq 0. \quad (7.55)$$

For future use, note that since $\mu_{d-2}(z) > 0$ for all z ,

$$0 \leq g_{d-2}(z) < \frac{2}{z^{d-2} f(z)^{1/2}}. \quad (7.56)$$

⁹To match their result, the appropriate change of variables is $A(r) = \log\left(\frac{\ell_{UV}}{z}\right)$, $A'(r) = \frac{\sqrt{f(z)}}{\ell_{UV}}$.

Finally, taking the limit $z = \epsilon \rightarrow 0$ and recalling that $f(\epsilon) \rightarrow 1$ and $g_{d-2} = 0$ for AdS,¹⁰

$$\Delta\mu_{d-2} = -\frac{1}{2} \frac{1}{d-2} g_{d-2}(0) \leq 0. \quad (7.57)$$

When $d \rightarrow 2$, g_{d-2} becomes a total derivative and the logarithmic term in ΔS is recovered,

$$\frac{\Delta c}{3} = R \left. \frac{d\Delta S}{dR} \right|_{R^{d-2}} = \gamma_2 \left(f(\infty)^{-\frac{1}{2}} - f(0)^{-\frac{1}{2}} \right) = \frac{\ell_{\text{IR}}}{2G_N^{(3)}} - \frac{\ell_{\text{UV}}}{2G_N^{(3)}} = \frac{c_{\text{IR}} - c_{\text{UV}}}{3} \leq 0, \quad (7.58)$$

giving raise to the weak version of the holographic C-theorem. The central charge is identified via $c = \frac{3\ell}{2G_N^{(3)}}$ in $d = 2$ [264].

7.4.2 $\Delta\mu_{d-4}(z)$

After the previous warm-up, we now move to the R^{d-4} coefficient, for which there was no known holographic expression. Starting from the equation,

$$\mu'_{d-4}(z) = \frac{(d-2)^2}{2} \frac{z^{d-1}}{f(z)^{1/2}} \mu_{d-2}(z)^2, \quad (7.59)$$

the solution integrates to

$$\mu_{d-4}(z) = -\frac{(d-2)^2}{2} \int_z^\infty dv \frac{v^{d-1}}{f(v)^{1/2}} \left(\int_v^\infty \frac{du}{u^{d-1} f(u)^{1/2}} \right)^2. \quad (7.60)$$

The expression (7.60) satisfies $\mu_{d-4} < 0$ for all z . Therefore, the NEC gives the

¹⁰In general $\Delta\mu_{d-2k}$ has potentially the most divergent contributions coming from terms that go like $g_{d-2k}(z) = \int_z^\infty \frac{dv}{v^{d-2k}} \frac{f'(v)}{f(v)^{(2k+1)/2}}$ when $z \rightarrow 0$. However because $f(z) = 1 + (\mu z)^{2(d-\Delta)} + \dots$ in the UV limit (E.10), the integrand for such contributions goes like $\sim v^{d-2\Delta+2k-1}$. In the window $\Delta < \frac{d+2k}{2}$ (7.38) the integrand decays slower than v^{-1} for $v \rightarrow 0$, so $\Delta\mu_{d-2k}$ remains finite and cut-off independent when $\epsilon \rightarrow 0$ as discussed in Sec. 7.3.3.

following inequality,

$$\begin{aligned} \Delta\mu_{d-4}(z) &= -\frac{(d-2)^2}{2} \left[\int_z^\infty dv \frac{v^{d-1}}{f(v)^{1/2}} \left(\int_v^\infty \frac{du}{u^{d-1} f(u)^{1/2}} \right)^2 - \int_z^\infty dv v^{d-1} \left(\int_v^\infty \frac{du}{u^{d-1}} \right)^2 \right] \\ &\geq 0. \end{aligned} \tag{7.61}$$

Indeed, the AdS contribution is explicitly larger than the one corresponding to the holographic RG flow, since $f(z) > 1$ is a monotonically increasing function.

Ref. [43] proved $\Delta\mu_{d-4} \leq 0$ in QFT using the strong subadditivity for multiple boosted spheres. Here we have obtained the same result for theories with gravity duals and the NEC, in the large R expansion. It would be interesting to relate (7.60) to euclidean boundary correlators. This would help towards an euclidean proof of the A-theorem, with a corresponding sum rule.

Following what we did before for μ_{d-2} , let us rewrite (7.61) in order to make the holographic A-theorem manifest when $d \rightarrow 4$. From (7.54), we have

$$\mu_{d-2}(z)^2 = \frac{1}{(d-2)^2} \frac{1}{z^{2(d-2)} f(z)} - \frac{g_{d-2}(z)}{4(d-2)^2} \left(\frac{4}{z^{d-2} f(z)^{1/2}} - g_{d-2}(z) \right). \tag{7.62}$$

Replacing into (7.59) and integrating,

$$\mu_{d-4}(z) = -\frac{1}{2} \int_z^\infty \frac{dv}{v^{d-3} f(v)^{3/2}} + \frac{1}{8} \int_z^\infty dv \frac{v^{d-1}}{f(v)^{1/2}} g_{d-2}(v) \left(\frac{4}{v^{d-2} f(v)^{1/2}} - g_{d-2}(v) \right). \tag{7.63}$$

Finally, integrating by parts with respect to $1/v^{d-3}$ in the first term, and defining

$$g_{d-4}(z) \equiv \int_z^\infty \frac{dv}{v^{d-4}} \frac{f'(v)}{f(v)^{5/2}} \geq 0, \tag{7.64}$$

we arrive at

$$\begin{aligned} \mu_{d-4}(z) &= -\frac{1}{2(d-4)} \frac{1}{z^{d-4} f(z)^{3/2}} + \frac{3}{4(d-4)} g_{d-4}(z) \\ &\quad + \frac{1}{8} \int_z^\infty dv \frac{v^{d-1}}{f(v)^{1/2}} g_{d-2}(v) \left(\frac{4}{v^{d-2} f(v)^{1/2}} - g_{d-2}(v) \right). \end{aligned} \tag{7.65}$$

7.5 Beyond the SSA: the R^{d-6} term

Note that from the integration by parts,

$$\frac{1}{2} \int_z^\infty \frac{dv}{v^{d-3} f(v)^{3/2}} = \frac{1}{d-4} \frac{1}{z^{d-4} f(z)^{3/2}} - \frac{3}{2(d-4)} g_{d-4}(z) \geq 0 \quad (7.66)$$

we obtain the bound

$$0 \leq g_{d-4}(z) < \frac{2}{3} \frac{1}{z^{d-4} f(z)^{3/2}}. \quad (7.67)$$

Finally setting $z = \epsilon \rightarrow 0$ and subtracting the pure AdS result, we obtain the desired inequality

$$\Delta\mu_{d-4} = \frac{3}{4(d-4)} g_{d-4}(0) + \frac{1}{8} \int_0^\infty dv \frac{v^{d-1}}{f(v)^{1/2}} g_{d-2}(v) \left(\frac{4}{v^{d-2} f(v)^{1/2}} - g_{d-2}(v) \right) \geq 0. \quad (7.68)$$

The last term is positive semidefinite because of (7.56). It contributes by a finite amount to the entropy and depends on the full RG flow. In the window (7.38) for $k = 2$, this is finite for $\epsilon \rightarrow 0$ and hence we have a physical cut-off independent coefficient.

When $d \rightarrow 4$, g_{d-4} becomes a total derivative and the logarithmic term in ΔS is recovered,

$$-4\Delta a = R \frac{d\Delta S}{dR} \Big|_{R^{d-4}} = \frac{\gamma_4}{2} \left(f(0)^{-\frac{3}{2}} - f(\infty)^{-\frac{3}{2}} \right) = -\frac{\pi\ell_{\text{IR}}^3}{2G_N^{(5)}} + \frac{\pi\ell_{\text{UV}}^3}{2G_N^{(5)}} = -4(a_{\text{IR}} - a_{\text{UV}}) \geq 0, \quad (7.69)$$

where the a -anomaly is given by $a = \frac{\pi\ell^3}{8G_N^{(5)}}$ in $d = 4$. The extra terms in (7.68) contribute to the constant nonuniversal term when $d \neq 4$.

7.5 Beyond the SSA: the R^{d-6} term

In this section we give an integral expression of $\mu_{d-6}(z)$ in terms of $f(z)$ and provide a proof of the inequality $\Delta\mu_{d-6} \leq 0$ following an anomaly oriented procedure. This is the first term in the large R expansion whose RG flow is not constrained by the boosted strong subadditivity. Surprisingly, we find that the NEC in the large R expansion is sufficient to establish the inequality.

For the present case the equation is

$$\mu'_{d-6}(z) = \frac{(d-2)^4}{8} \frac{z^{3(d-1)}}{f(z)^{1/2}} \mu_{d-2}^4(z) + (d-2)(d-4) \frac{z^{d-1}}{f(z)^{1/2}} \mu_{d-2}(z) \mu_{d-4}(z). \quad (7.70)$$

Unlike what happens with the coefficients in Sec. 7.4, this is the first time there is a competition between two terms of opposite sign (because of (7.52) and (7.60)). Using (7.54) and (7.65), expanding the two terms in (7.70), and integrating,

$$\begin{aligned} \mu_{d-6}(z) = & \int_z^\infty dv \left[-\frac{1}{8} \frac{1}{v^{d-5} f(v)^{1/2}} + \frac{1}{4} \frac{v^3}{f(v)^2} g_{d-2}(v) - \frac{1}{16} \frac{v^{d+1}}{f(v)^{3/2}} g_{d-2}(v)^2 \right. \\ & \left. - \frac{1}{128} \frac{v^{3(d-1)}}{f(v)^{1/2}} g_{d-2}^2(v) \left(\frac{4}{u^{d-2} f(u)^{1/2}} - g_{d-2}(u) \right)^2 \right] \\ & + \int_z^\infty dv \left[\frac{1}{2} \frac{1}{v^{d-5} f(v)^{1/2}} - \frac{1}{4} \frac{v^3}{f(v)^2} g_{d-2}(v) - \frac{1}{2} \frac{v^{d-1}}{f(v)^{1/2}} \left(\frac{2}{v^{d-2} f(v)^{1/2}} - g_{d-2}(v) \right) \right. \\ & \left. \times \left(\frac{3}{4} g_{d-4}(v) + \frac{(d-4)}{8} \int_v^\infty du \frac{u^{d-1}}{f(u)^{1/2}} g_{d-2}(u) \left(\frac{4}{u^{d-2} f(u)^{1/2}} - g_{d-2}(u) \right) \right) \right]. \end{aligned} \quad (7.71)$$

Adding up the first two terms arising from both integrals gives

$$\frac{3}{8} \int_z^\infty \frac{dv}{v^{d-5} f(v)^{1/2}} = \frac{3}{8(d-6)} \frac{1}{z^{d-6} f(z)^{5/2}} - \frac{15}{16(d-6)} g_{d-6}(z) > 0, \quad (7.72)$$

where

$$g_{d-6}(z) \equiv \int_z^\infty \frac{dv}{v^{d-6}} \frac{f'(v)}{f(v)^{7/2}}, \quad (7.73)$$

and because of (7.72)

$$0 \leq g_{d-6}(z) < \frac{2}{5} \frac{1}{z^{d-6} f(z)^{5/2}}. \quad (7.74)$$

Finally, we arrive at

$$\begin{aligned} \mu_{d-6}(z) = & \frac{3}{8(d-6)} \frac{1}{z^{d-6} f(z)^{5/2}} - \frac{15}{16(d-6)} g_{d-6}(z) - \int_z^\infty dv \left[\frac{1}{16} \frac{v^{d+1}}{f(v)^{3/2}} g_{d-2}(v)^2 \right. \\ & + \frac{1}{128} \frac{v^{3(d-1)}}{f(v)^{1/2}} g_{d-2}^2(v) \left(\frac{4}{u^{d-2} f(u)^{1/2}} - g_{d-2}(u) \right)^2 + \frac{1}{2} \frac{v^{d-1}}{f(v)^{1/2}} \left(\frac{2}{v^{d-2} f(v)^{1/2}} - g_{d-2}(v) \right) \\ & \left. \times \left(\frac{3}{4} g_{d-4}(v) + \frac{(d-4)}{8} \int_v^\infty du \frac{u^{d-1}}{f(u)^{1/2}} g_{d-2}(u) \left(\frac{4}{u^{d-2} f(u)^{1/2}} - g_{d-2}(u) \right) \right) \right]. \end{aligned} \quad (7.75)$$

Upon setting $z = \epsilon \rightarrow 0$, and subtracting the pure AdS contribution, we find

$$\begin{aligned} \Delta\mu_{d-6} = & -\frac{15}{16(d-6)}g_{d-6}(0) - \int_0^\infty dv \left[\frac{1}{16} \frac{v^{d+1}}{f(v)^{3/2}} g_{d-2}(v)^2 + \frac{1}{128} \frac{v^{3(d-1)}}{f(v)^{1/2}} g_{d-2}^2(v) \right. \\ & \times \left(\frac{4}{u^{d-2}f(u)^{1/2}} - g_{d-2}(u) \right)^2 + \frac{1}{2} \frac{v^{d-1}}{f(v)^{1/2}} \left(\frac{2}{v^{d-2}f(v)^{1/2}} - g_{d-2}(v) \right) \\ & \left. \times \left(\frac{3}{4}g_{d-4}(v) + \frac{(d-4)}{8} \int_v^\infty du \frac{u^{d-1}}{f(u)^{1/2}} g_{d-2}(u) \left(\frac{4}{u^{d-2}f(u)^{1/2}} - g_{d-2}(u) \right) \right) \right]. \end{aligned} \quad (7.76)$$

Given (7.38), this is finite when $\epsilon \rightarrow 0$. From to the inequalities (7.56) and (7.67), it satisfies the inequality

$$\Delta\mu_{d-6} \leq 0. \quad (7.77)$$

Therefore, we have found that the NEC implies the decrease of the R^{d-6} term along holographic RG flows. Finally, when $d \rightarrow 6$ the function g_{d-6} becomes a total derivative and the logarithmic term is recovered

$$R \frac{d\Delta S}{dR} \Big|_{R^{d-6}} = \frac{3}{8} \gamma_6 \left(f(0)^{-\frac{5}{2}} - f(\infty)^{-\frac{5}{2}} \right) = \frac{\pi^2 \ell_{\text{IR}}^5}{4G_N^{(7)}} - \frac{\pi^2 \ell_{\text{UV}}^5}{4G_N^{(7)}} \leq 0. \quad (7.78)$$

It would be interesting to translate (7.76) into stress tensor correlators. This expression already has the desired features of satisfying the inequality (7.77) and reproducing a sum rule for $d \rightarrow 6$. So it may provide hints towards an A-theorem for $d = 6$.

7.6 Conclusion

In this chapter we analyzed the coefficients $\Delta\mu_{d-2k}$ in the large radius expansion (7.1) of the EE for field theories with gravity duals. These coefficients are finite for RG flows triggered by operators with dimension $\Delta < \frac{d+2}{2}$. Unlike the universal A and F terms, the $\Delta\mu_{d-2k}$ contain information about the full RG flow connecting the UV and IR fixed points. Starting from the Ryu-Takayanagi formula, we derived a Hamilton-Jacobi equation (7.25) for the holographic EE $S(\epsilon, R)$. The cut off ϵ modifies the EE not just by cutting the integral, but also modifying the minimal surfaces, allowing ϵ to take any

value. At large radius, the HJ equation reduces to first order differential equations for the μ_{d-2k} , which are straightforward to solve. We derived explicit holographic results for $\mu_{d-2}, \mu_{d-4}, \mu_{d-6}$ and established the inequalities

$$\Delta\mu_{d-2} \leq 0, \quad \Delta\mu_{d-4} \geq 0, \quad \Delta\mu_{d-6} \leq 0. \quad (7.79)$$

The first two inequalities have been proved before for general QFTs using the boosted strong subadditivity [43] (SSA). On the other hand, the inequality $\Delta\mu_{d-6} \leq 0$ is new and goes beyond the SSA.

Let us end by discussing future directions opened by these results. We have obtained integral expressions for $\Delta\mu_{d-4}$ and $\Delta\mu_{d-6}$ as a function of the metric scale factor. These expressions are a starting point for deriving expressions in terms of euclidean stress-tensor correlators. This would be interesting for different reasons. It could suggest a sum rule for the 4d A-theorem, generalizing the sum rule of $d = 2$ (which uses $\langle T_\mu^\mu(x)T_\nu^\nu(0) \rangle$) to $d = 4$. The $d = 6$ result in terms of stress-tensor correlators, on the other hand, may shed light on a possible A-theorem for that dimensionality.

Another important lesson is that the NEC together with a large radius expansion give rise to the inequality $\Delta\mu_{d-6} \leq 0$ that is stronger than current results using SSA. It would be very useful to translate this into quantum information conditions. It suggests thinking in terms of a large radius expansion in field theory.

Finally, it would be important to push the holographic analysis to the higher coefficients $\Delta\mu_{d-2k}$. The findings support the conjecture

$$(-1)^k \Delta\mu_{d-2k} \geq 0, \quad (7.80)$$

and it would be nice to prove this for theories with gravity duals. The analysis for $\Delta\mu_{d-8}$ and higher coefficients appears to be significantly more involved, possibly requiring new tools so that it can be made systematic.

Chapter 8

Conclusion and outlook

In this dissertation, we investigated various topics of Quantum Computing, including logical magic states preparation protocols, and real-time noise learning techniques for quantum hardware. Moreover, we also investigated the entanglement entropy of the vacuum for some Quantum Field Theories, and discussed the connection with the irreversibility of the Renormalization Group flow.

In Chapter 2, we introduced a novel low-overhead method for preparing high-fidelity logical magic states via code switching between color codes. Using the latter protocol, in Chapter 3, we performed the first experimental demonstration of code-switching between color codes on a trapped ion quantum processor and reported a state-of-the-art logical magic state fidelity. We also developed and realized a sample-efficient characterization method involving two copies of the logical magic state using a Bell basis measurement. Looking forward, extending our approach to higher-distance instances of the color code family may prove to be the next frontier once more qubits are available in future-generation devices. Some challenges of scaling up our protocol consist of generalizing the syndrome extraction circuits, developing a scalable post-selection strategy, and crafting a simulation technique that can handle lower error rates, which are hard to tackle with a naive Monte Carlo sampling approach.

In Chapter 4, we introduced the first scalable and efficient simulation method for logical magic state preparation protocols subjected to circuit-level noise. The efficiency

of our simulation method is rooted in a curious fact: every circuit-level Pauli error in these protocols propagates to a Clifford error at the end. As a proof of principle, we provided numerical results for the preparation of the Hadamard $+1$ -eigenstate on the Steane $[[7,1,3]]$ code. In the future, it would be beneficial to develop a software toolkit capable of handling large-scale simulations of generic magic state preparation protocols. Moreover, we could also develop more efficient decoders besides look-up tables, by gaining an analytic understanding of circuit-level Pauli noise in the presence of non-Clifford gates. Another open question is whether our method can also be generalized to alternative protocols, such as those based on Clifford stabilizer codes [157, 168].

In Chapter 5, we proposed a real-time adaptation method for noise channel estimates associated with quantum gates using extended flag gadgets, mid-circuit measurements and Bayesian inference. Our numerical studies suggest that the technique is very effective in the regime where a maximum number of extended flag gadgets is implemented, but rapidly becomes less effective as the number of flag gadgets is decreased. As a consequence, this technique is most useful in the low noise regime where one can afford to implement the maximum number of flag gadgets, and the impact of noise on their implementation is minimal. We leave the testing of this method using an experiment for future work.

In Chapter 6, we computed the entanglement entropy of the vacuum of a spherical region for free fermionic field theories on a four dimensional Minkowski space-time. Surprisingly, the area coefficient of the entanglement entropy diverges for a radial discretization but is finite for a geometric regularization induced by the mutual information. In conjunction with previous results for bosonic fields [48–50] and the spin-1/2 case [51], our findings contributed the culminating computation of universal logarithmic coefficients for relativistic free field theories with spin $h \leq 2$. Having explicitly computed these coefficients, it would be interesting to explore further how higher-spin theories ($h \geq \frac{3}{2}$), which lack a local gauge invariant stress-energy tensor, relate their universal logarithmic coefficients with possible RG flows of their UV completion.

In Chapter 7, we studied field theories that admit gravitational dual and computed the entanglement entropy of the vacuum of a spherical region in a large radius limit. As a result, we established irreversibility inequalities for sub-leading terms of the entanglement entropy, and reproduced known monotonicity results in particular cases. Looking forward, since the integral expressions for the first two sub-leading terms depend on the metric scale factor, they might be relevant for deriving equivalent expressions based on euclidean stress-tensor correlators. Particularly, this could suggest a sum rule for the 4d irreversibility A-theorem, generalizing the sum rule of $d = 2$ [238, 265], and might furnish key insights on a possible six-dimensional irreversibility A-theorem.

