

# Entanglement Entropy in Quantum Gravity

by

William Donnelly

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## Abstract

We study a proposed statistical explanation for the Bekenstein-Hawking entropy of a black hole in which entropy arises quantum-mechanically as a result of entanglement. Arguments for the identification of black hole entropy with entanglement entropy are reviewed in the framework of quantum field theory, emphasizing the role of renormalization and the need for a physical short-distance cutoff.

Our main novel contribution is a calculation of entanglement entropy in loop quantum gravity. The kinematical Hilbert space and spin network states are introduced, and the entanglement entropy of these states is calculated using methods from quantum information theory. The entanglement entropy is compared with the density of states previously computed for isolated horizons in loop quantum gravity, and the two are found to agree up to a topological term.

We investigate a conjecture due to Sorkin that the entanglement entropy must be a monotonically increasing function of time under the assumption of causality. For a system described by a finite-dimensional Hilbert space, the conjecture is found to be trivial, and for a system described by an infinite-dimensional Hilbert space a counterexample is provided.

For quantum states with Euclidean symmetry, the area scaling of the entanglement entropy is shown to be equivalent to the strong additivity condition on the entropy. The strong additivity condition is naturally interpreted in information-theoretic terms as a continuous analog of the Markov property for a classical random variable. We explicitly construct states of a quantum field theory on the one-dimensional real line in which the area law is exactly satisfied.

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## Dedication

This is dedicated to Jessica. All of my accomplishments over the past months pale in comparison to hers.

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# Chapter 1

## Introduction

The problem of finding a fundamental theory encompassing both quantum mechanics and general relativity is a major unanswered question of theoretical physics. The study of black hole physics has provided a wealth of insight into the problem of quantum gravity, as it incorporates general relativity, quantum theory and thermodynamics. This is seen in the Bekenstein-Hawking formula for the thermodynamic entropy of a black hole

$$S_{\text{BH}} = \frac{A}{4} \frac{c^3}{G\hbar} \quad (1.1)$$

which depends on the area  $A$  of the black hole horizon in units of the Planck length  $\ell_P = \sqrt{G\hbar/c^3}$ . The problem of deriving the Bekenstein-Hawking formula from a microscopic description is an important open question, and is expected to provide insight into the nature of quantum gravity.

There are a number of proposals for a microscopic derivation of the black hole entropy [1]. One proposal is the holographic principle of 't Hooft, in which the Bekenstein-Hawking entropy is taken as a measure of the number of internal states of a region of space [2, 3]. This line of reasoning has led to the conjecture that the degrees of freedom within a region of space are isomorphic to the degrees of freedom of a conformal field theory on its boundary, a proposal known as the AdS/CFT correspondence [4].

Another proposal is that the Bekenstein-Hawking entropy measures possible geometric states of the horizon [5]. This approach has been pursued in loop quantum gravity where it has led to a counting of degrees of freedom for isolated horizons [6]. This proposal will be described in greater detail in chapter 3.

The subject of this thesis is a third proposal due originally to Rafael Sorkin that the Bekenstein-Hawking entropy is a measure of entanglement of a quantum state [7]. An appealing aspect of this proposal is that it allows the Bekenstein-Hawking entropy to be understood as a consequence of ordinary quantum theory, rather than as a result of exotic gravitational physics. As we will see it also allows the Bekenstein-Hawking entropy to be studied using the methods of quantum information theory.



Thermodynamics	Black hole mechanics
Temperature $T$	Surface gravity $\kappa$
Entropy $S$	Horizon surface area $A$
Energy $E$	Black hole mass $M$

Figure 1.1: Correspondence between properties of thermodynamic systems vs. properties of black holes

## 1.1 Black hole thermodynamics

The problem of black hole entropy comes from the study of black hole thermodynamics [8]. A most surprising feature of general relativity is the existence of a set of laws of black hole mechanics in precise correspondence with the laws of thermodynamics [9]. The correspondence between properties of a black hole and properties of a thermodynamic system are summarized in figure 1.1.