To conclude, I hope the findings of this thesis further our understanding of the quantum behaviour of nature, and serve as an inspiration for future scientific endeavours.

Appendix A

Appendix: Experimental demonstration of high-fidelity logical magic states from code switching

This is the Appendix associated with Chapter 3.

A.1 Experimental setup

We used Quantinuum’s H2-1 trapped-ion processor based on a QCCD architecture [126] to perform the magic state preparation experiments. Regarding the quantum processor, the most recent randomized benchmarking experiments averaged over all four gate zones showed fidelities of $p_1 = 1.9(4) \times 10^{-5}$ and $p_2 = 1.05(8) \times 10^{-3}$ for single-qubit and two-qubit gates, respectively. SPAM errors are dominated by $|1\rangle$ state measurement errors $p_{|1\rangle} = 1.38(12) \times 10^{-3}$, over $|0\rangle$ state measurement errors $p_{|0\rangle} = 6.0(8) \times 10^{-4}$. Crosstalk errors from mid-circuit SPAM operations are $p_{\text{ct}} = 6.6(8) \times 10^{-6}$.

Memory errors per qubit were benchmarked in Ref. [126] using random circuits, resulting in an estimate for memory error per circuit layer (~ 60 ms) of $p_{\text{idle}} = 2.0(2) \times$

A.2 Experimental methods

10^{-4} . However, the circuits used in this work have a very different structure, with some qubits idling for multiple circuit layers. To mitigate coherent accumulation of memory error, we apply dynamical decoupling pulses approximately every 30 ms, ideally keeping the memory error in each layer of gates $\leq 2.0(2) \times 10^{-4}$ while adding a small amount of error from the decoupling pulses ($\sim 1.9(4) \times 10^{-5}$). Confirming these effects is difficult in simulation due to the incompatibility of stabilizer simulations with coherent error accumulation, and a comprehensive experimental characterization of individual error sources' impacts is beyond the scope of this work.

The experiments were prepared using the OPENQASM2.0 programming language, designed to represent quantum circuits. The quantum circuits are then converted to the `Circuit` class using the `pytket` module, so they can be submitted to the H-series compiler stack where they are converted into machine level instructions. In this process, no optimization is utilized. The quantum circuits are also designed such that no classically-controlled operations are applied, thus minimizing the latency time, though we note that previous experiments [105] have shown that real-time application of corrections can be done without significant error.

A.2 Experimental methods

In this Appendix we provide additional information about the data analysis. A summary of the experimental results and numerical emulations is shown in Table A.1.

Quantity	Error-correction		Post-selection	
	Value	Acceptance rate(%)	Value	Acceptance rate(%)
$F(\bar{\rho}, T\rangle\langle T)$	0.99949(27)	82.58	0.99985(11)	81.26
ϵ	$4.56(2.63) \times 10^{-4}$	65.73	$9.28(9.28) \times 10^{-5}$	61.83
$\langle X \rangle_{\bar{\rho}}$	0.6993(78)	83.56	0.6987(78)	82.66
$\langle Y \rangle_{\bar{\rho}}$	0.7193(77)	81.24	0.7197(77)	79.72
$\langle Z \rangle_{\bar{\rho}}$	0.0000(109)	82.96	-0.0007(110)	81.42

Table A.1: Experimental results for the single-and two copy experiments analyzed using an ideal round of error-correction or post-selection/error-detection. The fidelity lower bound is computed using (3.5). The fidelity acceptance rate is the average over the acceptance rates of the single-copy experiments.

In the single-copy experiments (Fig. 3.2) the output of a given shot is a binary string with 31 entries. Out of those 31 bits, 7 of them correspond to Steane code data

qubits, 15 to qRM code data qubits, 4 to Z -type qRM code stabilizers ($\{p_2, p_3, p_8, p_{13}\}$), and 5 to flags (2 from state initialization, and 3 from the Z -type stabilizer circuit measurements). We pre-select and analyze only those shots such that the 4 Z -type stabilizers and 5 flags are +1. Moreover, from the 15 entries corresponding to the X -type destructive measurements of the qRM code data qubits, we extract the qRM X -type syndrome using the definitions shown in Table 2.5. In case any of these X -type syndromes are non-trivial, we discard the shot. Finally, the information from the remaining 7 Steane code data qubits is analyzed to extract logical Pauli basis expected values $\langle \bar{P} \rangle_{\bar{\rho}}$ for $\bar{P} \in \{\bar{X}, \bar{Y}, \bar{Z}\}$. First, the Steane code syndrome is extracted using Table 2.3 (note that for the Steane code, $p_i^y = p_i^z p_i^x$ where p_i^P stands for the i -th P -type stabilizer), followed by a correction which is applied based on a look-up table decoder (in cases where post-selection is considered, only the instances with trivial syndromes are analyzed). Then, the logical operator $\bar{P}$ of the single-copy experiment is computed using the definitions shown in Eqns. (2.1) and (2.2) (note that for the Steane code $\bar{Y} = -Y_1 Y_2 Y_3$). Since the logical $\bar{Z}$ correction of Fig. 3.1 is not physically applied, when the logical $\bar{X}^{\text{qRM}} = -1$ in the qRM code, the resultant logical operator $\bar{P}$ is flipped if $\bar{P} = \bar{X}$ or $\bar{Y}$.

Similarly, the data analysis of the two-copy experiment of Fig. 3.2 entails decoding a 62 binary string for every shot. Only shots where the qRM X and Z -type stabilizers and flags are +1 for both copies are kept. Thus, the acceptance rate of the two-copy experiment is roughly the square of the acceptance rate of the single-copy experiment. To extract the logical $\bar{X}_1 \otimes \bar{Z}_2$ operator, similar to the decoding process of the single-copy experiment, $\bar{X}_1$ and $\bar{Z}_2$ are obtained for the respective Steane code copy. Since the logical $\bar{Z}$ corrections of the two copies of the protocol of Fig. 3.1 are not physically applied, they are considered in post-processing. Because $\overline{\text{CNOT}}_s(\bar{Z}_1^{a_1} \otimes \bar{Z}_2^{a_2})\overline{\text{CNOT}}_s = \bar{Z}_1^{a_1+a_2} \otimes \bar{Z}_2^{a_2}$ (where $a_i = (1 - \bar{X}_i^{\text{qRM}})/2$ indicates whether a correction has to be applied to the i -th copy), the logical measurement of the first copy $\bar{X}_1$ has to be flipped when $a_1 + a_2 \equiv 1 \pmod{2}$.

The values reported in Table A.1 correspond to the mean over all the post-selected

shots N_{post} , and the acceptance rate is the number of post-selected shots over the total number of shots N_{shots} . The reported acceptance rate for the fidelity in Tables 3.1 and A.1 is the average over the acceptance rates of the single-copy experiments.

The (1σ) confidence error bars are computed as $\Delta\langle\bar{P}\rangle_{\bar{\rho}} = \sqrt{\frac{\text{Var}(\bar{P})}{N_{\text{post}}}}$ for the single-copy experiments, where $\text{Var}(\bar{P})$ is the sample variance. For the two-copy experiment, the (1σ) error bar is computed using a Binomial distribution $\Delta\epsilon = \sqrt{\frac{p_f(1-p_f)}{N_{\text{post}}}}$, where $p_f = \frac{N_{|\bar{-1}\rangle}}{N_{\text{post}}}$ is the fraction of detected logical $|\bar{-1}\rangle$ states $N_{|\bar{-1}\rangle}$. In case where $N_{|\bar{-1}\rangle} = 0$, the (1σ) confidence interval is $[0, \frac{1.147}{N_{\text{post}}}]$ [266], so we choose $p_f = \Delta\epsilon = \frac{1.147}{2N_{\text{post}}}$. Finally, the (1σ) error bar for the fidelity lower bound for F (3.5) is computed assuming uncorrelated error propagation.

Appendix B

Appendix: Efficient simulation of logical magic state preparation protocols

This is the Appendix associated with Chapter 4.

B.1 Error Model

We consider an error model given by the standard circuit-level Pauli noise. That is, each quantum operation is modeled as a noiseless operation, preceded or followed by some stochastic Pauli error occurring with a given probability. Hence, this error model encompass initialization P_I , gate-specific $\{P_i\}$ and measurement P_M errors. For the numerical simulations we consider a uniform circuit-level error model with strength p , where:

- **Initialization errors P_I .** Preparation of $|0\rangle$ ($|+\rangle$) noisy physical states is given by the initialization of noiseless $|0\rangle$ states followed by X (Z) errors occurring with probability p . Similarly, preparation of physical magic states is followed by some Pauli error Q occurring with probability p ; see Appendix B.1.1 for the justification. For $|T\rangle$ and $|H\rangle$ magic states, the Pauli errors Q are single-qubit

Paulis Z and Y , respectively.

- **Gate errors $\{P_i\}$.** Single-qubit (two-qubit) gates are given by the respective noiseless gates followed by uniform single-qubit $\mathcal{D}_1(\rho)$ (two-qubit $\mathcal{D}_2(\rho)$) depolarizing noise channels of strength p ,

$$\mathcal{D}_1(\rho) = (1-p)\rho + \frac{p}{3} \sum_{Q \in \{X, Y, Z\}} Q\rho Q, \quad \mathcal{D}_2(\rho) = (1-p)\rho + \frac{p}{15} \sum_{Q \in \{I, X, Y, Z\}^{\otimes 2} \setminus \{I \otimes I\}} Q\rho Q. \quad (\text{B.1})$$

- **Gate errors $\{P_i\}$.** “Idling” qubits (i.e. qubits that are acted on trivially) are followed by single-qubit depolarizing noise channel $\mathcal{D}_1(\rho)$ of strength p . Note that for n consecutive idling operations the effective error channel is given by n -time composition of $\mathcal{D}_1^{\otimes n}(\rho) = (\mathcal{D}_1 \circ \dots \circ \mathcal{D}_1)(\rho)$, where

$$\mathcal{D}_1^{\otimes n}(\rho) = (1-p_n)\rho + \frac{p_n}{3} \sum_{Q \in \{X, Y, Z\}} Q\rho Q, \quad p_n = \frac{3}{4} \left[1 - \left(1 - \frac{4}{3}p \right)^n \right]. \quad (\text{B.2})$$

- **Measurement errors P_M .** Measurement of qubits in the Z basis (X basis) is preceded by an X error (Z error) occurring with probability p .

B.1.1 Initialization Error: PSC Eigenstates

Here we justify the Pauli initialization error for eigenstates of PSCs [Definition 1]. The main claim is that any error model acting on such a state can be converted to a Pauli-based error model. This is achieved by randomly applying the PSC. We first focus on the single-qubit PSCs.

Proposition 4. *Let C be a single-qubit order-2 PSC and $|\psi\rangle$ be its $+1$ eigenstate. Consider a twirling map $\mathcal{T}_C(\cdot) = \frac{1}{2}((\cdot) + C(\cdot)C^\dagger)$. For any channel $\mathcal{E}$,*

$$\mathcal{T}_C \circ \mathcal{E}(|\psi\rangle\langle\psi|) = (1-p)|\psi\rangle\langle\psi| + pP|\psi\rangle\langle\psi|P^\dagger \quad (\text{B.3})$$

for some Pauli P and $0 \leq p \leq 1$.

B.1 Error Model

Proof. Note that the ± 1 eigenstates of C are $|v^\pm\rangle = \frac{I \pm C}{2}|s\rangle$ for a stabilizer state $|s\rangle$. Therefore, for any single-qubit density matrix $\rho = \sum_{a,b \in \{+, -\}} \alpha_{ab} |v^a\rangle\langle v^b|$ and some complex coefficients α_{ab} , the twirling map acting on ρ decoheres it onto the eigenbasis of C ,

$$\mathcal{T}_C(\rho) = \alpha_{++}|v^+\rangle\langle v^+| + \alpha_{--}|v^-\rangle\langle v^-|. \quad (\text{B.4})$$

Further, if $|\psi\rangle \equiv |v^+\rangle$ we need to prove that exists a Pauli P such that $|v^-\rangle = P|\psi\rangle$. This is equivalent to proving that given C , there exists a Pauli P that anticommutes with U . Since $U^2 = 1$, the standard form (4.21) of $C = Qe^{i\frac{\pi}{4}Q'}$ for Paulis Q, Q' such that $\{Q, Q'\} = 0$ and $Q^2 = I$. Therefore, $P \equiv Q'$ is such that $\{P, C\} = 0$. Hence, in this case twirling a physical magic state $|\psi\rangle\langle\psi|$ subjected to any noise channel $\mathcal{E}$ guarantees that only Pauli error P influence it, which implies (B.3). $\square$

The result of Proposition 4 can be also generalized to a larger class of multi-qubit magic state as in Proposition 5.

Proposition 5. *Consider an l -qubit magic state $|V\rangle = V|+\rangle^{\otimes l}$, where V is a diagonal gate in $\mathcal{C}^{(3)}$. Let $S_V = \langle VX_i V^\dagger : i \in [l] \rangle$ and define the twirling map*

$$\mathcal{T}_V(\cdot) = \frac{1}{|S_V|} \sum_{s \in S_V} s(\cdot) s^\dagger. \quad (\text{B.5})$$

For any channel $\mathcal{E}$,

$$\mathcal{T}_V \circ \mathcal{E}(|V\rangle\langle V|) = \sum_{x \in \mathbb{F}_2^l} p_x Z_x |V\rangle\langle V| Z_x^\dagger, \quad (\text{B.6})$$

for some probability distribution $\{p_x\}$, where $Z_x := \bigotimes_{i=1}^l Z_i^{x_i}$ and $x \in \mathbb{F}_2^l$.

Proof. Let $|V\rangle = V|+\rangle^{\otimes l}$ be a l -qubit magic state, where V is a diagonal gate from the third level of the Clifford hierarchy. The stabilizer group S_V of $|V\rangle$ is generated by unitaries s_z such that $s_z|V\rangle = |V\rangle$, where

$$S_V = \left\{ s_z : s_z = V \left(\bigotimes_{i=1}^l X_i^{z_i} \right) V^\dagger, z \in \mathbb{F}_2^l \right\}. \quad (\text{B.7})$$

We now show that there is a twirling operator $\mathcal{T}_V(\rho)$ that decoheres any l -qubit density

matrix ρ into a basis $\mathcal{B}$ consisting of projectors $P|V\rangle\langle V|P^\dagger$ for some set of Paulis P . Indeed, the basis is defined as $\mathcal{B} = \left\{ |\tilde{x}\rangle\langle\tilde{x}| : |\tilde{x}\rangle = \left(\bigotimes_{i=1}^l Z_i^{x_i} \right) |V\rangle, x \in \mathbb{F}_2^l \right\}$, where $s_z|\tilde{x}\rangle = (-1)^{x \cdot z}|\tilde{x}\rangle$, $x, z \in \mathbb{F}_2^l$ and $x \cdot z = \sum_{i=1}^l x_i z_i$. The twirling operator is then

$$\mathcal{T}_V(\rho) = \frac{1}{2^l} \sum_{g_z \in S} s_z \rho s_z^\dagger. \quad (\text{B.8})$$

The action $\mathcal{T}_V(\rho)$ on basis elements $|\tilde{x}\rangle\langle\tilde{y}|$ of ρ , represented by respective binary strings $x, y \in \mathbb{F}_2^l$, is

$$\frac{1}{2^l} \sum_{s_z \in S} s_z |\tilde{x}\rangle\langle\tilde{y}| s_z^\dagger = \delta_{x,y} |\tilde{x}\rangle\langle\tilde{x}|, \quad (\text{B.9})$$

where the Kronecker delta $\delta_{x,y}$ is 1 if $x = y$ and 0 otherwise. Therefore, due to (B.9)

$$\rho = \sum_{x,y \in \mathbb{F}_2^l} \alpha_{xy} |\tilde{x}\rangle\langle\tilde{y}| \implies \mathcal{T}(\rho) = \sum_{x \in \mathbb{F}_2^l} \alpha_{xx} |\tilde{x}\rangle\langle\tilde{x}|, \quad (\text{B.10})$$

for some complex coefficients α_{xy} . Hence, in this case twirling a physical magic state $|V\rangle\langle V|$ subjected to any noise channel $\mathcal{E}$ guarantees that only Z -type Pauli errors P influence it, which implies (B.6). $\square$

Propositions 4 and 5 imply that applying stochastically C (or more generally, a group generated by a set of PSCs) to a physical magic state $|\psi\rangle$ stabilized by C , errors become at most a Pauli P . We conjecture that this property generalizes to any k -qubit magic state stabilized by k independent and commuting PSCs, which is left for future work.

B.2 Properties of PSC

In this Appendix we provide proofs of the statements in Section 4.4.

Lemma 1. *Let U be a unitary. U is a PSC if and only if controlled- U is in the third level of the Clifford hierarchy $\mathcal{C}^{(3)}$.*

Proof. The “only if” part of the statement follows straightforwardly from Eqs. (4.19) and (4.20). For the “if” part of the statement, our proof closely follows Theorem

A.2 from [158] for their $k = 3$ case. Notice that in Eq. (4.20), under our assumption that $C(U) \in \mathcal{C}^{(3)}$, the unitary $V = (X \otimes U)C(U^{\dagger 2})$ must be a Clifford gate. We can recursively apply the circuit identity of Eq. (4.20) too

$$\begin{array}{c} \text{---} \boxed{X} \text{---} \\ \text{---} \boxed{U^2} \text{---} \end{array} \text{---} \text{CNOT} \text{---} = \begin{array}{c} \text{---} \boxed{U^2} \text{---} \\ \text{---} \boxed{U^{\dagger 4}} \text{---} \end{array} \text{---} \boxed{U^2} \text{---} \text{---} \boxed{X} \text{---} \quad (\text{B.11})$$

Moreover, note that

$$V(X \otimes I)V^\dagger = C(U^2)(X \otimes I)C(U^{\dagger 2}). \quad (\text{B.12})$$

Since $V = (X \otimes U)C(U^{\dagger 2})$ is a Clifford, from Eqs. (B.11) and (B.12) we see that $W = (X \otimes U^2)C(U^{\dagger 4}) \in \mathcal{C}^{(1)}$. This implies $U^4 = I$ (up to a global phase) because there are no controlled gates in $\mathcal{C}^{(1)}$, as well as $U^2 \in \mathcal{C}^{(1)}$. Moreover, using the definition of V we can rewrite $X \otimes U = V \cdot C(U^2)$. Since U^2 is a Pauli then $C(U^2)$ is a Clifford. Therefore, because V is a Clifford, $V \cdot C(U^2) = X \otimes U$ is a Clifford too. By the group structure of Clifford gates, $X \otimes U$ being a Clifford implies that U must be a Clifford too. To conclude, U is a Clifford such that U^2 is a Pauli (hence, it is a PSC). $\square$

Proposition 1. *A unitary U is a PSC if and only if it can be written in the following form:*

$$U = \alpha P \exp \left(\frac{\pi i}{4} \sum_{j=1}^m Q_j \right), \quad (\text{4.21})$$

where P is a Pauli and $\{Q_j : j = 1, \dots, m\}$ is a commuting set of Paulis $[Q_i, Q_j] = 0$, and α is a complex number such that $\alpha^8 = 1$.

Proof. The “if” part of the statement can be shown easily from the following identity:

$$U^2 = \alpha^2 P e^{\frac{\pi i}{4} \sum_{j=1}^m Q_j} P e^{-\frac{\pi i}{4} \sum_{j=1}^m Q_j} e^{\frac{\pi i}{2} \sum_{j=1}^m Q_j}. \quad (\text{B.13})$$

Since $e^{\frac{\pi i}{4} \sum_{j=1}^m Q_j}$ is a Clifford, conjugating P by this operator results in a Pauli [Eq. (B.24)].

Moreover,

$$e^{\frac{\pi i}{2} \sum_{j=1}^m Q_j} = i^m \prod_{j=1}^m Q_j, \quad (\text{B.14})$$

which is again a Pauli. Since $\alpha^8 = 1$, $\alpha^2 = +1, -1, +i$, or $-i$. Thus U^2 is a Pauli.

Less obvious is the “only if” statement. To that end, note that two Cliffords U_1 and U_2 are equivalent (up to a global phase) if and only if

$$U_1 P U_1^\dagger = U_2 P U_2^\dagger \quad (\text{B.15})$$

for every Pauli P . Thus, if we can show that a conjugation by a PSC is equivalent to a conjugation by a unitary of the form of $P e^{\frac{\pi i}{4} \sum_{j=1}^m Q_j}$, we are done.

A convenient framework to study the action of the Cliffords up to Pauli is the symplectic representation, reviewed below. In this framework, each n -qubit Pauli can be written as a $2n$ -dimensional binary vector u and a Clifford can be expressed as a $2n \times 2n$ binary invertible matrix C that preserves the symplectic form:

$$C^T \omega C = \omega, \quad (\text{B.16})$$

where ω is the binary symplectic matrix

$$\omega = \begin{pmatrix} 0_{n \times n} & I_{n \times n} \\ I_{n \times n} & 0_{n \times n} \end{pmatrix}. \quad (\text{B.17})$$

In particular, the Clifford preserves the symplectic product, i.e., $\langle Cv, Cu \rangle = \langle v, u \rangle$, where $\langle v, u \rangle := v^T \omega u$. Moreover, two Paulis P and Q commute if and only if their corresponding binary vector has a zero symplectic inner product.

In the symplectic representation, a PSC is a symplectic matrix (B.16) that squares to the identity since Paulis have trivial form in this representation. Without loss of generality, let $C = I + N$. Then, $C^2 = I$ implies $N^2 = 0$ since N is a binary matrix, i.e., N is nilpotent. Furthermore, $C^2 = I$ also implies $\langle Nx, Ny \rangle = 0$ for any x, y and that $\langle Nx, y \rangle = \langle x, Ny \rangle$. Thus, for any $u, v \in \text{Im}(N)$, $\langle u, v \rangle = 0$. This implies that the

Paulis associated to the elements of $\text{Im}(N)$ must necessarily commute.

Now we claim that

$$N = \omega \sum_k u_k u_k^T, \quad (\text{B.18})$$

where $u_k \in \text{Im}(\omega N)$. To see why, note ωN is symmetric due to the relation $\langle Nx, y \rangle = \langle x, Ny \rangle$. Let $P = VV'$ be the projector onto $\text{Im}(\omega N)$, where V' is a $r \times n$ matrix for some $r \leq n$. Then,

$$\begin{aligned} \omega N &= P\omega NP^T \\ &= V(V'\omega N(V')^T)V^T, \end{aligned} \quad (\text{B.19})$$

where the matrix in the paranthesis is a symmetric $r \times r$ matrix. Because it is a symmetric matrix over $\mathbb{F}_2$, it can be written in the following form:

$$V'\omega N(V')^T = \sum_k v_k v_k^T, \quad (\text{B.20})$$

where $v_k \in \mathbb{F}_2^k$. Thus,

$$\omega N = N\omega = \sum_k u_k u_k^T \quad (\text{B.21})$$

for some $u_k \in \text{Im}(\omega N)$.

Now we decompose $N = \sum_k N_k$, where $N_k = u_k u_k^T \omega$. Note that because $u_k \in \text{Im}(\omega N)$, $\langle u_i, u_j \rangle = 0$ for all i, j . Therefore, $N_i N_j = 0$ for all i, j and in particular each N_i is nilpotent. Thus we arrive at the following decomposition,

$$C = I + \sum_{j=1}^m N_j = \prod_{j=1}^m (I + N_j). \quad (\text{B.22})$$

Note that $(I + N_j)(x)$ is in one-to-one correspondence with $e^{\frac{\pi i}{4} Q_j} P e^{-\frac{\pi i}{4} Q_j}$ (up to a Pauli), where Q_j is a Pauli associated with u_j and P is an arbitrary Pauli with binary representation x . Indeed, it can be checked that the equivalence in terms of Eq. (B.15) holds since $e^{\frac{\pi i}{4} Q_j}$ maps P as in Eq. (B.24), and $(I + N_j)(x) = x + \langle u_j, x \rangle u_j$, which is either x if $\langle u_j, x \rangle = 0$ or $x + u_j$ if $\langle u_j, x \rangle = 1$. Moreover, because any two elements in $\text{Im}(\omega N)$ have zero symplectic inner product, $[Q_j, Q_k] = 0$ for all j and k . This

completes the proof. $\square$

Proposition 2. *Let C and P be a PSC and a Pauli respectively, supported on t qubits*

$$\text{---} \xrightarrow{t} \boxed{P} \text{---} \boxed{C} \text{---} = \text{---} \xrightarrow{t} \boxed{C} \text{---} \boxed{P} \text{---} \boxed{Q} \text{---}, \quad (4.22)$$

where Q is a t -qubit Pauli that either commutes or anticommutes with C . Furthermore, $\text{Supp}(Q) \subseteq \text{Supp}(C)$.

Proof. Note Eq. (4.22) follows from the identity (4.19) when $U = P$, $V = C$ and $Q = CPC^\dagger P^\dagger$. Because C is a Clifford, it follows that Q is a Pauli. Below we show that Q either commutes or anticommutes with C .

From Proposition 1, it follows that C can be written in the following form

$$C = \alpha \tilde{P} \exp \left(\frac{\pi i}{4} \sum_{j=1}^m Q_j \right), \quad (B.23)$$

where $\tilde{P}$ is a Pauli and $\{Q_j\}$ is a set of commuting Paulis and α is a complex number with a unit modulus. Recall the following standard identity:

$$e^{-\frac{\pi i}{4} P'} P e^{\frac{\pi i}{4} P'} = \begin{cases} P & \text{if } [P, P'] = 0, \\ -i P' P & \text{if } \{P, P'\} = 0. \end{cases} \quad (B.24)$$

Repeatedly applying this identity, we obtain

$$Q = \alpha \prod_{j \in \mathcal{A}_P} Q_j, \quad (B.25)$$

where α is a scalar of modulus 1 and $\mathcal{A}_P$ is a subset of $\{Q_j : j = 1, \dots, m\}$ that anticommute with P .

By construction, the following commutation relation holds:

$$\left[\exp \left(\frac{\pi i}{4} \sum_{j=1}^m Q_j \right), Q \right] = 0. \quad (B.26)$$

Therefore, the commutation relation of C and Q is determined by that of $\tilde{P}$ and Q . Since both are Paulis, it follows that C and Q either commute or anticommute. $\square$

B.3 Error Propagation

In Appendix B.3.1, we provide a proof of the asymptotic gate complexity of a Clifford error resulting from error propagation through a standard logical PSC measurement-based protocol from Theorem 2 in Section 4.5.1.

B.3.1 Proof of Theorem 2

We consider the most general setting of MSP protocols consisting of repeated stabilizer and logical PSC measurements that are interleaved in an arbitrary way. Using Fig. 4.7, we can guarantee that circuit-level errors will *only* ever propagate to a Clifford. What remains to be studied is the gate complexity of the resulting Clifford error circuit. We show this grows modestly with various parameters of the protocol.

Theorem 2. *Let w_c and w_q be the maximum row and column weight of a parity check matrix H . Consider a standard protocol consisting of $r = r_S + r_L$ rounds of stabilizer (r_S) and PSC (r_L) measurements. Any single-qubit circuit-level error propagates through this protocol to a Clifford error consisting of $O(r^2 w_q (w_c + \ell))$ one- and two-qubit Clifford gates, for ℓ the number of PSC tensor factors V_i in $\bar{U}$.*

Proof. Without loss of generality, it suffices to consider single-qubit errors occurring on either data or ancilla qubits. Furthermore, at any given time errors will be propagated through a round of stabilizer measurements or a round of logical PSC measurements.

Propagation through a data qubit. Given a data qubit is involved in at most w_q stabilizer checks, propagation through a round of stabilizer measurements yields at most an additional w_q single-qubit Pauli errors on ancillae. Hence across r_S rounds, at most $r_S w_q$ additional single-qubit Pauli errors are propagated to ancillae. Moreover, since we do not consider ancilla qubit resets, these Pauli errors will not propagate any further in a nontrivial way.

For propagation through a logical PSC measurement round, a given data qubit is in the support of a *single* PSC V_i [Definition 2] and therefore, in the support of $C(V_i)$'s target. By Proposition 2, a single-qubit Pauli error will propagate an additional controlled-Pauli $C(Q)$ for Q a Pauli that either commutes or anticommutes with V_i and satisfies $\text{supp}(Q) \subseteq \text{supp}(V_i)$. As per our assumption, this latter fact implies that Q must be an $O(1)$ -qubit Pauli. Across r_L rounds of logical PSC measurement, r_L $C(Q)$ errors are propagated. Further, each $C(Q)$ will propagate additional $C(Z)$ errors [Eq. (4.27)]. In particular, each data qubit in the target of $C(Q)$ is involved in at most w_q stabilizer checks. Hence, each of the r_L $C(Q)$ s will propagate at most $r_S w_q$ additional $C(Z)$ gates. Further, each of the r_L $C(Q)$ errors will encounter r_L $C(V_i)$ s from logical PSC measurement rounds, resulting in at most an additional $r_L^2 C(Z)$.

Hence, propagation of single-qubit circuit-level errors from data qubits results in a Clifford error with $O(r_S r_L w_q + r_L^2)$ one- and two-qubit gates.

Propagation through an ancilla qubit. Ancilla qubits may be used for stabilizer measurement of PSC measurement. We treat each case separately.

We start with the former case. Given each stabilizer check involves at most w_c data qubits, a single-qubit Pauli error will propagate to at most w_c single-qubit Pauli errors on data qubits. Unlike ancillae, data qubits are used throughout the protocol and can therefore continue to propagate non-trivial errors. From the analysis of the error propagation on data qubits, it follows that each of the (at most) w_c single-qubit Pauli errors propagates to a Clifford error with $O(r_S r_L w_q + r_L^2)$ gates.

We now consider the latter case. Each such logical PSC measurement ancilla will be the control for ℓ $C(V_i)$ gates [Definition 2]. Thus across r_L rounds of logical PSC measurement, a single-qubit circuit-level error on such an ancilla propagates to an additional (at most) $\ell r_L C(Q)$ gates and $\ell r_L V_i$ gates [Eq. (4.20)]. From above, we know that $\ell r_L C(Q)$ gates will propagate an additional $O(\ell r_S r_L w_q + \ell r_L^2) C(Z)$ gates. Then, each of the ℓr_L PSC gates V_i will trivially propagate past logical PSC measurements as each V_i has disjoint support and V_i necessarily commutes with V_j for $i \neq j$. For stabilizer measurements, each of the $O(1)$ qubits in the support of V_i are involved in

at most w_q stabilizer checks. Thus, each of ℓr_L V_i gates will propagate an additional $C(R)$ gate, defined similarly to $C(Q)$ above. Finally, each of the ℓr_L $C(R)$ gates will also propagate to additional $O(\ell r_S r_L w_q + \ell r_L^2)$ $C(Z)$ gates.

Hence, propagation of single-qubit circuit level errors from ancilla qubits results in a Clifford error with $O((w_c + \ell)(r_S r_L w_q + r_L^2))$ one- and two-qubit gates.

In summary, any single-qubit error propagates to a Clifford error with a number of $O(r^2 w_q (w_c + \ell))$ one- and two-qubit gates as desired. $\square$

B.4 Magic state $|\bar{H}\rangle$ simulation details

In this Appendix we give additional details about the simulation technique for the specific magic $|\bar{H}\rangle$ state preparation protocol of Fig. 4.9 from Section 4.7.2.

We recall the propagation rules for Pauli errors (and phase gates) through CH gates introduced in Section 4.3,

$$\begin{array}{c} \text{---} [X] \text{---} \\ | \\ \text{---} [H] \text{---} \end{array} = \begin{array}{c} \text{---} \\ | \\ \text{---} [H] \text{---} [H] \end{array} \quad , \quad \begin{array}{c} \text{---} [S^a] \text{---} \\ | \\ \text{---} [H] \text{---} \end{array} = \begin{array}{c} \text{---} \\ | \\ \text{---} [H] \end{array} \text{---} [S^a] \quad , \quad (\text{B.27})$$

$$\begin{array}{c} \text{---} \\ | \\ \text{---} [X] \text{---} [H] \end{array} = \begin{array}{c} \text{---} \\ | \\ \text{---} [H] \text{---} [X] \end{array} \text{---} [Y] \text{---} [S] \quad , \quad \begin{array}{c} \text{---} \\ | \\ \text{---} [Z] \text{---} [H] \end{array} = \begin{array}{c} \text{---} \\ | \\ \text{---} [H] \text{---} [Z] \end{array} \text{---} [Y] \text{---} [S^\dagger] \quad . \quad (\text{B.28})$$

Note that $a \in \{0, 1, 2, 3\}$ and that $S^2 = Z$ and $S^3 = S^\dagger$. To propagate errors through the measurement of $\bar{H}$ of Fig. 4.9 we label error locations with a number and a color; see Fig. B.1.

The numerical simulation of the MSP protocol considers a circuit-level noise model that we describe in Appendix B.1. The different types of errors arising during the measurement of $\bar{H}$ in Fig. 4.9 can be labeled as follows,

	t_1	t_2	t_3	t_4	t_5	t_6	t_7	t_8	t_9	t_{10}
Qubit 1	39	40								42
Qubit 2	31	32						34	35	
Qubit 3	26	27					29	30		
Qubit 4	21	22				24	25			
Qubit 5	16	17			19	20				
Qubit 6	11	12		14	15					
Qubit 7	2	4	5							
Qubit 8	1	3	8	13	18	23	28	33	36	41
Qubit 9	6	7	9	10					37	38

Figure B.1: Error locations for the flag-based measurement of $\bar{H}$ from Fig. 4.9 labeled with numbers and colors. Blue boxes represent Pauli errors due to the non-fault-tolerant encoding circuit. White boxes represent idling errors, orange boxes represent initialization errors, and green boxes represent 2-qubit depolarizing errors.

- **Blue boxes** correspond to Pauli errors coming from the non fault-tolerant preparation of $|\bar{H}\rangle$. These errors have as binary representation for $a_i, b_i \in \{0, 1\}$

$$X_1^{a_{39}} Z_1^{b_{39}} \otimes X_2^{a_{31}} Z_2^{b_{31}} \otimes X_3^{a_{26}} Z_3^{b_{26}} \otimes X_4^{a_{21}} Z_4^{b_{21}} \otimes X_5^{a_{16}} Z_5^{b_{16}} \otimes X_6^{a_{11}} Z_6^{b_{11}} \otimes X_7^{a_2} Z_7^{b_2}. \quad (\text{B.29})$$

- **Orange boxes** correspond to ancilla qubits initialization errors with $a_i, b_i \in \{0, 1\}$,

$$X_8^{a_1} Z_8^{b_1} \otimes X_9^{a_6} Z_9^{b_6}. \quad (\text{B.30})$$

For the error model being under consideration $a_1 = b_6 = 0$.

- **Blue boxes** correspond to two-qubit depolarizing channel errors applied after each two-qubit *CNOT* or *CH* gate. The set of errors is given by

$$X_7^{a_4} Z_7^{b_4} \otimes X_8^{a_3} Z_8^{b_3} \quad , \quad X_8^{a_8} Z_8^{b_8} \otimes X_9^{a_9} Z_9^{b_9} \quad , \quad X_8^{a_{13}} Z_8^{b_{13}} \otimes X_6^{a_{14}} Z_6^{b_{14}} \quad , \quad \dots \quad , \quad (\text{B.31})$$

for $a_i, b_i \in \{0, 1\}$.

- **White boxes** correspond to idling errors given implemented via single-qubit depolarizing channels. Note that for idling errors starting at step t_i and ending at step t_j , they can effectively be sampled from a depolarizing channel $\mathcal{D}_1^{\otimes n}(\rho)$ with $n = j - i + 1$, see Eq. (B.2). The set of errors is given by

$$X_1^{a_{40}} Z_1^{b_{40}} \quad , \quad X_2^{a_{32}} Z_2^{b_{32}} \quad , \quad X_3^{a_{35}} Z_3^{b_{35}} \quad , \quad X_3^{a_{27}} Z_3^{b_{27}} \quad , \quad \dots \quad , \quad (\text{B.32})$$

for $a_i, b_i \in \{0, 1\}$.

The final propagated Clifford error C_{prop} has an analytic form that can be written as the product

$$C_{\text{prop}} = E_9 E_8 \cdots E_1 . \quad (\text{B.33})$$

Each of the errors E_i for $i = 1, \dots, 7$ is given by

$$E_7 = (X_7^{a_4+a_5} Z_7^{b_4+b_5} H_7^{a_1} X_7^{a_2} Z_7^{b_2}) (C_8 Y_7)^{a_2+b_2} , \quad (\text{B.34})$$

$$E_6 = (X_6^{a_{14}+a_{15}} Z_6^{b_{14}+b_{15}} H_6^{a_1+a_3+a_8} X_6^{a_{11}+a_{12}} Z_6^{b_{11}+b_{12}}) (C_8 Y_6)^{a_{11}+a_{12}+b_{11}+b_{12}} , \quad (\text{B.35})$$

$$E_5 = (X_5^{a_{19}+a_{20}} Z_5^{b_{19}+b_{20}} H_5^{a_1+\sum_{i=1}^3 a_{5i-2}} X_5^{a_{16}+a_{17}} Z_5^{b_{16}+b_{17}}) (C_8 Y_5)^{a_{16}+a_{17}+b_{16}+b_{17}} , \quad (\text{B.36})$$

$$E_4 = (X_4^{a_{24}+a_{25}} Z_4^{b_{24}+b_{25}} H_4^{a_1+\sum_{i=1}^4 a_{5i-2}} X_4^{a_{21}+a_{22}} Z_4^{b_{21}+b_{22}}) (C_8 Y_4)^{a_{21}+a_{22}+b_{21}+b_{22}} , \quad (\text{B.37})$$

$$E_3 = (X_3^{a_{29}+a_{30}} Z_3^{b_{29}+b_{30}} H_3^{a_1+\sum_{i=1}^5 a_{5i-2}} X_3^{a_{26}+a_{27}} Z_3^{b_{26}+b_{27}}) (C_8 Y_3)^{a_{26}+a_{27}+b_{26}+b_{27}} , \quad (\text{B.38})$$

$$E_2 = (X_2^{a_{34}+a_{35}} Z_2^{b_{34}+b_{35}} H_2^{a_1+\sum_{i=1}^6 a_{5i-2}} X_2^{a_{31}+a_{32}} Z_2^{b_{31}+b_{32}}) (C_8 Y_2)^{a_{31}+a_{32}+b_{31}+b_{32}} , \quad (\text{B.39})$$

$$E_1 = (X_1^{a_{42}} Z_1^{b_{42}} H^{a_1+\sum_{i=1}^6 a_{5i-2}+a_{36}} X_1^{a_{39}+a_{40}} Z_1^{b_{39}+b_{40}}) (C_8 Y_1)^{a_{39}+a_{40}+b_{39}+b_{40}} . \quad (\text{B.40})$$

The contribution for the ancillas E_8 and E_9 is

$$E_9 = X_9^{a_6+a_7+a_9+a_{10}+\sum_{i=2}^6 a_{5i-2}+a_{37}+a_{38}} Z_9^{b_6+b_7+b_9+b_{10}+b_{37}+b_{38}} , \quad (\text{B.41})$$

$$\begin{aligned}
 E_8 = & X_8^{a_1 + \sum_{i=1}^6 a_{5i-2} + a_{36} + a_{41}} Z_8^{b_1 + a_2 + a_3 + b_8 + b_9 + b_{10} + \sum_{i=1}^5 a_{5i+6} + a_{5i+7} + b_{5i+8} + b_{36} + a_{39} + a_{40} + b_{41}} \times \\
 & \times S_8^{a_2 + b_2 + \sum_{i=1}^5 a_{5i+6} + a_{5i+7} + b_{5i+6} + b_{5i+7} + a_{39} + a_{40} + b_{39} + b_{40}} .
 \end{aligned}
 \tag{B.42}$$

In a numerical simulation, given a sampled initialization Pauli error frame (B.29), the remaining of the coefficients a_i, b_i can be sampled from the respective probability distributions dictated by their type (color and position following Fig. B.1). Therefore, since the measurement $\bar{H}$ gadget acts trivially on the noiseless encoded state, all the non-Clifford gates can be effectively removed from the circuits at the expense of introducing stochastic Clifford errors C_{prop} acting on a noiseless logical magic state. The numerical results using this technique in a stabilizer-based emulator matches the numerical results obtained via state-vector simulations; see Figs. 4.10 and 4.11 in the main text.

B.5 Simulation via stabilizer rank decomposition

In this Appendix, we revisit the *phase-sensitive* Clifford simulation method [145], providing an alternative to the phase-insensitive simulation method introduced in Section 4.6 (which is based on the Pauli rank decomposition of the magic state).

From the discussion in Section 4.5, it follows that any circuit-level Pauli noise propagates to a Clifford error at the end of the circuit. More precisely, the state obtained after the error propagation is of the following form:

$$C_{\text{prop}}(|\bar{\phi}\rangle + \dots + \rangle), \tag{B.43}$$

where $|\bar{\phi}\rangle$ is the magic state encoded in the code subspace and $|\dots + \rangle$ represent the syndrome register, whose measurement is deferred to the end. We envision measuring the syndrome register, applying a correction (or post-selection) to the noisy code state, and then computing the overlap of the resulting state with $|\bar{\phi}\rangle$. (We note that the syndrome register may contain additional qubits that are part of the flag gadgets.)