Though there exist black hole analogues of all four laws of thermodynamics, of particular interest are the first and second laws. The first law of thermodynamics states that when energy  $dE$  at temperature  $T$  is added to thermodynamic system via a reversible process, the entropy increases by an amount  $dS$  satisfying

$$dE = TdS.$$

Similarly the first law of black hole mechanics says that when matter is added to a black hole with surface gravity  $\kappa$  the area of its event horizon will increase by an amount  $dA$  such that

$$dM = \frac{\kappa}{8\pi} dA. \tag{1.2}$$

The second law of thermodynamics states that the entropy of a closed system cannot decrease. The black hole analogue of the second law of thermodynamics is the theorem of Hawking, stating that the surface area of a black hole's event horizon is non-decreasing in time [10]. This theorem relies only on the assumption of cosmic censorship, and applies very generally even to systems where multiple black holes collide and merge. Note that the asymmetry of this law with respect to time reversal is a result of the asymmetry in the definition of a black hole.

From the perspective of classical physics, the assignment of a temperature to a black hole has no clear interpretation. Classically, no matter can escape the horizon of a black hole, and an observer in the vacuum outside a black hole will measure no temperature. Without quantum physics the similarity between black hole mechanics and thermodynamics can be no more than an analogy.

Indications that the black hole area represents a true thermodynamic entropy were provided by thought experiments in which thermodynamic entropy of a system is decreased by lowering matter into a black hole [11]. These thought experiments

led Bekenstein to postulate the generalized second law, according to which the sum of the black hole entropy and entropy of matter cannot decrease.

The strongest indication that the black hole entropy is a real physical entropy was provided by Hawking, who showed that in the presence of quantum fields a black hole radiates thermally at the *Hawking temperature*

$$T_{\text{H}} = \frac{\kappa}{2\pi} \frac{\hbar c^3}{Gk} \quad (1.3)$$

proportional to its surface gravity  $\kappa$ . This cemented the status of the laws of black hole mechanics as real laws of thermodynamics, and the black hole area as a physical entropy. Substituting the relation between temperature and surface gravity (1.3) into the first law of black hole mechanics (1.2) and identifying the black hole energy with its mass, one arrives directly at the expression for the Bekenstein-Hawking entropy (1.1).

This thermodynamic behaviour is not specific to black holes, but extends to other types of causal horizons. Gibbons and Hawking considered an analogous situation in de Sitter space, in which an observer has a cosmological horizon due to the exponential expansion of space [12]. In de Sitter space, the thermal state has a temperature related to the rate of expansion, which has the same relation to the surface gravity at the horizon as the Hawking temperature

$$T_C = \frac{\kappa}{2\pi} \frac{\hbar c^3}{Gk}.$$

An important difference between cosmological horizons and black holes is the observer-dependence of the cosmological horizon. The black hole horizon is defined as the boundary of the past of future null infinity, which is clearly observer-independent. It may be equivalently defined as the boundary of the past of the world line of any observer that does not eventually cross the horizon. All such observers will agree on the location of the horizon. This is not the case in de Sitter space, where different observers will have different past horizons.

There is also an analogue of black hole radiation in flat Minkowski spacetime. A uniformly accelerating observer in Minkowski space has a horizon, called the Rindler horizon. This is because a constant acceleration allows the observer to outrun certain light rays. If the observer is modelled as a particle detector locally coupled to the field with acceleration  $a$ , it would behave as if immersed in a thermal bath at the *Unruh temperature* [13]

$$T_{\text{U}} = \frac{a}{2\pi} \frac{\hbar c^3}{Gk}.$$

The similarities between the temperature associated with these different types of horizons suggest that they have a common physical origin. In fact the Rindler geometry in the Unruh effect can be seen as a limit of the exterior geometry of a

black hole in the limit of large mass. By the equivalence principle, it may also be viewed as the limit where the observer approaches the horizon.

These considerations have led to the suggestion that the black hole entropy should extend to every causal horizon, defined as the boundary of the past of any time-like curve with infinite proper length [14]. This definition encompasses all three of the previously-mentioned cases, and there are indications that the laws of black hole mechanics extend to general causal horizons. This suggests that any statistical derivation of black hole entropy must apply to all causal horizons.

At the heart of the derivation of black hole temperature is the fact that in quantum field theory the very concept of a particle is observer-dependent. Different observers will in general disagree about which modes are of positive frequency, and therefore disagree on which state represents the true vacuum. Since the vacuum may be described either as a pure state or as a mixed state depending on the observer, any statistical derivation of the black hole entropy must account for the observer-dependence of the entropy.

Although the black hole temperature is derived directly, the black hole entropy is derived indirectly via the laws of black hole mechanics. We know from statistical mechanics that entropy has an interpretation as a quantitative measure of the lack of information about the microscopic state of a system. The problem of black hole entropy is to account for the Bekenstein-Hawking entropy without appealing to the first law of black hole mechanics.

## 1.2 Entanglement entropy

In quantum theory a pure state of a composite system  $AB$  is described by a state in a tensor product Hilbert space

$$|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B.$$

If there exist vectors  $|\psi^A\rangle \in \mathcal{H}_A$  and  $|\psi^B\rangle \in \mathcal{H}_B$  such that  $|\psi\rangle = |\psi^A\rangle \otimes |\psi^B\rangle$  then  $|\psi\rangle$  is *unentangled*, otherwise it is *entangled*.

In order to quantify the degree of entanglement,  $|\psi\rangle$  may be expressed as a Schmidt decomposition. There exist positive real numbers  $\{\lambda_i\}_{i \in \mathcal{I}}$  called *Schmidt coefficients*, and orthonormal sets  $\{|\psi_i^A\rangle\}_{i \in \mathcal{I}} \subset \mathcal{H}_A$  and  $\{|\psi_i^B\rangle\}_{i \in \mathcal{I}} \subset \mathcal{H}_B$  such that

$$|\psi\rangle = \sum_{i \in \mathcal{I}} \lambda_i |\psi_i^A\rangle \otimes |\psi_i^B\rangle.$$

The number of non-zero Schmidt coefficients  $|\mathcal{I}|$  is called the *Schmidt rank*, which may be either finite or countably infinite. In particular we see that  $|\psi\rangle$  is unentangled if and only if its Schmidt rank is one.

The density matrix  $\rho = |\psi\rangle\langle\psi|$  is sufficient to recover statistics for any measurement done on the system  $AB$ . If one is concerned only with measurements on system  $A$  then it is sufficient to consider the *partial trace*

$$\rho_A = \text{Tr}_{\mathcal{H}_B}\rho = \sum_{i \in \mathcal{I}} \rho_i |\psi_i^A\rangle\langle\psi_i^A|$$

where  $\rho_i = \lambda_i^2$ . One can do the same for system  $B$  yielding the state

$$\rho_B = \text{Tr}_{\mathcal{H}_A}\rho = \sum_{i \in \mathcal{I}} \rho_i |\psi_i^B\rangle\langle\psi_i^B|.$$

The rank of  $\rho_A$  is the Schmidt rank of the state  $|\psi\rangle$ . An important property of the density matrices  $\rho_A$  and  $\rho_B$  is that they have the same non-zero spectrum, which is entirely determined by the Schmidt coefficients.

The physical entropy of a quantum system is given by the von Neumann entropy

$$S(\rho) = -\text{Tr}(\rho \log \rho).$$

If  $|\psi\rangle$  is entangled, then the states  $\rho_A$  and  $\rho_B$  will each have positive entropy given by

$$S(\rho_A) = S(\rho_B) = -\sum_{i \in \mathcal{I}} \rho_i \log \rho_i.$$

This quantity is called the *entanglement entropy* of the state  $|\psi\rangle$ . The entanglement entropy is symmetric and measures the degree of entanglement between systems  $A$  and  $B$ .