Without loss of generality, let the measurement basis be $\{|\tilde{x}\rangle : x \in \mathbb{F}_2^m\}$, where $|\tilde{x}\rangle = (\otimes_{i=1}^m H_i)|x\rangle$ and U_x be the corresponding Pauli correction operation.¹ (Here we are assuming that the syndrome register has m qubits.) The state obtained after the correction is a density matrix of the following form

$$\rho = \sum_x (U_x \otimes \langle \tilde{x}|) C_{\text{prop}}(|\bar{\phi}\rangle\langle \bar{\phi}| \otimes |+\dots+\rangle\langle +\dots+|) C_{\text{prop}}^\dagger (U_x^\dagger \otimes |\tilde{x}\rangle). \quad (\text{B.44})$$

Thus, the overlap between ρ and $|\phi\rangle$ becomes

$$\langle \bar{\phi} | \rho | \bar{\phi} \rangle = \sum_x p_x |\langle \bar{\phi} | \tilde{\phi}_x \rangle|^2, \quad (\text{B.45})$$

where

$$\begin{aligned} p_x &= \|(U_x \otimes \langle \tilde{x}|) C_{\text{prop}}(|\bar{\phi}\rangle \otimes |+\dots+\rangle)\|^2, \\ |\tilde{\phi}_x\rangle &= (U_x \otimes \langle \tilde{x}|) C_{\text{prop}}(|\bar{\phi}\rangle \otimes |+\dots+\rangle) / \sqrt{p_x}. \end{aligned} \quad (\text{B.46})$$

Therefore, estimation of the overlap is reduced the problem of (i) sampling over the probability distribution $\{p_x : x \in \mathbb{F}_2^m\}$ and (ii) estimating the overlap $|\langle \bar{\phi} | \tilde{\phi}_x \rangle|^2$. Both problems can be solved using the stabilizer rank decomposition of $|\phi\rangle$. Without loss of generality, let $|\bar{\phi}\rangle = \sum_{i=1}^q \alpha_i |s_i\rangle$, where $\{|s_i\rangle\}$ is a set of normalized stabilizer states, $\{\alpha_i\}$ is a set of complex amplitudes, and q is the stabilizer rank. Importantly, the stabilizer rank remains unchanged under stabilizer operations, e.g., Clifford unitary and measurement of Paulis. Moreover, the state can be updated efficiently under these operations. As we show below, these facts let us solve the aforementioned problems.

Let us first briefly note that the stabilizer rank decomposition lets us efficiently compute overlap of two stabilizer states, even including the phase. This is possible because any stabilizer state can be written in the so called CH-form [145]. Let n_{tot} be the total number of qubits. The CH form of the stabilizer state is

$$|\Omega\rangle = \omega U_C U_H |s\rangle, \quad (\text{B.47})$$

¹In principle, U_x can be chosen as a Clifford correction. However, it is unclear if that leads to an advantage over Pauli correction.

with a complex global phase ω , a ‘control’-type Clifford U_C generated by $\{S, CX, CZ\}$, a ‘Hadamard’-type Clifford U_H generated by $\{I, H\}$, and a computational basis vector $|s\rangle \in \{0, 1\}^{\otimes n_{\text{tot}}}$. Upon application of a ‘control’-type Clifford gate, the CH-form of any state $|\Omega\rangle$ can be updated in $O(n_{\text{tot}})$ time. Moreover, upon the application of a ‘Hadamard’-type gate or a projective Pauli measurement, the CH-form of any state $|\Omega\rangle$ can be updated in $O(n_{\text{tot}}^2)$ time; see [145, Proposition 4]. Using this update rule, we can compute the overlap as follows. Let $|\Omega'\rangle = \omega' U'_C U'_H |s\rangle$ be another stabilizer state in a CH-form. Using the update rule, $\langle\Omega'|\Omega\rangle = \tilde{\omega} \langle s' | \tilde{U}_C \tilde{U}_H |s\rangle$ for some complex number $\tilde{\omega}$ and Cliffords $\tilde{U}_C \tilde{U}_H$. $\tilde{U}_C$ can be absorbed into $\langle s' |$, updating it into a new basis vector and a phase. The matrix element of the Hadamard-type Clifford can be computed straightforwardly at this point. Thus $\langle\Omega'|\Omega\rangle$ can be computed in time polynomial in n_{tot} .

Using this overlap estimation as a subroutine, we now describe how to (i) sample over $\{p_x\}$ and (ii) compute $|\langle\bar{\phi}|\tilde{\phi}_x\rangle|^2$. The sampling can be done by recursively sampling each bit in the following way. Without loss of generality, consider measuring one of the qubits in the syndrome register. The post-measurement state for both outcomes can be written as a q -fold linear combination of stabilizer states. In particular, the norm of each post-measurement state can be estimated from $O(q^2)$ overlap estimations. Once these norms are estimated, one can sample over this binary probability distribution and pick the corresponding post-measurement state. Since the stabilizer rank of the post-measurement state is still at most q , this process can be repeated with the same complexity until the entire syndrome register is measured. Computing $|\langle\bar{\phi}|\tilde{\phi}_x\rangle|^2$ can be done in a similar way. Note that the stabilizer rank of the post-measurement state is still at most q . Therefore, the overlap can be again computed using $O(q^2)$ overlap estimations.

To summarize, using the stabilizer rank decomposition, we can estimate the logical error rate in the following way. First, sample over the circuit-level noise and propagate it to an end-of-circuit Clifford error using the method in Section 4.4. Next, estimate Eq. (B.45) by averaging $|\langle\bar{\phi}|\tilde{\phi}_x\rangle|^2$ over the probability distribution $\{p_x\}$. Since all the

sampling, error propagation, and overlap estimation can be done efficiently (insofar as q is small), the logical error rate can be estimated efficiently.

One advantage of the stabilizer rank decomposition method, compared to the Pauli rank method [Section 4.6], is its smaller variance. The Pauli rank based method has $\Theta(1)$ variance. However, for the stabilizer rank based method, the logical error rate is an average of $1 - |\langle \bar{\phi} | \tilde{\phi}_x \rangle|^2 \in [0, 1]$. If the mean value is p_L , the variance is bounded from above by $p_L(1 - p_L)$, which can be substantially smaller than that of the Pauli rank based method when $p_L \ll 1$. Indeed, if X is a random variable in $[0, 1]$, the variance is $\mathbb{E}[X^2] - \mathbb{E}[X]^2 \leq \mathbb{E}[X] - \mathbb{E}[X]^2 = p_L(1 - p_L)$ (Here $\mathbb{E}$ is the expected value). However, from an implementation perspective, the stabilizer rank method is arguably more complicated. For future work, it will be desirable to compare the practical efficiencies of the two methods.

B.5.1 Pauli rank and stabilizer rank are not related

Although Pauli rank and stabilizer rank are both suitable non-stabilizerness metrics, it was shown in Ref. [146] that one can always find an n -qubit state for which these non-stabilizerness metrics are exponentially-separated and therefore not related. In particular, consider the state $|\psi_n\rangle \propto |0\rangle^{\otimes n} + |+\rangle^{\otimes n}$. Clearly this state has stabilizer rank $q = 2$ for all such n -qubit states. Additionally, we know that the Pauli rank of a stabilizer state is exactly 2^n (this can be shown by writing the density matrix of a stabilizer state $|\phi\rangle$ as a product of n projectors onto $+1$ -eigenspaces of stabilizer operators for $|\phi\rangle$). Since $|\psi_n\rangle$ is not a stabilizer state, its Pauli rank must be strictly greater than 2^n . In fact, one can show that the Pauli rank of $|\psi_n\rangle$ is at least $p \geq 3^n - 1$, hence providing a non-trivial example of a state with an exponential gap between its Pauli rank and stabilizer rank.

Appendix C

Appendix: Real-time adaptation of quantum noise channel estimates

This is the Appendix associated with Chapter 5.

C.1 Flag gadgets for the CNOT gate

C.1.1 4-layered flag gadgets

In this Appendix we provide details regarding the 4-layered flag gadgets utilized for updating the noise channel estimates associated to a CNOT gate. In Fig. C.1, we show the explicit construction of the flag gadgets. Note that single-controlled multi-qubit gates can be decomposed as a sequence of single-controlled single-qubit gates. For the case in question, $C_3X_1X_2 = C_3X_1 \circ C_3X_2$ and $C_3Z_1Z_2 = C_3Z_1 \circ C_3Z_2$.

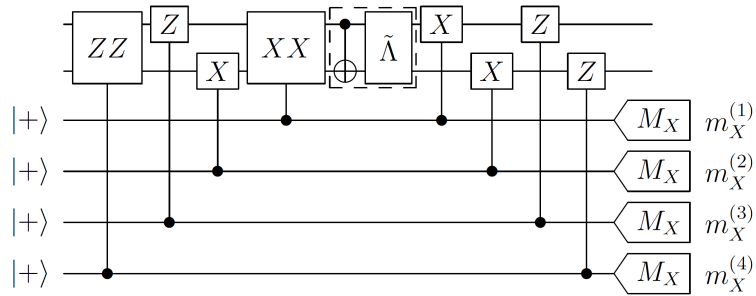


Figure C.1: 4-layered gadget for a noisy CNOT gate. The dashed region represents a noisy CNOT gate, modeled as a noiseless CNOT gate followed by a Pauli channel $\tilde{\Lambda}$.

$m_X^{(1)}$	$m_X^{(2)}$	$m_X^{(3)}$	$m_X^{(4)}$	$P(m_X \vec{\lambda})$
+1	+1	+1	+1	λ_{II}
+1	+1	+1	-1	λ_{IX}
+1	+1	-1	+1	λ_{XI}
+1	-1	+1	+1	λ_{IZ}
-1	+1	+1	+1	λ_{ZI}
+1	+1	-1	-1	λ_{XX}
+1	-1	+1	-1	λ_{IY}
-1	+1	+1	-1	λ_{ZX}
+1	-1	-1	+1	λ_{XZ}
-1	+1	-1	+1	λ_{YI}
-1	-1	+1	+1	λ_{ZZ}
+1	-1	-1	-1	λ_{XY}
-1	+1	-1	-1	λ_{YX}
-1	-1	+1	-1	λ_{ZY}
-1	-1	-1	+1	λ_{YZ}
-1	-1	-1	-1	λ_{YY}

Table C.1: Likelihood probability of measuring m_X given a prior probability distribution $P(\vec{\lambda})$ for a 4-layered flag gadget acting on a 2-qubit unitary. The right column was constructed using (5.17), and indices $i \in [1, 16]$ where replaced by $i \in \{I, X, Y, Z\}^{\otimes 2}$, respectively. This table represents the 2-qubit generalization of Table 5.1.

In Table C.1, we show the likelihood probability (5.20) which depends on the measurement outcome m_X of Fig. C.1.

C.1.2 1-layered flag gadgets

In this Appendix we provide details regarding the 1-layered flag gadgets utilized for updating the noise channel estimates associated to a CNOT gate. As it was mentioned in Fig. 5.9, the 1-layered flag gadgets were chosen uniformly at random from the 2-qubit Pauli group excluding the identity $\mathcal{P}_2/\{I \otimes I\}$. The set $[g]$ (5.17) associated to with every gadget $R \in \mathcal{P}_2/\{I \otimes I\}$ is described in Table C.2. We opted to use the convention of Table C.3 as a label for the indices of λ_i .

R	L	$[g] : m_X = +1$	$[g] : m_X = -1$
X_2	X_2	[1, 2, 5, 6, 9, 10, 13, 14]	[3, 4, 7, 8, 11, 12, 15, 16]
Y_2	$Z_1 Y_2$	[1, 3, 5, 7, 9, 11, 13, 15]	[2, 4, 6, 8, 10, 12, 14, 16]
Z_2	$Z_1 Z_2$	[1, 4, 5, 8, 9, 12, 13, 16]	[2, 3, 6, 7, 10, 11, 14, 15]
X_1	$X_1 X_2$	[1, 2, 3, 4, 5, 6, 7, 8]	[9, 10, 11, 12, 13, 14, 15, 16]
Y_1	$Y_1 X_2$	[1, 2, 3, 4, 9, 10, 11, 12]	[5, 6, 7, 8, 13, 14, 15, 16]
Z_1	Z_1	[1, 2, 3, 4, 13, 14, 15, 16]	[5, 6, 7, 8, 9, 10, 11, 12]
$X_1 X_2$	X_1	[1, 2, 5, 6, 11, 12, 15, 16]	[3, 4, 7, 8, 9, 10, 13, 14]
$X_1 Y_2$	$Y_1 Z_2$	[1, 3, 5, 7, 10, 12, 14, 16]	[2, 4, 6, 8, 9, 11, 13, 15]
$X_1 Z_2$	$-Y_1 Y_2$	[1, 4, 5, 8, 10, 11, 14, 15]	[2, 3, 6, 7, 9, 12, 13, 16]
$Y_1 X_2$	Y_1	[1, 2, 7, 8, 9, 10, 15, 16]	[3, 4, 5, 6, 11, 12, 13, 14]
$Y_1 Y_2$	$-X_1 Z_2$	[1, 3, 6, 8, 9, 11, 14, 16]	[2, 4, 5, 7, 10, 12, 13, 15]
$Y_1 Z_2$	$X_1 Y_2$	[1, 4, 6, 7, 9, 12, 14, 15]	[2, 3, 5, 8, 10, 11, 13, 16]
$Z_1 X_2$	$Z_1 X_2$	[1, 2, 7, 8, 11, 12, 13, 14]	[3, 4, 5, 6, 9, 10, 15, 16]
$Z_1 Y_2$	Y_2	[1, 3, 6, 8, 10, 12, 13, 15]	[2, 4, 5, 7, 9, 11, 14, 16]
$Z_1 Z_2$	Z_2	[1, 4, 6, 7, 10, 11, 13, 16]	[2, 3, 5, 8, 9, 12, 14, 15]

Table C.2: Set of 1-layered flag gadgets for a unitary $U = \text{CNOT}_{1 \rightarrow 2}$ including: right unitaries $R \in \mathcal{P}_2 / \{I \otimes I\}$, left unitaries satisfying $RUL = U$ (5.6), and set of indices $[g]$ dependent on the measurement outcome m_X (5.15). The indices conventions for the Pauli estimates λ_i can be found in Fig. C.3.

λ_j	II	IX	IY	IZ	XI	XX	XY	XZ	YI	YX	YY	YZ	ZI	ZX	ZY	ZZ
j	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16

Table C.3: Labeling for Pauli error estimates λ_i associated to 2-qubit gates.

To construct Table C.2 it was necessary to use the fundamental properties of Fig. C.2,

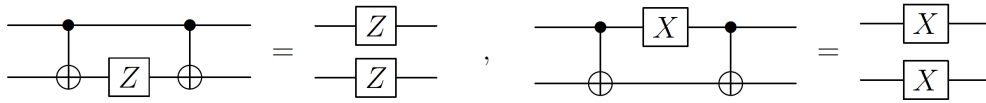


Figure C.2: Non-trivial gate identities for the conjugation of single qubit $X(Z)$ gates under CNOT gates.

C.2 Proof of the approximate update rule

In this Appendix we derive the approximate update rule (5.49) from the exact expression (5.29), which we reproduce here again

$$\langle \lambda_j \rangle_{P^{(n)}} = \frac{\sum_{i_n \in [g_n]} \cdots \sum_{i_1 \in [g_1]} \langle \lambda_j \lambda_{i_n} \cdots \lambda_{i_1} \rangle_{P^{(0)}}}{\sum_{i_n \in [g_n]} \cdots \sum_{i_1 \in [g_1]} \langle \lambda_{i_n} \cdots \lambda_{i_1} \rangle_{P^{(0)}}}. \quad (\text{C.1})$$

Given that product of high moments of a Dirichlet distribution have a close form expression (5.46) in terms of the generalized beta function (5.31), we can employ the recursive property of the Gamma function $\Gamma(x+1) = x\Gamma(x)$ to express

$$\langle \lambda_j \lambda_{i_n} \dots \lambda_{i_1} \rangle_{P^{(0)}} = \langle \lambda_{i_n} \dots \lambda_{i_1} \rangle_{P^{(0)}} \left(\frac{\alpha_0}{\alpha_0 + n} \langle \lambda_j \rangle_{P^{(0)}} + \frac{1}{\alpha_0 + n} (\delta_{j,i_1} + \dots + \delta_{j,i_n}) \right). \quad (\text{C.2})$$

Replacing (C.2) into (C.1) gives

$$\langle \lambda_j \rangle_{P^{(n)}} = \frac{\alpha_0}{\alpha_0 + n} \langle \lambda_j \rangle_{P^{(0)}} + \frac{1}{\alpha_0 + n} \sum_{t=1}^n \frac{\sum_{i_n} \dots \sum_{i_1} \langle \lambda_{i_n} \dots \lambda_{i_1} \rangle_{P^{(0)}} \delta_{j,i_t}}{\sum_{i_n} \dots \sum_{i_1} \langle \lambda_{i_n} \dots \lambda_{i_1} \rangle_{P^{(0)}}}. \quad (\text{C.3})$$

Note that we introduced the notation that a sum over i_k denotes a sum over $i_k \in [g_k]$. To proceed, we can expand out the correlators even further using $n-1$ times the recursive relation

$$\begin{aligned} \langle \lambda_{i_n} \dots \lambda_{i_1} \rangle_{P^{(0)}} &= \prod_{k=1}^n \frac{1}{\alpha_0 + k - 1} \left(\alpha_0 \langle \lambda_{i_k} \rangle_{P^{(0)}} + \sum_{p=1}^{k-1} \delta_{i_k, i_p} \right) \\ &= \frac{\Gamma(\alpha_0 + n - 1)}{\Gamma(\alpha_0 + 1)} \alpha_0^n \left(\prod_{p=1}^n \langle \lambda_{i_p} \rangle \right) \left(1 + \alpha_0^{-1} \sum_{k=1}^n \sum_{q=1}^{k-1} \frac{\delta_{i_k, i_q}}{\langle \lambda_{i_k} \rangle} + \Omega(\alpha_0^{-2} n^3) \right). \end{aligned} \quad (\text{C.4})$$

In the last step, we expanded out the numerator in powers of α_0 and we also removed the $P^{(0)}$ label from the expected values. At order α_0^{-p} in (C.4) the individual terms have the product of exactly p different Kronecker deltas. This expansion property explains the correlation between different iterations discussed in Section 5.3.4. For instance, at order α_0^{-1} , upon taking the respective sums there will be indices belonging to the intersection of sets from two different iterations, i.e., $[g_k] \cap [g_q]$ with $k \neq q$ and $k, q = 1, \dots, n$.