As a consequence of entanglement the density matrix  $\rho$  may have zero entropy  $S(\rho) = 0$ , while the states  $\rho_A$  and  $\rho_B$  both have positive entropy. Note that this does not occur in classical probability theory. There the entropy is given by the Shannon entropy, which for a discrete probability distribution  $p : \mathbb{N} \rightarrow \mathbb{R}$  is given by

$$H(p) = -\sum_{i=1}^{\infty} p(i) \log p(i).$$

We can therefore consider the analogous case where the density matrix  $\rho$  is replaced with a probability distribution  $p_{AB} : \mathbb{N}^2 \rightarrow \mathbb{R}$  where  $p_{AB}(a, b) \geq 0$  and  $\sum_{a,b} p_{AB}(a, b) = 1$ . The analogue of  $\rho_A$  is the function  $p_A : \mathbb{N} \rightarrow \mathbb{R}$  given by  $p_A(a) = \sum_b p_{AB}(a, b)$ . It is a theorem of classical information theory that  $H(p_A) \leq H(p)$ , in other words the entropy of a system is larger than the entropy of any of its subsystems [15]. For quantum systems there is no equivalent restriction on the von Neumann entropy  $S$ . This fact has been summarized by saying that “quantum information can be negative” [16].

### 1.3 Black hole entropy as entanglement

The idea that entanglement entropy could provide a microscopic explanation for the Bekenstein-Hawking entropy was first proposed by Sorkin and collaborators [7, 17]. They observed that in quantum field theory, regions of space are subsystems. In particular, in the presence of a horizon the degrees of freedom on a Cauchy surface can be partitioned into those inside the horizon and those outside the horizon. It is then possible for the state on the full Cauchy surface to be a pure state such as the vacuum state, while the state of the subsystem outside the horizon is a mixed state such as a thermal state of non-zero temperature.

This naturally explains why a horizon has entropy. In thermodynamics entropy arises because some variables are considered observable such as the total energy of the system, while others such as the exact positions of particles are unobservable. A horizon provides a natural division of the degrees of freedom into those outside the horizon which are observable, and those behind the horizon which are unobservable.

Note that the entanglement entropy is not the same as ignorance of the state of the region beyond the horizon. The entanglement entropy is a measure of ignorance about the state of the exterior region which arises because of an observer's inability to measure beyond the horizon.

Any statistical derivation of the Bekenstein-Hawking entropy must explain the area law, which is the proportionality of the entropy and the area of the horizon. This is contrary to the expectation from thermodynamics that the entropy of a system should be proportional to the system's volume.

For example, consider a large but finite lattice with a finite number  $d$  of degrees of freedom at each point. Given a subset of  $n$  lattice points, it is clear that the total number of degrees of freedom grows like  $N = d^n$ . If all states are equally likely then the von Neumann entropy reduces to the Boltzmann entropy  $S = \log N = n \log d$  which is proportional to the volume of the region considered.

One reason why the entanglement entropy cannot scale with volume is that the entanglement entropy is symmetric. Recall that if  $A$  and  $B$  are two systems and  $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$  then the entropy of system  $A$  is equal to the entropy of system  $B$ . However it is clear that the volume of a general subset of lattice points is not the same as the volume of its complement. This rules out the possibility of an exact volume scaling of the entanglement entropy. The area law is not ruled out, since the boundary of  $A$  is the same as the boundary of its complement  $B$ .

In fact, the area-scaling of the entanglement entropy has been confirmed for a scalar quantum field theory in flat spacetime by both analytic and numerical methods [17, 18, 19]. In all cases the entanglement entropy of the vacuum state has been found to scale linearly with the surface area of the region traced over. This is described in greater detail in chapter 2.