We are now ready to replace (C.4) into (C.3). The non-trivial denominator of (C.3)

can be then written as

$$\begin{aligned} \sum_{i_n} \cdots \sum_{i_1} \langle \lambda_{i_n} \cdots \lambda_{i_1} \rangle_{P^{(0)}} &= \frac{\Gamma(\alpha_0 + n - 1)}{\Gamma(\alpha_0 + 1)} \alpha_0^n \left[\prod_{p=1}^n \left(\sum_{i_p} \langle \lambda_{i_p} \rangle \right) \right] \left(1 + \right. \\ &\quad \left. + \alpha_0^{-1} \sum_{k=1}^n \sum_{q=1}^{k-1} \frac{(\sum_{i \in [g_k] \cap [g_q]} \langle \lambda_i \rangle)}{(\sum_{i_k} \langle \lambda_{i_k} \rangle)(\sum_{i_q} \langle \lambda_{i_q} \rangle)} + \Omega(\alpha_0^{-2} n^3) \right). \end{aligned} \quad (C.5)$$

The analysis of the non-trivial numerator of (C.3) is a bit more subtle, because of the additional delta function

$$\begin{aligned} \sum_{i_n} \cdots \sum_{i_1} \langle \lambda_{i_n} \cdots \lambda_{i_1} \rangle_{P^{(0)}} \delta_{j, i_t} &= \frac{\Gamma(\alpha_0 + n - 1)}{\Gamma(\alpha_0 + 1)} \alpha_0^n \left[\prod_{p=1}^n \left(\sum_{i_p} \langle \lambda_{i_p} \rangle \right) \right] \langle \lambda_j \rangle \left(\frac{\delta(j, [g_t])}{(\sum_{i_t} \langle \lambda_{i_t} \rangle)} + \right. \\ &\quad + \alpha_0^{-1} \frac{\delta(j, [g_t])}{(\sum_{i_t} \langle \lambda_{i_t} \rangle)} \sum_{k=1, k \neq t}^n \sum_{q=1, q \neq t}^{k-1} \frac{(\sum_{i \in [g_k] \cap [g_q]} \langle \lambda_i \rangle)}{(\sum_{i_k} \langle \lambda_{i_k} \rangle)(\sum_{i_q} \langle \lambda_{i_q} \rangle)} \\ &\quad \left. + \alpha_0^{-1} \sum_{k=1, k \neq t}^n \frac{\delta(j, [g_k] \cap [g_t])}{(\sum_{i_k} \langle \lambda_{i_k} \rangle)(\sum_{i_t} \langle \lambda_{i_t} \rangle)} + \Omega(\alpha_0^{-2} n^3) \right). \end{aligned} \quad (C.6)$$

Putting (C.6) and (C.5) together into (C.3) provides a proof for the approximate update rule (5.49)

$$\langle \lambda_j \rangle_{P^{(n)}} = \frac{\alpha_0}{\alpha_0 + n} \langle \lambda_j \rangle_{P^{(0)}} + \frac{1}{\alpha_0 + n} \sum_{t=1}^n \frac{X_1(t) + \alpha_0^{-1} X_2(t) + \Omega(\alpha_0^{-2} n^3)}{1 + \alpha_0^{-1} Y_2 + \Omega(\alpha_0^{-2} n^3)}. \quad (C.7)$$

Where the quantities $X_1(t)$, $X_2(t)$ and Y_2 are

$$X_1(t) = \langle \lambda_j \rangle \frac{\delta(j, [g_t])}{(\sum_{i_t} \langle \lambda_{i_t} \rangle)}, \quad (C.8)$$

$$X_2(t) = \langle \lambda_j \rangle \frac{\delta(j, [g_t])}{(\sum_{i_t} \langle \lambda_{i_t} \rangle)} \sum_{k=1, k \neq t}^n \left(\frac{\delta(j, [g_k])}{(\sum_{i_k} \langle \lambda_{i_k} \rangle)} + \sum_{q=1, q \neq t}^{k-1} \frac{(\sum_{i \in [g_k] \cap [g_q]} \langle \lambda_i \rangle)}{(\sum_{i_k} \langle \lambda_{i_k} \rangle)(\sum_{i_q} \langle \lambda_{i_q} \rangle)} \right), \quad (C.9)$$

$$Y_2 = \langle \lambda_j \rangle \sum_{k=1}^n \sum_{q=1}^{k-1} \frac{(\sum_{i \in [g_k] \cap [g_q]} \langle \lambda_i \rangle)}{(\sum_{i_k} \langle \lambda_{i_k} \rangle)(\sum_{i_q} \langle \lambda_{i_q} \rangle)}. \quad (C.10)$$

C.3 Numerical Methods

The numerical simulations are done using the stabilizer circuit simulator Stim [96] in Python. In Stim qubits are by default initialized in the computational basis $|0\rangle$ states. Clifford gates and single qubit destructive measurements are supported. Error models can be incorporated before or after the desired operations, and they are parametrized by some noise strength parameters, respectively.

Regarding error models, for Figs. 5.7, 5.8, 5.9 and 5.11 the prior expected values $\langle\lambda_i\rangle_{P^{(0)}}$ are chosen at random from a $K = 16$ variable Dirichlet distribution (5.30) with hyperparameters $\alpha_i = 1$ using the library NumPy in Python. We believe that our method should work regardless of the chosen prior distribution. For the aforementioned figures, the physical error rates $\langle\lambda_i\rangle_{P_{\text{phy}}}$ are obtained by considering a small perturbation of the prior expected values. Specifically, each $\langle\lambda_i\rangle_{P_{\text{phy}}} = \langle\lambda_i\rangle_{P^{(0)}} + \chi$ can be modified by adding a random number χ sampled from the uniform distribution with support in $[-\delta, \delta]$ and by subsequently renormalizing the expected values such that their sum is $\sum_i \langle\lambda_i\rangle_{P_{\text{phy}}} = 1$. In our case we consider $\delta = 0.02$, additionally, all the figures utilize the same physical and prior error rates.

To account for the errors introduced by the noisy flag gadgets (see Section 5.3.5), we utilize a circuit-level error model of strength p , where each component of a quantum circuit is followed or preceded by a noisy process, see Fig. 5.10. Concretely, for the preparation of noisy $|+\rangle$ states, we model them as noiseless $|+\rangle$ states followed by a phase flip (Z) error occurring with probability p . Similarly, for noisy X -type measurements, we model them as noiseless X -type measurements preceded by a phase flip error occurring with probability p . Finally, for two qubit entangling gates between data and ancilla qubits, we model them as noiseless gates followed by a depolarizing error channel with strength p ,

$$\mathcal{D}_2(\rho) = (1 - p)\rho + \sum_{P \in \mathcal{P}_2/\{I \otimes I\}} \frac{p}{15} P\rho P, \quad (\text{C.11})$$

where $\mathcal{P}_2 = \{I, X, Y, Z\}^{\otimes 2}$ is the Pauli group acting on 2-qubits.

The updated expected values $\langle \lambda_i \rangle_{P(n)}$ are computed using equation (5.44) for Fig. 5.7, 5.8 and 5.11, and equation (5.49) for Fig. 5.9. All the simulations utilize $\alpha_0 = 2000$. The number of sampled shots is: $n = 10000$ for Fig. 5.7 and 5.8, $n = 1000$ for Fig. 5.9 and $n \in [1, 20000]$ for Fig. 5.11. The error bars represent one standard deviation obtained from the square root of the variance from equation (5.45). Finally, on Fig. 5.11 the TVD distance is computed using equation (5.57).

Appendix D

Appendix: Entanglement entropy of a Rarita-Schwinger field in a sphere

This is the Appendix associated with Chapter 6.

D.1 Spherical harmonics

D.1.1 Spinor spherical harmonics

The spinor spherical harmonics are a complete basis of the space of spinor functions on the sphere S^2 . They are simultaneously eigenfunctions of the total angular momentum operator squared $\hat{J}^2$ and the orbital angular momentum squared $\hat{L}^2$. The spinor spherical harmonics are useful for problems involving spinor fields on central potential (see for example [267]). For the convenience of the calculation, we will use the basis for spin 1/2 spinors presented in [216], which defines the spinor spherical harmonics $\Omega_{\kappa\mu}$ in terms of the standard spherical harmonics¹ Y_{lm} as

$$\Omega_{\kappa\mu}(\theta, \varphi) = \begin{pmatrix} \text{sgn}(-\kappa) \sqrt{\frac{\kappa + \frac{1}{2} - \mu}{2\kappa + 1}} Y_{l, \mu - 1/2}(\theta, \varphi) \\ \sqrt{\frac{\kappa + \frac{1}{2} + \mu}{2\kappa + 1}} Y_{l, \mu + 1/2}(\theta, \varphi) \end{pmatrix}, \quad (\text{D.1})$$

¹The scalar spherical harmonics $Y_{lm}(\theta, \varphi)$ involved in the definition are the usual ones, given in terms of the associated Legendre functions of the first kind $P_l^{(m)}(x)$ as $Y_{lm}(\theta, \varphi) = \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^{(m)}(\cos(\theta)) e^{im\varphi}$.

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where $0 \leq \theta \leq \pi$ and $0 \leq \varphi \leq 2\pi$ are the angular coordinates that parameterize S^2 , and the quantum numbers κ and μ are discretized as

$$\kappa = \pm 1, \pm 2, \dots, \quad \mu = -|\kappa| + \frac{1}{2}, -|\kappa| + \frac{3}{2}, \dots, |\kappa| - \frac{1}{2}. \quad (\text{D.2})$$

From here, the eigenvalues of the orbital angular momentum squared and the total angular momentum squared denoted by l and j , respectively, can be recovered via

$$l = \left| \kappa + \frac{1}{2} \right| - \frac{1}{2} = \begin{cases} \kappa & \text{for } \kappa > 0 \\ -\kappa - 1 & \text{for } \kappa < 0 \end{cases}, \quad j = |\kappa| - \frac{1}{2}. \quad (\text{D.3})$$

In fact, the orbital angular momentum operator, given by $\vec{L} = -i\vec{r} \times \vec{\nabla}$, yields

$$\hat{L}^2 \Omega_{\kappa\mu}(\theta, \phi) = \kappa(\kappa + 1) \Omega_{\kappa\mu}(\theta, \phi) = l(l + 1) \Omega_{\kappa\mu}(\theta, \phi), \quad (\text{D.4})$$

and the total angular momentum defined for spin 1/2 as $\vec{J} = \vec{L} + \vec{\sigma}/2$ gives

$$\hat{J}^2 \Omega_{\kappa\mu}(\theta, \phi) = (\kappa^2 - 1/4) \Omega_{\kappa\mu}(\theta, \phi) = j(j + 1) \Omega_{\kappa\mu}(\theta, \phi). \quad (\text{D.5})$$

It is important to stress that the set of spherical harmonics (D.1) does not diagonalize the Dirac operator $-i\not{\nabla}$ on S^2 . Notwithstanding, they can be written as a linear combination of functions that do so [268].

In addition, the orthonormality relations for spinor spherical harmonics are given by

$$\int_{S^2} d\Omega \Omega_{\kappa'\mu'}^\dagger(\theta, \varphi) \Omega_{\kappa,\mu}(\theta, \varphi) = \delta_{\kappa\kappa'} \delta_{\mu\mu'}, \quad (\text{D.6})$$

which follows from the standard orthonormality conditions of scalar spherical harmonics.

An extended list of further properties can be found in [216]. For the EE calculations,

these are the relevant ones

$$(\vec{\sigma} \cdot \hat{r})\Omega_{\kappa\mu}(\theta, \varphi) = -\Omega_{-\kappa\mu}(\theta, \varphi), \quad (\text{D.7})$$

$$(\vec{\sigma} \cdot \vec{L})\Omega_{\kappa\mu}(\theta, \varphi) = -(\kappa + 1)\Omega_{\kappa\mu}(\theta, \varphi), \quad (\text{D.8})$$

$$(\vec{\sigma} \cdot \vec{p})f(r)\Omega_{\kappa\mu}(\theta, \varphi) = i \left(\frac{\partial}{\partial r} + \frac{\kappa + 1}{r} \right) f(r)\Omega_{-\kappa\mu}(\theta, \varphi), \quad (\text{D.9})$$

where $\vec{p} = -i\vec{\nabla}$, $\vec{L} = \vec{r} \times \vec{p}$ and $\hat{r} = \frac{\vec{r}}{|\vec{r}|}$. Note that the equation (D.9) follows from applying the differential operator $\vec{\sigma} \cdot \vec{p}$ in spherical coordinates

$$\vec{\sigma} \cdot \vec{p} = (\vec{\sigma} \cdot \hat{r}) \left(-i \frac{\partial}{\partial r} + \frac{i\vec{\sigma} \cdot \vec{L}}{r} \right). \quad (\text{D.10})$$

D.1.2 Vector-spinor spherical harmonics

Following the construction of the orthonormal basis of spinor spherical harmonics from scalar spherical harmonics, we define the vector-spinor spherical harmonics on S^2 from their vectorial counterparts as

$$\vec{\Omega}_{\kappa\mu}^s(\theta, \varphi) = \begin{pmatrix} \text{sgn}(-\kappa) \sqrt{\frac{\kappa + \frac{1}{2} - \mu}{2\kappa + 1}} \vec{Y}_{l, \mu - 1/2}^s(\theta, \varphi) \\ \sqrt{\frac{\kappa + \frac{1}{2} + \mu}{2\kappa + 1}} \vec{Y}_{l, \mu + 1/2}^s(\theta, \varphi) \end{pmatrix}, \quad s = r, e, m, \quad (\text{D.11})$$

where $\vec{Y}_{lm}^r$, $\vec{Y}_{lm}^e$ and $\vec{Y}_{lm}^m$ are the radial, electric, and magnetic vector spherical harmonics conveniently defined as

$$\vec{Y}_{lm}^r(\theta, \varphi) = Y_{lm}(\theta, \varphi) \hat{r}, \quad l \geq 0 \quad -l \leq m \leq l \quad (\text{D.12})$$

$$\vec{Y}_{lm}^e(\theta, \varphi) = \frac{r \vec{\nabla} Y_{lm}(\theta, \varphi)}{\sqrt{l(l+1)}}, \quad l \geq 1 \quad -l \leq m \leq l \quad (\text{D.13})$$

$$\vec{Y}_{lm}^m(\theta, \varphi) = \frac{\vec{r} \times \vec{\nabla} Y_{lm}(\theta, \varphi)}{\sqrt{l(l+1)}}, \quad l \geq 1 \quad -l \leq m \leq l \quad (\text{D.14})$$

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Note that electric $\vec{Y}_{lm}^e$ and magnetic $\vec{Y}_{lm}^m$ vector spherical harmonics are not defined for zero orbital angular momentum $l = 0$. According to (D.3), this corresponds to $\kappa = -1$. Thus, the vector-spinor spherical harmonics $\vec{\Omega}_{-1\mu}^e$ and $\vec{\Omega}_{-1\mu}^m$ are not defined either.

Many of the properties of vector-spinor spherical harmonics are inherited from the properties of vector spherical harmonics, which can be found in [49, 50, 269, 270]. For instance, we can check that orthonormality conditions hold as

$$\int_{S^2} d\Omega \vec{\Omega}_{\kappa'\mu'}^{\dagger s'}(\Omega) \cdot \vec{\Omega}_{\kappa\mu}^s(\Omega) = \delta_{ss'} \delta_{\kappa\kappa'} \delta_{\mu\mu'}, \quad (\text{D.15})$$

which follows from the orthonormality of vector spherical harmonics given by

$$\int_{S^2} d\Omega \vec{Y}_{l'm'}^{\dagger s'}(\Omega) \cdot \vec{Y}_{lm}^s(\Omega) = \delta_{ss'} \delta_{ll'} \delta_{mm'}. \quad (\text{D.16})$$

The directional and differential properties can be obtained in an analogous manner

$$\vec{\nabla} \cdot \vec{\Omega}_{\kappa\mu}^r = \frac{2}{r} \Omega_{\kappa\mu}, \quad \hat{r} \cdot \vec{\Omega}_{\kappa\mu}^r = \Omega_{\kappa\mu}, \quad (\text{D.17})$$

$$\vec{\nabla} \cdot \vec{\Omega}_{\kappa\mu}^e = -\frac{\sqrt{\kappa(\kappa+1)}}{r} \Omega_{\kappa\mu}, \quad \hat{r} \cdot \vec{\Omega}_{\kappa\mu}^e = 0, \quad (\text{D.18})$$

$$\vec{\nabla} \cdot \vec{\Omega}_{\kappa\mu}^m = 0, \quad \hat{r} \cdot \vec{\Omega}_{\kappa\mu}^m = 0. \quad (\text{D.19})$$

$$\vec{\nabla} \times \vec{\Omega}_{\kappa\mu}^r = -\frac{\sqrt{\kappa(\kappa+1)}}{r} \vec{\Omega}_{\kappa\mu}^m, \quad \hat{r} \times \vec{\Omega}_{\kappa\mu}^r = 0, \quad (\text{D.20})$$

$$\vec{\nabla} \times \vec{\Omega}_{\kappa\mu}^e = \frac{1}{r} \vec{\Omega}_{\kappa\mu}^m, \quad \hat{r} \times \vec{\Omega}_{\kappa\mu}^e = \vec{\Omega}_{\kappa\mu}^m, \quad (\text{D.21})$$

$$\vec{\nabla} \times \vec{\Omega}_{\kappa\mu}^m = -\frac{\sqrt{\kappa(\kappa+1)}}{r} \vec{\Omega}_{\kappa\mu}^r - \frac{1}{r} \vec{\Omega}_{\kappa\mu}^e, \quad \hat{r} \times \vec{\Omega}_{\kappa\mu}^m = -\vec{\Omega}_{\kappa\mu}^e. \quad (\text{D.22})$$

For EE calculations involving the Rarita-Schwinger field, the following properties were

also employed

$$\vec{\sigma} \cdot \vec{\Omega}_{\kappa\mu}^r = (\vec{\sigma} \cdot \hat{r})\Omega_{\kappa\mu} = -\Omega_{-\kappa\mu} , \quad (\text{D.23})$$

$$\vec{\sigma} \cdot \vec{\Omega}_{\kappa\mu}^e = \frac{ir(\vec{\sigma} \cdot \vec{p})}{\sqrt{\kappa(\kappa+1)}}\Omega_{\kappa\mu} = -\sqrt{\frac{\kappa+1}{\kappa}}\Omega_{-\kappa\mu} , \quad (\text{D.24})$$

$$\vec{\sigma} \cdot \vec{\Omega}_{\kappa\mu}^m = \frac{i\vec{\sigma} \cdot \vec{L}}{\sqrt{\kappa(\kappa+1)}}\Omega_{\kappa\mu} = -i\sqrt{\frac{\kappa+1}{\kappa}}\Omega_{\kappa\mu} . \quad (\text{D.25})$$

D.2 Lattice fermions

D.2.1 Numerical simulations

In this Appendix, we explain how to compute EE and mutual information numerically for a free Dirac field in the half-line (6.17), following the procedure discussed in [40, 219]. First, we consider the model on a lattice with $r = na$ for $n \in \{1, 2, \dots, M\}$, infrared cutoff M and lattice spacing a , which is set to $a = 1$. For simplicity, we suppress the (κ, μ) indices and use the notation $\Psi_{\kappa\mu}(r) \rightarrow \psi_n$. Thus, the lattice version of the Hamiltonian (6.17) for each mode reads

$$\hat{H}^\kappa = \sum_{n=1}^M \left[\frac{i}{2} \left(\psi_{n+1}^\dagger \alpha_r \psi_n - \psi_n^\dagger \alpha \psi_{n+1} \right) + \frac{\kappa}{n} \psi_n^\dagger \beta_r \psi_n \right] \equiv \sum_{n,m=1}^M \psi_m^\dagger \hat{H}_{mn}^\kappa \psi_n . \quad (\text{D.26})$$

We also impose the open chain boundary condition, i.e. $\psi_{M+1}, \psi_{M+1}^\dagger = 0$, since we do not expect correlations between ψ_1 and ψ_M for large M . The lattice Hamiltonian is described by a $2M \times 2M$ matrix $\hat{H}_{mn}^\kappa$ because there are two degrees of freedom per site, with eigenvalues $\omega_q^\pm$ and eigenvectors $\vec{\Phi}_q^\pm$,

$$\hat{H}^\kappa \vec{\Phi}_q^\pm = \omega_q^\pm \vec{\Phi}_q^\pm, \quad \vec{\Phi}_q^\pm = \left(\Phi_q^\pm(1) \dots \Phi_q^\pm(l) \dots \Phi_q^\pm(M) \right)^T, \quad q, l = 1, \dots, M. \quad (\text{D.27})$$

In this context, $\pm$ means positive/negative energy, respectively, and $\Phi_q^\pm(k)$ without a vector symbol indicates that it is a two component spinor. The correlator involving fields in two sites m, n can be computed as a sum over the outer product of negative energy spinors [271]

$$C_{mn} = \langle \psi_m^\dagger \psi_n \rangle \equiv \langle G | \psi_m^\dagger \psi_n | G \rangle = \sum_{q=1}^M \Phi_q^{-\dagger}(m) \Phi_q^-(n). \quad (\text{D.28})$$

We only need $\omega_q^- = -\omega_q^+ \leq 0$ because the expectation values are computed with respect to the ground state $|G\rangle$, which is filled by all the negative energy states. For this construction, it is important that the eigenvectors $\vec{\Phi}_q^\pm$ are properly normalized to the unity. In models with translational invariance, it is possible to write down closed form expressions for C_{mn} [272]. However, in the former case, C_{mn} must be constructed by numerically diagonalizing $\hat{H}_\kappa$ and employing (D.28).

Since the theory is quadratic on the fields, the ground state $|G\rangle$ is Gaussian and the EE associated with any region can be computed using the eigenvalues of (D.28). If we restrict to a spatial subsystem A , we only need the eigenvalues of $C_A \equiv (C_{mn})_{m,n \in A}$, and the entropy can be computed as

$$S(A) = -\text{Tr} [C_A \log(C_A) + (1 - C_A) \log(1 - C_A)]. \quad (\text{D.29})$$

For a finite line starting at the origin $(0, R)$, the corresponding discretization is achieved for $R = N + \frac{1}{2}$ and $m, n \in [1, N]$. For a finite line (R_1, R_2) with $R_1 < R_2$, the corresponding discretization is achieved by $R_i = N_i + \frac{1}{2}$ and $m, n \in [N_1 + 1, N_2]$. Also, it is important to recall that for $d = 2$ spacetime dimensions, because of the fermion doubling, the numerical results for the EE must be divided by 2 to be consistent with the continuum limit.

The mutual information for regions A and B can be defined in terms of the EE as $I(A, B) = S(A) + S(B) - S(A \cup B)$. Therefore, its numerical computation is straightforward and extends from the previous discussion. Particularly, it is useful for computing the regularized EE as discussed in Section 6.2.2.

D.2.2 Large angular momentum behavior

In this Appendix, we prove that the leading order behavior of the EE for large angular momentum κ , for spherical region of radius $R = N + \frac{1}{2}$ on a lattice of size M , is independent of M for $\kappa \gg M$ and is given by (6.20).

To begin with, we apply perturbation theory over the tridiagonal matrix $\hat{H}_{mn}^\kappa$ defined by the Dirac Hamiltonian on the lattice (D.26). Subsequently we split $\hat{H}_{mn}^\kappa$ in a leading diagonal part $\hat{H}_{mn}^0$ of order $\mathcal{O}(\kappa)$ and in a subleading non diagonal one V_{mn} of order $\mathcal{O}(1)$. More precisely, we write

$$\hat{H}_{mn}^\kappa = \hat{H}_{mn}^0 + gV_{mn}, \quad \hat{H}_{mn}^0 = \frac{\kappa}{n} \beta_r \delta_{mn}, \quad V_{mn} = \frac{i}{2} \alpha_r (\delta_{mn+1} - \delta_{m+1n}), \quad (\text{D.30})$$

where we have introduced the parameter g to keep track of the perturbation order. The eigenvalues and eigenvectors of the diagonal matrix $\hat{H}_{mn}^0$ are given by

$$\hat{H}_{mn}^0 \vec{\Phi}_q^{\pm(0)} = \omega_q^{\pm(0)} \vec{\Phi}_q^{\pm(0)}, \quad \omega_q^{\pm(0)} = \pm \frac{\kappa}{q}, \quad \vec{\Phi}_q^{\pm(0)}(n) = \frac{\delta_{qn}}{\sqrt{2}} \begin{pmatrix} \mp i \\ 1 \end{pmatrix}. \quad (\text{D.31})$$

Carrying out the perturbation up to second order gives the lattice Hamiltonian eigenvalues

$$\omega_q^{\pm(2)} = \omega_q^{\pm(0)} \pm \frac{g^2}{4\kappa} \left[\left(\frac{1}{q} + \frac{1}{q-1} \right)^{-1} + \left(\frac{1}{q} + \frac{1}{q+1} \right)^{-1} \right]. \quad (\text{D.32})$$

On the other hand, the eigenvectors are

$$\begin{aligned} \vec{\Phi}_q^{\pm(2)} = \vec{\Phi}_q^{\pm(0)} + \frac{g}{2\kappa} \left[b(q) \vec{\Phi}_{q+1}^{\mp(0)} - c(q) \vec{\Phi}_{q-1}^{\mp(0)} \right] \\ - \frac{g^2}{4\kappa^2} \left[\frac{1}{2} a(q) \vec{\Phi}_q^{\pm(0)} + d(q) \vec{\Phi}_{q+2}^{\pm(0)} + e(q) \vec{\Phi}_{q-2}^{\pm(0)} \right], \end{aligned} \quad (\text{D.33})$$

with coefficients

$$a(q) = b^2(q) + c^2(q), \quad b(q) = \left(\frac{1}{q} + \frac{1}{q+1} \right)^{-1}, \quad c(q) = \left(\frac{1}{q} + \frac{1}{q-1} \right)^{-1}, \quad (\text{D.34})$$

$$d(q) = \left(\frac{1}{q} + \frac{1}{q+1} \right)^{-1} \left(\frac{1}{q} - \frac{1}{q+2} \right)^{-1}, \quad e(q) = \left(\frac{1}{q} + \frac{1}{q-1} \right)^{-1} \left(\frac{1}{q} - \frac{1}{q-2} \right)^{-1}. \quad (\text{D.35})$$

These eigenvectors are also normalized to the unity

$$\langle \vec{\Phi}_q^{\pm(2)} | \vec{\Phi}_{q'}^{\pm(2)} \rangle = \delta_{qq'} + \mathcal{O}(g^3). \quad (\text{D.36})$$

In this set-up, we can compute the leading order correction to the correlation matrix C_{mn} by simply replacing (D.33) in the definition (D.28). As a result, one obtains the matrix up to second order in g

$$C_{n,n} = \frac{1}{2} \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} - \frac{g^2}{4\kappa^2} a(n) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad (\text{D.37})$$

$$C_{n+1,n} = -C_{n,n+1} = \frac{g}{2\kappa} b(n) \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \quad (\text{D.38})$$

$$C_{n+2,n} = -C_{n,n+2} = -\frac{g^2}{8\kappa^2} [d(n) + e(n+2) - c(n+1)b(n+1)] \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad (\text{D.39})$$

with the remainder of the coefficients being zero. Surprisingly, the entries of this matrix are independent of the total lattice size M . We have explicitly verified this phenomenon in our numerical simulations.

The EE of a spherical region of radius $R = N + \frac{1}{2}$ can be computed from the eigenvalues of $C_A = (C_{mn})_{m,n \in A}$ as in (D.29). At zeroth order in g , the matrix C_A is diagonal, with eigenvalues 0 and 1, and eigenvectors $\vec{\Phi}_q^{+(0)}$ and $\vec{\Phi}_q^{-(0)}$, respectively, yielding a net zero entropy $S(A) = 0$. Corrections to the eigenvalues can be computed by applying degenerate perturbation theory to C_A . At first order in g , there are no corrections. However, at second order, the degenerate formalism is quite tedious to apply. It is simpler to compute the corrections to the eigenvalues by examining the characteristic polynomial of C_A at the lowest non trivial order in g . Rewriting the

eigenvalues as

$$\lambda = \lambda^{(0)} + g^2 \lambda^{(2)}, \quad (\text{D.40})$$

with $\lambda^{(0)} = 0, 1$, it turns out that

$$\begin{aligned} 0 &= \det [C_A - \lambda \mathbb{I}_{2N}] \\ &= f(\lambda^{(0)}, \lambda^{(1)}) + g^{2N} \left[(\lambda^{(2)})^{N-1} \left(\lambda^{(2)} + (2\lambda^{(0)} - 1) \frac{\xi(N)}{\kappa^2} \right) \right] + \mathcal{O}(g^{2(N+1)}), \end{aligned} \quad (\text{D.41})$$

with

$$\xi(N) = \frac{N^2(N+1)^2}{4(2N+1)^2}. \quad (\text{D.42})$$

The function f contains all of the terms up to $\mathcal{O}(g^{2(N-1)})$ and vanishes when $\lambda^{(0)} = 0, 1$ for all $\lambda^{(2)}$. Finally, the eigenvalues at second order are then given by 0 and 1 with multiplicity $N - 1$, in addition to ξ/κ^2 and $(1 - \xi/\kappa^2)$. Hence, the EE at first non trivial order for $\kappa \gg M$

$$\begin{aligned} 4\kappa S_{\text{sphere}}^\kappa(N, M) &= -4\kappa \left[\frac{\xi}{\kappa^2} \log \left(\frac{\xi}{\kappa^2} \right) + \left(1 - \frac{\xi}{\kappa^2} \right) \log \left(1 - \frac{\xi}{\kappa^2} \right) \right] \\ &\sim 8\xi(N) \frac{\log(\kappa)}{\kappa} + 4\xi(N) [1 - \log(\xi(N))] \frac{1}{\kappa} + \dots, \end{aligned} \quad (\text{D.43})$$

where we have accounted for a factor of two due to the fermion doubling.

D.3 Scale vs conformal invariance

The free massless Rarita-Schwinger theory exhibits Poincaré and scale invariance; thus, in this appendix, we study whether such symmetry can be enhanced to include the full conformal group in $d = 4$. On the one hand, we have stated that the theory describes massless particles of spin $3/2$. Therefore, the Weinberg-Witten theorem [208] precludes the existence of a local symmetric gauge invariant stress-energy tensor that can be integrated to produce the generators of the Poincaré group. This failure can be considered an argument against the theory having conformal symmetry. In this context, the theory does not satisfy the usual CFT axioms appearing in the bootstrap

literature, which assume the existence of such a current [273, 274]². On the other hand, the lack of a well-defined stress-energy tensor does not imply the absence of conformal symmetry [277]. Indeed, this is the case for free higher integer spin theories in $d = 4$, which have been explicitly shown to have such symmetry [278, 279].

Considering the spin-3/2 case, the corresponding free massless relativistic wave equation has been proven to be conformal [280, 281]. Moreover, all the free, massless, irreducible representations of the conformal group have been classified in [282, 283], where the representations $(3/2, 0)$ and $(0, 3/2)$ of $SO(4, 2)$ are given by a spinor self/anti-self dual 2-forms fields satisfying the gamma-traceless condition. These are the same symmetries and equations of motion of the chiral/anti-chiral parts of $F_{\mu\nu}$ (6.43). Further, the field strength $F_{\mu\nu}$ and its adjoint are the lowest dimensional operators appearing in the gauge invariant phase space, with their scaling dimension $\Delta = 5/2$ saturating the unitarity bound [284].

In this context, we will proceed in the same vein as the proofs of conformal invariance presented for the Maxwell field [285] and the linearized graviton field [278]. Specifically, we check that the two-point function of the spinor field strength $F_{\mu\nu}$ coincides with the correlation function of a spin-3/2 conformal primary, and that it transforms covariantly under conformal transformations. Moreover, because the theory is free, by Wick's theorem, all higher point correlators are defined solely in terms of two-point functions, which implies that the properties we proved extend to all of the correlators of the theory. In other words, the free massless Rarita-Schwinger theory in $d = 4$ describes a free conformal field theory with the field strength $F_{\mu\nu}$ as a gauge invariant conformal primary of spin 3/2.

We now proceed to compute the two-point function to verify that $F_{\mu\nu}$ is a primary operator of the theory. The propagator of the vector-valued spinor field $\psi_\nu(x)$ can be obtained by properly inverting the quadratic action (6.27) while taking into account

²Because of the lack of a well-defined stress-tensor, the Rarita-Schwinger field evades many general results about the enhancement of the Poincaré+scale-invariant symmetries [275, 276], as it does not satisfy their assumptions.

the gauge redundancies [212]

$$\langle \psi_\mu(x) \bar{\psi}_\nu(y) \rangle = \frac{1}{4\pi^2} \left[\eta_{\mu\nu} \not{x-y} + \frac{1}{2} \gamma_\mu \not{x-y} \gamma_\nu \right] \frac{1}{(x-y)^2} + [\text{gauge terms}], \quad (\text{D.44})$$

Therefore, the field strength and its adjoint yield by direct computation the correlator³

$$\begin{aligned} \langle F_{\mu\nu}(x) \bar{F}_{\lambda\sigma}(y) \rangle = & -\frac{4}{\pi^2} \frac{(x-y)}{(x-y)^6} \left[\mathcal{I}_{\mu\lambda}(x-y) \mathcal{I}_{\nu\sigma}(x-y) - (\mu \leftrightarrow \nu) \right] \\ & - \frac{1}{\pi^2} \frac{1}{(x-y)^6} \left[\mathcal{I}_{\mu\lambda}(x-y) \gamma_\nu \not{x-y} \gamma_\sigma + \mathcal{I}_{\nu\sigma}(x-y) \gamma_\mu \not{x-y} \gamma_\lambda - (\mu \leftrightarrow \nu) \right] \\ & - \frac{(x-y)}{\pi^2 (x-y)^6} i \gamma^5 \epsilon_{\mu\nu}{}^{\alpha\beta} \left[\mathcal{I}_{\alpha\lambda}(x-y) \mathcal{I}_{\beta\sigma}(x-y) - (\alpha \leftrightarrow \beta) \right], \end{aligned}$$

where $\mathcal{I}_{\mu\nu}$ denotes the usual inversion tensor

$$\mathcal{I}_{\mu\nu}(x-y) = \eta_{\mu\nu} - 2 \frac{(x-y)_\mu (x-y)_\nu}{(x-y)^2}. \quad (\text{D.45})$$

It is possible to check that (D.45) coincides with the two-point function of an irreducible spin- $\frac{3}{2}$ conformal primary using technology from a six-dimensional embedding space where conformal transformations are linearly realized [226, 286]. This technique is briefly reviewed in Appendix D.3.1, where we also give the expression in the six-dimensional space, which after being projected out to four dimensions reproduces (D.45).

In addition, we can check that (D.45) transforms covariantly under conformal transformations. This is self-evident for Poincaré or scale transformations; therefore, it remains to be proven for special conformal transformations. These transformations are tedious to implement, so another approach consists of demonstrating its covariance under spatial inversions [287, 288]

$$x'^\mu = -\frac{x^\mu}{x^2}, \quad (\text{D.46})$$

³The presence of γ^5 does not indicate a $O(4, 2)$ invariance breaking to $SO(4, 2)$. Indeed, considering the definition $\gamma^5 = \frac{i}{4!} \epsilon_{\mu\nu\rho\sigma} \gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma$ we get $i \gamma^5 \epsilon^{\mu\nu\alpha\beta} = -\frac{1}{4!} \gamma^\lambda \gamma^\sigma \gamma^\rho \gamma^\eta \epsilon_{\lambda\sigma\rho\eta} \epsilon^{\mu\nu\alpha\beta} = \frac{1}{4!} \gamma^\lambda \gamma^\sigma \gamma^\rho \gamma^\eta \eta_{\lambda\sigma\rho\eta}^{\mu\nu\alpha\beta}$, where $\eta_{\lambda\sigma\rho\eta}^{\mu\nu\alpha\beta}$ is the generalized Minkowski metric.

which implies covariance under special transformations, as these are compositions of inversions and translations. Indeed, we can compute

$$\langle F_{\mu\nu}^i(x) \bar{F}_{\lambda\sigma}^j(y) \rangle = (x^2 y^2)^{-\frac{5}{2}} \mathcal{I}_\mu^\alpha(x) \mathcal{I}_\nu^\beta(x) \mathcal{I}_\lambda^\rho(y) \mathcal{I}_\sigma^\delta(y) S^{ik}(x) S^{lj}(y) \langle F_{\alpha\beta}^k(x') \bar{F}_{\rho\delta}^l(y') \rangle, \quad (\text{D.47})$$

with the fermionic inversion operator being defined as

$$S^{ij}(x) = \frac{x^\mu \gamma_\mu^{ij}}{|x|}. \quad (\text{D.48})$$

The result (D.47) follows from properties of the inversion tensor [289]. In particular, we consider that

$$\mathcal{I}_{\mu\nu}(x) = \mathcal{I}_{\mu\nu}(x'), \quad \mathcal{I}_{\mu\nu}(x' - y') = \mathcal{I}_\mu^\rho(x) \mathcal{I}_\nu^\sigma(x) \mathcal{I}_{\rho\sigma}(x - y), \quad (\text{D.49})$$

$$\mathcal{I}_\mu^\sigma(x) \mathcal{I}_{\sigma\nu}(x) = \eta_{\mu\nu}, \quad \mathcal{I}_\mu^\alpha(x) \mathcal{I}_\nu^\beta(x) \mathcal{I}_\rho^\lambda(x) \mathcal{I}_\delta^\sigma(x) \epsilon_{\alpha\beta}^{\rho\delta} = -\epsilon_{\mu\nu}^{\lambda\sigma}, \quad (\text{D.50})$$

as well as the following relations for the fermionic inversion operator

$$S^{ik}(x) S^{kl}(x' - y') S^{lj}(y) = S^{ij}(x - y), \quad (\text{D.51})$$

$$\mathcal{I}_\mu^\lambda(x) \mathcal{I}_\nu^\sigma(y) S^{ik}(x) \gamma_\lambda^{kl} S^{lm}(x' - y') \gamma_\sigma^{mn} S^{nj}(y) = \gamma_\mu^{ip} S^{pq}(x - y) \gamma_\nu^{qj}. \quad (\text{D.52})$$

These results demonstrate that the gauge invariant field strength correlators for the free massless Rarita-Schwinger field in $d = 4$ have conformal symmetry. However, the theory does not have a local gauge invariant stress tensor, which prevents the construction of the generators of the conformal group. Conveniently, the existence of operators, called twists, that implement the symmetry over a given space-time region is secured by the weak version of Noether's theorem [290]. The only requirement of the theorem is that the split property holds for every space-time region. This follows from two premises: the validity of the time slice axiom, and the fact that the degrees of freedom of the theory do not increase rapidly in the UV, namely, that there is no Hagedorn temperature. Both are expected to hold for the free Rarita-Schwinger field

on a Minkowski background.

For instance, twist operators for space-time translations can be constructed in the following manner. Translational invariance of the theory provides a canonical stress tensor $\Theta_{\mu\nu}$ as a consequence of the usual Noether's theorem,

$$\Theta_{\mu\nu} = -\frac{1}{2} \left[\epsilon_{\mu\alpha\beta\gamma} \bar{\psi}^\alpha \gamma^5 \gamma^\beta \partial_\nu \psi^\gamma - \eta_{\mu\nu} (\epsilon_{\alpha\beta\gamma\delta} \bar{\psi}^\alpha \gamma^5 \gamma^\beta \partial^\gamma \psi^\delta) \right]. \quad (\text{D.53})$$

Such tensor is not symmetric nor gauge invariant and the standard Belinfante procedure does not provide an improvement to make it gauge invariant [212, 222]. This can be interpreted as a direct consequence of the Weinberg-Witten theorem. Nevertheless, it can be used to provide a gauge invariant generator for spacetime translations when integrated over the complete manifold [212]. It can also be used to provide twist operators generating space-time translations in a given region if the correct boundary terms are added (see [231] for some examples).

D.3.1 Embedding space

In this Appendix, we briefly review the six-dimensional embedding space formalism that gives a framework for computing correlation functions of primary fields in four-dimensional CFTs. We mainly follow the conventions presented in [226, 286]. Furthermore, we present explicit expressions for terms in the embedding space whose projection to four dimensions reproduces the field strength correlator (D.45) of the free massless Rarita-Schwinger theory.

The basic idea of this method is that conformal transformations associated with the four dimensional group $SO(4, 2)$ can be realized as linear transformations in a six-dimensional projective space defined via the hypercone condition

$$\eta_{KL} X^K X^L = 0, \quad (\text{D.54})$$

where for every non zero λ the coordinates $X^K \sim \lambda X^K$ are identified. The capital indices $K, L, .. = 1, 2, ..6$ are Lorentz indices on the six-dimensional embedding space

where the metric is given by⁴

$$\eta_{11} = \eta_{22} = \eta_{33} = \eta_{55} = +1, \quad \eta_{00} = \eta_{66} = -1. \quad (\text{D.55})$$

The action of four-dimensional conformal transformations coincides with the action of the Lorentz group in this six-dimensional embedding space, which is described by

$$X^K = \Lambda^K_L X^L, \quad \eta_{KL} \Lambda^K_M \Lambda^L_N = \eta_{MN}, \quad \det(\Lambda) = 1. \quad (\text{D.56})$$

Further, the four dimensional coordinates x^μ can be projected out from the six dimensional ones X^μ by virtue of the transformation

$$x^\mu = \frac{X^\mu}{X^5 + X^6}. \quad (\text{D.57})$$

As a warm-up, we consider primary tensor fields belonging to the irreducible representations $(l, 0)$ or $(0, l)$ for an integer l in four dimensions. These are given by tensors $f_{\mu_1 \nu_1, \mu_2 \nu_2, \dots, \mu_l \nu_l}(x)$, with l pairs of skew-symmetric indices $[\mu_i \nu_i]$. Following the discussion in [286], these tensor fields can be projected out from a tensor field $F_{K_1 L_1, K_2 L_2, \dots, K_l L_l}(X)$ with the same symmetries living in the six-dimensional space

$$f_{\mu_1 \nu_1, \mu_2 \nu_2, \dots, \mu_l \nu_l}(x) = (X^5 + X^6)^\Delta e_{\mu_1}^{K_1}(x) e_{\nu_1}^{L_1}(x) \dots e_{\mu_l}^{K_l}(x) e_{\nu_l}^{L_l}(x) F_{K_1 L_1, K_2 L_2, \dots, K_l L_l}(X) \Big|_{\text{cone}}, \quad (\text{D.58})$$

where $e_\mu^K(x)$ are the projection operators defined as

$$e_\nu^\mu(x) = \delta_\nu^\mu, \quad e_\mu^5(x) = -x_\mu, \quad e_\mu^6(x) = x_\mu. \quad (\text{D.59})$$

The six dimensional terms involving $F_{K_1 L_1, K_2 L_2, \dots, K_l L_l}$ must be homogeneous under rescaling

$$F_{K_1 L_1, K_2 L_2, \dots, K_l L_l}(\lambda X) = \lambda^{-\Delta} F_{K_1 L_1, K_2 L_2, \dots, K_l L_l}(X), \quad (\text{D.60})$$

⁴The signature in the four-dimensional sector $\eta_{\mu\nu} = (-+++)$ for $\mu, \nu = 0, \dots, 3$ is the opposite of the signature used throughout the chapter. Since tensorial expressions will not depend on the specific signature, in this Appendix, we opted to use the same conventions as [226, 286].

with Δ as the scaling dimension of the four-dimensional conformal primary. In addition, they must satisfy the transversality condition for every free Lorentz index

$$X^{K_1} F_{K_1 L_1, K_2 L_2, \dots, K_l L_l}(X) = 0. \quad (\text{D.61})$$

For instance, the correlator of a spin-1 conformal 2-form primary can be recovered from the corresponding correlator of the 2-form $F_{KL}(X)$ in the six-dimensional space. The most general two-point function is simply given by

$$\langle F_{MN}(X) F_{KL}(Y) \rangle = \frac{I_{MK} I_{NL} - I_{ML} I_{NK}}{(XY)^\Delta}, \quad (\text{D.62})$$

where I_{KL} denotes the tensor

$$I_{KL}(X, Y) = \eta_{KL} - \frac{X_L Y_K}{XY}, \quad (\text{D.63})$$

which obeys the useful transversality properties

$$X^K I_{KL} = 0, \quad Y^L I_{KL} = 0, \quad (\text{D.64})$$

thus implying that (D.62) obeys the transversality condition (D.61). Picking $\Delta = 2$ saturates the spin 1 unitarity bound, and the four dimensional conformal correlator recovers the field theoretical result from the Maxwell field in $d = 4$ [285].

The introduction of spin-1/2 fermions in the embedding space is more subtle. First, a set of gamma matrices that satisfy the six-dimensional Clifford algebra $\{\Gamma^K, \Gamma^L\} = 2\eta^{KL}$ needs to be put in place. Those gamma matrices can explicitly be written as [226, 286]

$$\Gamma^\mu = \begin{pmatrix} 0 & i\gamma^5 \gamma^\mu \\ i\gamma^5 \gamma^\mu & 0 \end{pmatrix}, \quad \Gamma^5 = \begin{pmatrix} 0 & \gamma^5 \\ \gamma^5 & 0 \end{pmatrix}, \quad \Gamma^6 = \begin{pmatrix} 0 & \mathbb{I}_4 \\ -\mathbb{I}_4 & 0 \end{pmatrix}, \quad (\text{D.65})$$

where γ^μ are four-dimensional gamma matrices that satisfy the four-dimensional Clif-

ford algebra $\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}$, and also generate $\gamma^5 = -i\gamma^0\gamma^1\gamma^2\gamma^3$. As a result of this choice, a spinorial field $\Psi(X)$ in the embedding space can be decomposed in its chiral parts by

$$\Psi(X) = \begin{pmatrix} \Psi_+(X) \\ \Psi_-(X) \end{pmatrix}. \quad (\text{D.66})$$

The corresponding spin-1/2 field in the four-dimensional space $\psi(x)$ is obtained as

$$\psi(x) = (X^5 + X^6)^{\Delta - \frac{1}{2}} \left[\left(\frac{1 - \gamma^5}{2} \right) \Psi_+(X) + \left(\frac{1 + \gamma^5}{2} \right) \Psi_-(X) \right] \Big|_{\text{cone}}, \quad (\text{D.67})$$

provided that $\Psi(X)$ obeys

$$\Psi(\lambda X) = \lambda^{-\Delta + \frac{1}{2}} \Psi(X), \quad (\Gamma \cdot X) \Psi(X) = 0. \quad (\text{D.68})$$

The two-point function of spin-1/2 conformal primaries follows from the projection of the correlator

$$\langle \Psi(X) \bar{\Psi}(Y) \rangle = \frac{(\Gamma \cdot X)(\Gamma \cdot Y)}{(XY)^{\Delta + \frac{1}{2}}}, \quad (\text{D.69})$$

which has the right scaling and transversality condition, considering that

$$(\Gamma \cdot X)^2 \Big|_{\text{cone}} = \frac{1}{2} \{ \Gamma_A, \Gamma_B \} X^A X^B \Big|_{\text{cone}} = 0. \quad (\text{D.70})$$

Picking $\Delta = 3/2$ saturates the unitarity bound for spin 1/2 fields, and the four dimensional projection of (D.69) coincides with the two-point function of a free fermion field in $d = 4$.

Finally, tensor-spinors in four dimensions transforming as $(l + \frac{1}{2}, 0)$ or $(0, l + \frac{1}{2})$ for an integer l are described by $\mathcal{F}_{\mu_1\nu_1, \mu_2\nu_2, \dots, \mu_l\nu_l}(x)$. Indeed, they can be represented in the embedding space by

$$\mathcal{F}_{K_1 L_1, K_2 L_2, \dots, K_l L_l}(X) = \begin{pmatrix} \mathcal{F}_{K_1 L_1, K_2 L_2, \dots, K_l L_l}^+(X) \\ \mathcal{F}_{K_1 L_1, K_2 L_2, \dots, K_l L_l}^-(X) \end{pmatrix}. \quad (\text{D.71})$$

The corresponding reduction to the four-dimensional space is thus

$$\begin{aligned} \mathcal{F}_{\mu_1\nu_1,\mu_2\nu_2,\dots,\mu_l\nu_l}(x) &= (X^5 + X^6)^{\Delta-\frac{1}{2}} e_{\mu_1}^{K_1}(x) e_{\nu_1}^{L_1}(x) \dots e_{\mu_l}^{K_l}(x) e_{\nu_l}^{L_l}(x) \times \\ &\times \left[\left(\frac{1-\gamma^5}{2} \right) \mathcal{F}_{K_1L_1,K_2L_2,\dots,K_lL_l}^+(X) + \left(\frac{1+\gamma^5}{2} \right) \mathcal{F}_{K_1L_1,K_2L_2,\dots,K_lL_l}^-(X) \right] \Big|_{\text{cone}}, \end{aligned} \quad (\text{D.72})$$

where Δ is the scaling dimension of the conformal primary in four dimensions, and

$$\mathcal{F}_{K_1L_1,K_2L_2,\dots,K_lL_l}(\lambda X) = \lambda^{-\Delta+\frac{1}{2}} \mathcal{F}_{K_1L_1,K_2L_2,\dots,K_lL_l}(X), \quad (\text{D.73})$$

along with the constraints

$$X^{K_i} \mathcal{F}_{K_1L_1,\dots,K_iL_i,\dots,K_lL_l}(X) = 0, \quad (\Gamma \cdot X) \mathcal{F}_{K_1L_1,K_2L_2,\dots,K_lL_l}(X) = 0. \quad (\text{D.74})$$

For these higher-spin fields, extra irreducibility conditions must be imposed on $\mathcal{F}$. This is the double gamma-traceless requirement $\gamma^{\mu_1}\gamma^{\nu_1}\mathcal{F}_{\mu_1\nu_1,\mu_2\nu_2,\dots,\mu_l\nu_l}(x) = 0$ that eliminates degrees of freedom that do not correspond to spin $l + \frac{1}{2}$ fields. This can be also imposed in the embedding space by means of $\Gamma^{K_1}\Gamma^{L_1}\mathcal{F}_{K_1L_1,K_2L_2,\dots,K_lL_l}(X) = 0$ [226]. However, it is simpler to impose this condition in the four-dimensional space after reduction.

When considering the case of interest, a spinor 2-form field $\mathcal{F}_{KL}$, we found three terms in the embedding space that independently satisfy the transversality constraints (D.74). These are given by combinations of the tensor (D.63) and the gamma matrices (D.65) as

$$\begin{aligned} \langle \mathcal{F}_{MN}(X) \bar{\mathcal{F}}_{KL}(Y) \rangle &= \frac{(\Gamma \cdot X)}{(XY)^{\Delta+\frac{1}{2}}} \left[a_1 (I_{MK}I_{NL} - I_{ML}I_{NK}) + \right. \\ &+ a_2 (I_{MK}\Gamma_N\Gamma_L - I_{ML}\Gamma_N\Gamma_K + I_{NL}\Gamma_M\Gamma_K - I_{NK}\Gamma_M\Gamma_L) + \\ &\left. + a_3 \Gamma^A\Gamma^B\Gamma^C\Gamma^D (I_{MA}I_{NB} - I_{MB}I_{NA})(I_{CK}I_{DL} - I_{CL}I_{DK}) \right] (\Gamma \cdot Y), \end{aligned} \quad (\text{D.75})$$

for a priori arbitrary constants a_1 , a_2 and a_3 . The first term, proportional to a_1 , and the second term, proportional to a_2 , respectively, reduce to the first and second line of

(D.45). The third term, proportional to a_3 , reduces to a linear combination of the three lines of (D.45). Thus, they represent a set of three independent terms that can recover the Rarita-Schwinger correlator in four dimensions. The gamma tracelessness condition $\gamma^\mu \langle F_{\mu\nu}(x) \bar{F}_{\lambda\sigma}(y) \rangle = 0$ and the divergenceless condition $\partial^\mu \langle F_{\mu\nu}(x) \bar{F}_{\lambda\sigma}(y) \rangle = 0$ uniquely fix the relative weight of each coefficient a_i once the correlator (D.75) is projected out to four dimensions. The final result coincides with the field strength correlator (D.45) of the Rarita-Schwinger theory for the proper scaling dimension $\Delta = 5/2$.

Appendix E

Appendix: Holographic entanglement entropy inequalities beyond strong subadditivity

This is the Appendix associated with Chapter 7.

E.1 Gravity dual equations of motion

The action for an arbitrary minimally coupled scalar field $\phi(z)$ in the bulk is

$$S = \frac{1}{16\pi G_N^{(d+1)}} \int d^d x \, dz \, \sqrt{-g} \left(R^{(d+1)} - g^{MN} \partial_M \phi \partial_N \phi - V(\phi) \right) - \frac{1}{8\pi G_N^{(d+1)}} \int d^d x \, \sqrt{\gamma} K. \quad (\text{E.1})$$

Here we consider the Einstein-Hilbert action with the standard Gibbons-Hawking boundary term and some arbitrary potential $V(\phi)$ for the scalar field. The equations of motion are

$$R_{MN} - \frac{1}{2} g_{MN} R = \partial_M \phi \partial_N \phi - \frac{1}{2} g_{MN} [(\partial_z \phi)^2 + V(\phi)], \quad (\text{E.2})$$

and

$$\frac{1}{\sqrt{-g}} \partial_M (\sqrt{-g} g^{MN} \partial_N \phi) - \frac{1}{2} \frac{dV}{d\phi} = 0. \quad (\text{E.3})$$

E.1 Gravity dual equations of motion

If the potential has a critical point $\frac{dV}{d\phi}(\phi_c) = 0$ with $V(\phi_c) = -\frac{d(d-1)}{2\ell_c^2}$, then pure AdS_{d+1} with radius ℓ_c is a solution in the class of (7.11) for the equations of motion with

$$f(z) = \left(\frac{\ell_{\text{UV}}}{\ell_c}\right)^2, \quad \phi(z) = \phi_c \quad \forall z. \quad (\text{E.4})$$

Replacing the metric (7.11) in the equations of motion (E.2) and (E.3)¹ and combining them yields two coupled nonlinear ODEs in z

$$\phi''(z) - \left(\frac{d-1}{z} - \frac{f'(z)}{2f(z)}\right) \phi'(z) - \frac{\ell_{\text{UV}}^2}{2z^2 f(z)} \frac{dV(\phi)}{d\phi} = 0, \quad (\text{E.5})$$

$$\frac{d-1}{z} \frac{f'(z)}{f(z)} = 2\phi'(z)^2. \quad (\text{E.6})$$

These equations cannot be solved in closed form for a general potential in arbitrary d , but notable features emerge after expanding the solutions near the critical points. Around the UV fixed point the bulk potential can be expanded as

$$V(\phi) \approx -\frac{d(d-1)}{2\ell_{\text{UV}}^2} + m^2 \phi^2 + \dots, \quad (\text{E.7})$$

so that the equations of motion can be solved order by order. To begin with, at zeroth order $f(z) = 1$ for all z and

$$\phi(z) \approx \phi_{\text{UV}} z^{d-\Delta} + \phi_{\Delta} z^{\Delta} \quad z \rightarrow 0, \quad m^2 \ell_{\text{UV}}^2 = \Delta(\Delta - d), \quad (\text{E.8})$$

solves (E.5). The constant ϕ_{Δ} corresponds to the normalizable fall-off and it is proportional to the vacuum expectation value (VEV) of the field which is set to zero; ϕ_{UV} is dual to the source of the relevant boundary operator $\mathcal{O}$ of conformal dimension Δ and so the mass is tachyonic, *viz.* $m^2 = \Delta(\Delta - d) < 0$. This explains why the UV is a local maximum in Figure 7.1. Subsequently equation (E.6) can be integrated using $f(0) = 1$,

$$f(z) \approx 1 + \frac{d-\Delta}{d-1} \phi_{\text{UV}}^2 z^{2(d-\Delta)}. \quad (\text{E.9})$$

¹For the metric (7.11) we find $R_{zz} = \frac{d}{2} \frac{(-2f+zf')}{z^2 f}$ and $R_{\mu\nu} = \eta_{\mu\nu} \frac{(-2df+zf')}{2z^2}$.

A similar procedure can be followed around the IR fixed point. The limit $z \rightarrow \infty$ corresponds to the IR asymptotic region where $\phi(z \rightarrow \infty) = \phi_{IR} z^{d-\tilde{\Delta}}$. The irrelevant boundary operator $\mathcal{O}$ has conformal dimension $\tilde{\Delta}$ with $d - \tilde{\Delta} < 0$. The zeroth order in $f(z)$ is given by $f(\infty) = \ell_{UV}^2 / \ell_{IR}^2$. This analysis justifies the following generic expansion for $f(z)$

$$f(z) \approx \begin{cases} 1 + (\mu z)^{2\alpha} + \dots & z \rightarrow 0 \quad (\text{UV}) \\ \frac{\ell_{UV}^2}{\ell_{IR}^2} \left(1 - \frac{1}{(\tilde{\mu} z)^{2\tilde{\alpha}}}\right) + \dots & z \rightarrow \infty \quad (\text{IR}) \end{cases}, \quad (\text{E.10})$$

where $\alpha = d - \Delta$ and $\tilde{\alpha} = \tilde{\Delta} - d$ are both positive. The constants μ and $\tilde{\mu}$ are mass scales fixed by potential's couplings, ϕ_{UV} and ϕ_{IR} respectively. These mass scales define the UV and IR regimes when $\mu z \ll 1$ and $\tilde{\mu} z \gg 1$.

In General Relativity it is common to impose constraints to the matter content in order to discard non physical solutions. This is the case for the singularity theorems[291]. Among the standard pointwise energy conditions the Null Energy Condition (NEC) is the weakest one. It states that $T_{MN}\eta^M\eta^N \geq 0$ for any null vector $\eta^M = (\eta^z, \eta^0, \vec{\eta})$. Using the metric (7.11) any null vector is constrained by

$$0 = g_{MN}\eta^M\eta^N \quad \implies \quad (\eta^0)^2 = \frac{1}{f(z)}(\eta^z)^2 + (\vec{\eta})^2. \quad (\text{E.11})$$

Given the contraction

$$\begin{aligned} T_{MN}\eta^M\eta^N &= \frac{\ell_{UV}^2}{z^2} \left(\frac{1}{f(z)} T_z^z (\eta^z)^2 - T_0^0 (\eta^0)^2 + T_i^i (\vec{\eta})^2 \right) \\ &= \frac{\ell_{UV}^2}{z^2} \left(\frac{1}{f(z)} (T_z^z - T_0^0) (\eta^z)^2 + (T_i^i - T_0^0) (\vec{\eta})^2 \right), \end{aligned} \quad (\text{E.12})$$

then, $T_z^z - T_0^0 \geq 0$. Moreover, using Einstein's equations

$$T_z^z - T_0^0 = R_z^z - R_0^0 = \frac{z^2}{\ell_{UV}^2} (f(z) R_{zz} + R_{00}) = (d-1) \frac{z f'(z)}{2 \ell_{UV}^2} \geq 0 \implies f'(z) \geq 0. \quad (\text{E.13})$$

Since for arbitrary holographic RG flows $f(0) = 1$ and $f(\infty) = (\ell_{UV}/\ell_{IR})^2$, the NEC

implies

$$1 \leq f(z) \leq \left(\frac{\ell_{\text{UV}}}{\ell_{\text{IR}}} \right)^2, \quad 0 \leq f'(z). \quad (\text{E.14})$$

E.2 Euler-Lagrange approach

In the main part of the work we calculated explicitly the large radius expansion of the holographic EE using the Hamilton-Jacobi equation. Here we will show how the same results can be derived by solving the equation of motion (7.18) that results from extremizing the area, and evaluating it on-shell. We reproduce the equation here for convenience,

$$\rho(z)z^{d-1}\sqrt{\rho'(z)^2 + \frac{1}{f(z)}}\partial_z \left(\frac{\rho'(z)}{z^{d-1}\sqrt{\rho'(z)^2 + \frac{1}{f(z)}}} \right) - \frac{(d-2)}{f(z)} = 0. \quad (\text{E.15})$$

The Hamilton Jacobi approach is more direct; on the other hand, solving the Euler Lagrange equations gives a better understanding of the geometry of the minimal surface. So both methods are complementary. We start with the simpler cases of AdS and $d = 2$. Then we pass to the general case and study the large R expansion.

E.2.1 Simpler cases

Pure AdS _{$d+1$}

This is the case where $f(z)$ is constant for all z and there is no RG flow. If we start with the UV theory, then $f(z) = 1$ and the solution to the equation (7.18) is simply

$$\rho_{\text{UV}}(z) = \sqrt{z_t^2 - z^2}. \quad (\text{E.16})$$

It satisfies the boundary conditions if

$$z_t^{UV} = \sqrt{R^2 + \epsilon^2}. \quad (\text{E.17})$$

The minimal surface is a hemisphere centered at $z = \rho = 0$, with radius z_t^{UV} . This is the radius at $z = 0$, which is different than the size R of the entangling region at $z = \epsilon$.

Similarly, in the IR theory, $f(z) = \ell_{UV}^2/\ell_{IR}^2$ and the solution reads

$$\rho_{IR}(z) = \frac{\ell_{IR}}{\ell_{UV}} \sqrt{z_t^2 - z^2}. \quad (\text{E.18})$$

In this case the boundary conditions imply that

$$z_t^{IR} = \sqrt{\frac{\ell_{UV}^2}{\ell_{IR}^2} R^2 + \epsilon^2}. \quad (\text{E.19})$$

These solutions are valid for all d .

Evaluating the UV solution (E.16) in the holographic EE formula (7.14) we reobtain the solution (7.29)

$$S_{UV} = \gamma_d \int_{\epsilon/z_t^{UV}}^1 d\omega \, \omega^{1-d} (1 - \omega^2)^{\frac{d-3}{2}}. \quad (\text{E.20})$$

Two dimensional case and c-theorem

When $d = 2$ the $\rho(z)$ dependence disappears in the equation (E.15) leaving an equation involving just $\rho'(z)$ and $\rho''(z)$. Therefore the variational problem contains a conserved quantity and the solution can be written as

$$\rho(z) = R - \int_{\epsilon}^z \frac{dz}{f(z)^{1/2}} \frac{1}{\sqrt{(z_t/z)^2 - 1}}. \quad (\text{E.21})$$

The turning point is fixed by

$$\rho(z_t) = 0 \implies R = \int_{\epsilon}^{z_t} \frac{dz}{f(z)^{1/2}} \frac{1}{\sqrt{(z_t/z)^2 - 1}}. \quad (\text{E.22})$$

As a consequence of the NEC (7.12), $f(z) \geq 1$, so for an arbitrary z_t

$$R \leq \int_{\epsilon}^{z_t} dz \frac{1}{\sqrt{(z_t/z)^2 - 1}} = \sqrt{z_t^2 - \epsilon^2}. \quad (\text{E.23})$$

From (E.17), $R = \sqrt{(z_t^{\text{UV}})^2 - \epsilon^2}$, so (E.23) implies $z_t^{\text{UV}} \leq z_t$. Similarly, because $f(z) \leq \left(\frac{\ell_{\text{UV}}}{\ell_{\text{IR}}}\right)^2$, we have $z_t \leq z_t^{\text{IR}}$. The combined inequalities give

$$z_t^{\text{UV}} \leq z_t \leq z_t^{\text{IR}}. \quad (\text{E.24})$$

The first derivative of S with respect to R can be written as an expression in terms $\rho(z)$ evaluated at the cut-off ϵ , see (7.22). In particular for $d = 2$,

$$R \frac{dS}{dR} = \gamma_2 \frac{R}{z_t}. \quad (\text{E.25})$$

This defines a running c-function by comparing (E.25) between the UV fixed point and the holographic flow,

$$\frac{\Delta c}{3} = \frac{c(R)}{3} - \frac{c^{\text{UV}}(R)}{3} = R \frac{dS}{dR} - R \frac{dS^{\text{UV}}}{dR} = \gamma_2 R \left(\frac{1}{z_t} - \frac{1}{z_t^{\text{UV}}} \right) \leq 0. \quad (\text{E.26})$$

In the large R limit, $z_t \approx \frac{\ell_{\text{UV}}}{\ell_{\text{IR}}} R$ and the expression extracts the universal coefficient in $d = 2$

$$\frac{\Delta c}{3} = R \frac{d\Delta S}{dR} \Big|_{\tilde{\mu} R \gg 1} = \frac{\ell_{\text{UV}}}{2G_N^{(3)}} - \frac{\ell_{\text{IR}}}{2G_N^{(3)}} = \frac{(c_{\text{IR}} - c_{\text{UV}})}{3} \leq 0, \quad (\text{E.27})$$

where we identify the holographic central charge $c = \frac{3\ell}{2G_N^{(3)}}$ [264]. Eqs. (E.26) and (E.27) give a holographic proof of the irreversibility theorem in $d = 2$ [41, 239, 240].

E.2.2 Larger dimensions

For dimensions $d > 2$ the variational problem associated to (E.15) does not have a conserved quantity, and the equation of motion cannot be solved analytically for arbitrary $f(z)$. Instead, we will follow a matching procedure similar to what was originally done by [242, 243].

The idea is to write two different expansions for $\rho(z)$. The first expansion is written in powers of R in the large R limit, where each coefficient depends on z (Section E.2.2). This expansion is valid near $z = 0$ but it is not suitable near the turning point z_t , so

all coefficients in the expansion have an unknown parameter. The second expansion is written in powers of the IR mass scale $\tilde{\mu}$. We refer to this as the large z expansion (Section E.2.2). There we can impose the turning point boundary condition but not $\rho(\epsilon) = R$. In the limit where R and z are both large, both expansions overlap and this allows to fix the unknown parameters (Section E.2.2). In Fig. E.1, we depict a schematic profile for $\rho(z)$ including all the scales present, and the overlap range.

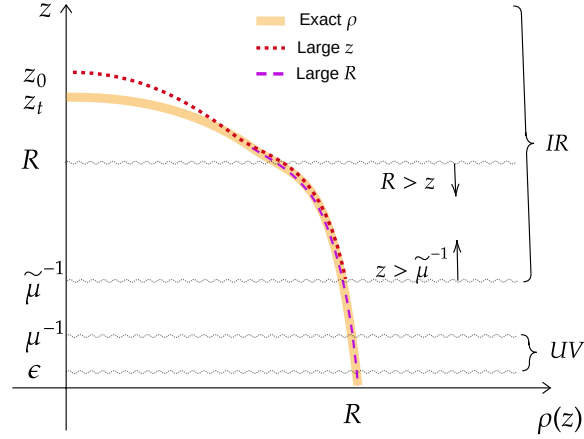


Figure E.1: Different approximations for the profile $\rho(z)$ of the minimal surface including all the scales present in the problem. The exact solution of $\rho(z)$, which is unknown for $d > 2$, is depicted in broad plot with turning point z_t . In long dashed lines there is a schematic plot of the large R expansion (E.45) and in short dashed lines there is an schematic plot of the large z expansion (E.40) to order z_0^{-1} . The UV is defined for $\epsilon < z < \mu^{-1}$, where ϵ is an UV cut-off and μ an UV energy scale; the IR is defined for $\tilde{\mu} < z$ where, $\tilde{\mu}$ is an IR energy scale. The matching procedure is done when z is between $\tilde{\mu}^{-1} < z < R$, where R is the sphere's radius of the spatial region at the boundary.

Large R expansion

For the large R expansion, let us begin proposing

$$\rho(z, R) = R - \frac{\rho_1(z)}{R^a}. \quad (\text{E.28})$$

This ansatz satisfies the UV boundary condition if $\rho_1(\epsilon) = 0$. The minus sign is explicitly chosen because we expect ρ to decrease with z as depicted in Figure 7.2. The linearized equation of motion (E.15) for $\rho_1(z)$ is

$$\frac{z^{d-1}}{\sqrt{f(z)}} \left(\frac{\sqrt{f(z)}}{z^{d-1}} \rho_1'(z) \right)' = -\frac{(d-2)}{f(z)} R^{a-1}. \quad (\text{E.29})$$

To satisfy that $\rho_1(z)$ is independent from R we need $a = 1$. The equation can be integrated to obtain the first correction

$$\rho_1(z) = b_1 \int_{\epsilon}^z du \frac{u^{d-1}}{\sqrt{f(u)}} + (d-2) \int_{\epsilon}^z du \frac{u^{d-1}}{\sqrt{f(u)}} \int_u^{\infty} dv \frac{1}{v^{d-1} \sqrt{f(v)}}. \quad (\text{E.30})$$

The ansatz (E.28) is valid for $\frac{\rho_1(z)}{R^2} \ll 1$. Here b_1 an arbitrary constant that multiplies the homogeneous solution. This reflects the fact that we cannot impose the IR boundary condition $\rho(z_t) = 0$ in this expansion.

The next corrections involve higher odd powers of $1/R$. The general solution also includes non-integer powers of $1/R$ that satisfy the homogeneous equation without source. These terms contribute nonlocal corrections to the EE that go to zero at large R , so we will not focus on them. In summary, we have

$$\rho(z) = R - \frac{\rho_1(z)}{R} - \frac{\rho_3(z)}{R^3} - \dots - \frac{\rho_\nu(z)}{R^\nu} - \dots. \quad (\text{E.31})$$

Expanding the Euler-Lagrange equation in $1/R$ gives equations for each ρ_n ,

$$\frac{z^{d-1}}{\sqrt{f(z)}} \left(\frac{\sqrt{f(z)}}{z^{d-1}} \rho'_n(z) \right)' = s_n(z), \quad (\text{E.32})$$

where $s_n(z)$ is a source term for $\rho_n(z)$, which depends on $\rho_m(z)$ with $m < n$. The first values for the sources are

$$s_1(z) = -\frac{(d-2)}{f(z)}, \quad s_3(z) = -\rho_1(z) \frac{(d-2)}{f(z)} - (d-2) \rho'_1(z)^2 + \frac{(d-1)}{z} f(z) \rho'_1(z)^3. \quad (\text{E.33})$$

Integrating (E.32) gives the solutions

$$\rho_n(z) = b_n \int_{\epsilon}^z du \frac{u^{d-1}}{\sqrt{f(u)}} - \int_{\epsilon}^z du \frac{u^{d-1}}{\sqrt{f(u)}} \int_u^{\infty} dv \frac{\sqrt{f(v)}}{v^{d-1}} s_n(z), \quad (\text{E.34})$$

with the b_n undetermined at this stage.

Large z expansion

Now we look for approximate solutions of the Euler-Lagrange equation in the IR regime $\tilde{\mu}z \gg 1$. Since $z < z_t$, in this limit we have $\tilde{\mu}z_t \gg 1$. In the IR zone we expect the solution to be similar to the pure AdS_{d+1} solution. We add a correction σ_1 that should be suppressed by powers of $\tilde{\mu}z$,

$$\rho(z) = \frac{\ell_{IR}}{\ell_{UV}} \sqrt{z_0^2 - z^2} + \frac{\ell_{IR}}{\ell_{UV}} \sigma_1(z), \quad (\text{E.35})$$

for some constant z_0 .

In the strict IR limit $z_0 = z_t^{\text{IR}}$ as discussed in (E.18). Using the IR approximation (E.10) of $f(z)$ in (E.15), the linearized equation for the correction becomes

$$\begin{aligned} \sqrt{z_0^2 - z^2} \left((d-2+\tilde{\alpha})z_0^2 z - (\tilde{\alpha}-1)z^3 \right) \frac{1}{(\tilde{\mu}z)^{2\tilde{\alpha}}} = \sigma_1(z)(d-2)z_0^2 z + \sigma_1'(z) \left(2z^4 + (d-3)z_0^2 z^2 \right. \\ \left. - (d-1)z_0^4 \right) + \sigma_1''(z) \left(z^5 + z z_0^4 - 2z^3 z_0^2 \right). \end{aligned} \quad (\text{E.36})$$

The solution to this equation is an integral involving hypergeometric functions, but the exact expression is not illuminating. However, we only need the solution at large R , which simplifies as we describe next.

The first thing we learn from this equation is that $\sigma_1(z)$ is suppressed by $(\tilde{\mu}z)^{-2\tilde{\alpha}}$. The value of z_t can be obtained at this order of approximation from the IR condition $\rho(z_t) = 0$,

$$z_0^2 = z_t^2 + \sigma_1^2(z_t). \quad (\text{E.37})$$

Thus, $z_0 \sim z_t$ plus corrections of order $(\tilde{\mu}z_t)^{-2\tilde{\alpha}}$. From the pure AdS_{d+1} case we expect the turning point to be of order $z_t \sim R$; we will check this self-consistently after finding the solution for $\rho(z)$. Since we want to match (E.31) with (E.35) we need to expand (E.35) in the large z_0 limit. The large z_0 expansion applied to (E.36) gives a linear equation for $\sigma_1(z)$ at order z_0^{-1}

$$\frac{z}{z_0} \frac{(d-2+\tilde{\alpha})}{(\tilde{\mu}z)^{2\tilde{\alpha}}} = -(d-1)\sigma_1'(z) + z\sigma_1''(z), \quad (\text{E.38})$$

with solution²

$$\sigma_1(z) = c_0 + \frac{z^2}{2z_0} \frac{1}{(\tilde{\mu}z)^{2\tilde{\alpha}}} \frac{(\tilde{\alpha} + d - 2)}{(\tilde{\alpha} - 1)(2\tilde{\alpha} + d - 2)} + \mathcal{O}\left(\frac{1}{z_0^2}\right). \quad (\text{E.39})$$

Replacing this solution into (E.35) and expanding the square root, we find the double expansion in z and z^0 we were looking for

$$\rho(z) = \frac{\ell_{IR}}{\ell_{UV}} z_0 - \frac{\ell_{IR}}{\ell_{UV}} \frac{z^2}{2z_0} \left(1 - \frac{1}{(\tilde{\mu}z)^{2\tilde{\alpha}}} \frac{(\tilde{\alpha} + d - 2)}{(\tilde{\alpha} - 1)(2\tilde{\alpha} + d - 2)} + \dots \right) + c_0 + \dots \quad (\text{E.40})$$

The first ‘ $\dots$ ’ refers to additional subleading powers of $(\tilde{\mu}z)^{2\tilde{\alpha}}$ whereas the second ‘ $\dots$ ’ refers to additional subleading powers of $1/z_0$. Both terms receive extra contributions if we consider higher corrections in (E.35).

Matching the expansions

The ρ_n corrections (E.34) have b_n as unspecified parameters. To obtain their values we need information from the IR region. For such reason we expand the integrals in (E.34) for $\tilde{\mu}z \gg 1$ using $f(z)$ (E.10) in the IR zone. The idea is to get an expression that looks like (E.40) in order to extract b_n .

The first correction (E.30) has two terms. To expand the first term, we split the integral introducing an arbitrary value Z in the IR zone $\tilde{\mu}Z \gg 1$, so that in the interval (z, Z) the IR approximation is valid. The result is independent of Z up to order $(\tilde{\mu}Z)^{-2\tilde{\alpha}}$, so we opt to consider the limit when $Z \rightarrow \infty$. Namely,

$$\begin{aligned} \int_{\epsilon}^z du \frac{u^{d-1}}{\sqrt{f(u)}} &\approx \int_{\epsilon}^Z du \frac{u^{d-1}}{\sqrt{f(u)}} + \frac{\ell_{IR}}{\ell_{UV}} \int_Z^z du u^{d-1} \left(1 + \frac{1}{2}(\tilde{\mu}u)^{-2\tilde{\alpha}} + \dots \right) \\ &= \tilde{\Sigma} + \frac{z^d}{d} \frac{\ell_{IR}}{\ell_{UV}} \left(1 + \frac{1}{(\tilde{\mu}z)^{2\tilde{\alpha}}} \frac{d}{2(d - 2\tilde{\alpha})} + \dots \right), \end{aligned} \quad (\text{E.41})$$

²We do not consider the homogeneous solution $\sigma_1^{\text{hom}}(z)$ since the corresponding matching expression is only related with the non integer powers of R .

where $\tilde{\Sigma}$ is defined as

$$\tilde{\Sigma} = \lim_{Z \rightarrow \infty} \int_{\epsilon}^Z du \frac{u^{d-1}}{\sqrt{f(u)}} - \frac{Z^d}{d} \frac{\ell_{IR}}{\ell_{UV}} \left(1 + \frac{1}{(\tilde{\mu}Z)^{2\tilde{\alpha}}} \frac{d}{2(d-2\tilde{\alpha})} + \dots \right). \quad (\text{E.42})$$

We use the same method for the second term expansion

$$\begin{aligned} -(d-2) \int_{\epsilon}^z du \frac{u^{d-1}}{\sqrt{f(u)}} \int_{\infty}^u dv \frac{1}{v^{d-1}\sqrt{f(v)}} &\approx -(d-2) \int_{\epsilon}^Z du \frac{u^{d-1}}{\sqrt{f(u)}} \int_{\infty}^u dv \frac{1}{v^{d-1}\sqrt{f(v)}} \\ &\quad + (d-2) \frac{\ell_{IR}^2}{\ell_{UV}^2} \int_Z^z du u^{d-1} \left(1 + \frac{1}{2(\tilde{\mu}u)^{2\tilde{\alpha}}} \right) \times \\ &\quad \times \int_{\infty}^u dv v^{1-d} \left(1 + \frac{1}{2(\tilde{\mu}v)^{2\tilde{\alpha}}} \right) \\ &= \tilde{\Gamma} + \frac{\ell_{IR}^2}{\ell_{UV}^2} \frac{z^2}{2} \left(1 - \frac{1}{(\tilde{\mu}z)^{2\tilde{\alpha}}} \frac{(\tilde{\alpha} + d - 2)}{(\tilde{\alpha} - 1)(2\tilde{\alpha} + d - 2)} + \dots \right), \end{aligned} \quad (\text{E.43})$$

where $\tilde{\Gamma}$ is defined as

$$\begin{aligned} \tilde{\Gamma} = \lim_{Z \rightarrow \infty} \left[-(d-2) \int_{\epsilon}^Z du \frac{u^{d-1}}{\sqrt{f(u)}} \int_{\infty}^u \frac{dv}{v^{d-1}\sqrt{f(v)}} \right] \\ - \left[\frac{\ell_{IR}^2}{\ell_{UV}^2} \frac{Z^2}{2} \left(1 - \frac{1}{(\tilde{\mu}Z)^{2\tilde{\alpha}}} \frac{(\tilde{\alpha} + d - 2)}{(\tilde{\alpha} - 1)(2\tilde{\alpha} + d - 2)} + \dots \right) \right]. \end{aligned} \quad (\text{E.44})$$

As a result, the following double expansion holds for $\rho(z)$,

$$\begin{aligned} \rho(z) = R - \frac{1}{R} \left[b_1 \tilde{\Sigma} + \tilde{\Gamma} + \frac{\ell_{IR}^2}{\ell_{UV}^2} \frac{z^2}{2} \left(1 - \frac{1}{(\tilde{\mu}z)^{2\tilde{\alpha}}} \frac{(\tilde{\alpha} + d - 2)}{(\tilde{\alpha} - 1)(2\tilde{\alpha} + d - 2)} + \dots \right) \right. \\ \left. + b_1 \frac{\ell_{IR}}{\ell_{UV}} \frac{z^d}{d} \left(1 + \frac{1}{(\tilde{\mu}z)^{2\tilde{\alpha}}} \frac{d}{2(d-2\tilde{\alpha})} + \dots \right) \right] + \dots \quad (\text{E.45}) \end{aligned}$$

Now that we have both expansions (E.45) and (E.40) in the same form we can match the coefficients in them,

$$R = \frac{\ell_{IR}}{\ell_{UV}} z_0, \quad b_1 = 0, \quad c_0 = -\frac{\tilde{\Gamma}}{R}. \quad (\text{E.46})$$

It is important to observe in (E.45) that the correction with the first power of R has two terms that go like z^2 and z^d . The unknown parameter b_1 is the coefficient of the

E.2 Euler-Lagrange approach

term $\frac{z^d}{R}$. A similar scenario occurs when higher orders are considered in the expansion. In that case $\rho(z)$ looks like

$$\rho(z) = R - \frac{\ell_{IR}}{\ell_{UV}} \frac{z^d}{d} \left(\frac{b_1}{R} + \frac{b_3}{R^3} + \dots \right) - d_2 \frac{z^2}{R} - d_4 \frac{z^4}{R^3} - \dots, \quad (\text{E.47})$$

for some coefficients d_{2k} . Then (E.47) suggests that the b_n coefficients must be identified by looking at the terms $\sim z^d/R^n$ in the large z expansion of $\rho(z)$ (E.35). Since $\sigma_1(z)$ is of order $(\tilde{\mu}z)^{-2\tilde{\alpha}}$ only the square root term might contribute to b_n . Its expansion for large z is

$$\frac{\ell_{IR}}{\ell_{UV}} \sqrt{z_0^2 - z^2} = \frac{\ell_{IR}}{\ell_{UV}} \sum_{k=0}^{\infty} \binom{1/2}{k} (-1)^k \frac{z^{2k}}{z_0^{2k-1}}. \quad (\text{E.48})$$

Finally,

$$b_n = \begin{cases} 0 & n \neq d-1 \\ -d(-1)^{\frac{d}{2}} \binom{1/2}{d/2} \left(\frac{\ell_{IR}}{\ell_{UV}} \right)^{d-1} & n = d-1 \text{ \& } d = \text{even} \end{cases}. \quad (\text{E.49})$$

To make computations shorter, we work with non-integer dimensions d , so we can effectively consider $b_n = 0$ for all n . Taking the limit to the integer dimensions recovers the correct result.

E.2.3 Entropy expansion

Having obtained the approximate solution $\rho(z)$ at large R , we are ready to evaluate the entropy. To make more explicit the R dependence of the entropy using the Euler-Lagrange approach, we rewrite (7.14) as

$$S = \gamma_d R^{d-2} \int_{\epsilon}^{z_t} \frac{dz}{z^{d-1}} \left(\frac{\rho(z)}{R} \right)^{d-2} \sqrt{\rho'(z)^2 + \frac{1}{f(z)}}. \quad (\text{E.50})$$

Both terms $\frac{\rho(z)}{R}$ and $\rho'(z)$ contain only inverse odd powers of R , thus the large R limit of the integrand reproduces the structure (7.1). The upper limit of integration z_t is also R -dependent, and this only contributes to finite terms because at first order $z_t \sim R$. So in order to obtain the μ_{d-2k} it is sufficient to take $z_t \rightarrow \infty$.

The first term from this expansion reproduces the area law and coincides with the

result of the HJ formalism (7.52) when $z_t \rightarrow \infty$:

$$S^{(d-2)} = \gamma_d R^{d-2} \int_{\epsilon}^{\infty} \frac{dz}{z^{d-1}} \frac{1}{\sqrt{f(z)}}. \quad (\text{E.51})$$

The second term depends on $\rho_1(z)$, so it needs to be evaluated using the solution (E.30) with $b_1 = 0$. In particular, we have

$$\rho_1'(z) = (d-2) \frac{z^{d-1}}{\sqrt{f(z)}} \int_z^{\infty} \frac{dv}{v^{d-1}} \frac{1}{\sqrt{f(v)}}. \quad (\text{E.52})$$

This matches the HJ solution (7.60) when $z_t \rightarrow \infty$,

$$\begin{aligned} S^{(d-4)} &= \gamma_d R^{d-4} \int_{\epsilon}^{\infty} \frac{dz}{z^{d-1}} \frac{1}{\sqrt{f(z)}} \left(\frac{1}{2} f(z) \rho_1'(z)^2 - (d-2) \rho_1(z) \right) \\ &= -\frac{\gamma_d}{2} R^{d-4} \int_{\epsilon}^{\infty} \frac{dz}{z^{d-1}} \sqrt{f(z)} \rho_1'(z)^2 \\ &= -\gamma_d \frac{(d-2)^2}{2} R^{d-4} \int_{\epsilon}^{\infty} dz z^{d-1} f(z) \left(\int_z^{\infty} \frac{dv}{v^{d-1}} \frac{1}{\sqrt{f(v)}} \right)^2. \end{aligned} \quad (\text{E.53})$$

In the second step the equation of motion for $\rho_1(z)$ (E.29) was applied in order to combine both terms,

$$-\int_{\epsilon}^{\infty} dz \rho_1(z) \frac{(d-2)}{z^{d-1} \sqrt{f(z)}} = -\int_{\epsilon}^{\infty} \frac{dz}{z^{d-1}} \sqrt{f(z)} \rho_1'(z)^2 + \underbrace{\rho_1(z) \frac{\sqrt{f(z)} \rho_1'(z)}{z^{d-1}}}_{=0} \Big|_{\epsilon}^{\infty}. \quad (\text{E.54})$$

The procedure can be applied to calculate the higher order terms μ_{d-2k} . In the main text we have instead focused on the HJ method since we found it was more economic than using the minimal surface equation of motion.

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