The entanglement entropy is divergent in quantum field theory, and must be regulated by introducing an ultraviolet cutoff scale  $\epsilon$ . The entanglement entropy

of  $\nu$  non-interacting scalar fields depends linearly on the number of fields and the boundary area  $A$  as

$$S \propto \frac{\nu A}{\epsilon^2}. \quad (1.4)$$

The exact coefficient of proportionality may differ depending on the regularization method. While the dependence on area matches the Bekenstein-Hawking entropy, there are two aspects in which (1.4) differs from the Bekenstein-Hawking formula. The first is that this expression diverges in the limit  $\epsilon \rightarrow 0$ , whereas  $S_{\text{BH}}$  is finite. The second is that (1.4) has the wrong dependence on the number of fields, an issue which has been called the *species problem*.

The divergence of the entanglement entropy is not surprising if the black hole entropy and entropy of entanglement are the same quantity. If this is the case, then the entanglement entropy ought to satisfy the Bekenstein-Hawking formula when both quantum theory and general relativity are taken into account. The scalar quantum field theory neglects the gravitational influence of the quantum fields on spacetime, and therefore describes a theory where  $G = 0$ . When  $G = 0$ ,  $S_{\text{BH}}$  is infinite, so it is not surprising that these entanglement entropy calculations yield divergent results.

This would seem to imply that this divergence will be present unless we take into account the effect of matter on spacetime. The simplest model that takes this influence into account is semiclassical gravity. In this model the Einstein tensor is set equal to the expectation value of the quantum energy momentum tensor

$$G_{ab} = 8\pi G \langle T_{ab} \rangle.$$

It is not hard to see that this does not help to regulate the entanglement entropy. This is because the entanglement entropy diverges for the vacuum state in Minkowski spacetime, for which  $G_{ab} = \langle T_{ab} \rangle = 0$ . In order to regulate the divergence of entanglement entropy we must treat gravity as a quantum field.

In order to understand the divergence of entanglement entropy and the species problem it is important to consider that the gravitational constant  $G$  is not a constant, but depends on the energy scale at which it is observed. There is a bare constant  $G_0$  which appears in the classical action and a renormalized constant  $G_R$  which appears in the effective action. The relationship between  $G_0$  and  $G_R$  depends on the number and type of fields, giving a resolution of the species problem described in section 2.3.

While renormalization of  $G$  resolves the species problem, it shows that the problem of constructing a theory with a finite entanglement entropy between regions of space is equivalent to the problem of constructing a theory with a non-zero renormalized gravitational constant. Gravity is known to be non-renormalizable, suggesting that the entanglement entropy is also non-renormalizable.

The divergence of the entanglement entropy suggests the need for a physical ultraviolet cutoff at the Planck scale. It is expected on general grounds that a fundamental theory of quantum gravity will provide exactly such a cutoff, solving both

the ultraviolet problem of quantum gravity and the divergence of the entanglement entropy.

In chapter 3 we consider the entanglement entropy in loop quantum gravity. Loop quantum gravity is a quantum theory of pure gravity without matter in which space is represented by a discrete structure, a spin network. We show that the entanglement entropy obeys a discrete version of the area law which reduces to the exact area law for a certain class of Euclidean-invariant states.

In order for the entropy of entanglement to be considered as a physically meaningful entropy, it should satisfy some form of the second law of thermodynamics. It has been argued by Sorkin that the entanglement entropy should satisfy the second law exactly when the surface under consideration is a horizon [20]. The important property distinguishing a horizon is that the state of the region beyond the horizon does not influence the evolution of the rest of the universe. The increase of black hole entropy is therefore a manifestation of two factors: entanglement from quantum theory, and causality from general relativity. Sorkin's argument is evaluated in chapter 4.

Inspired by the problem of regularizing the entanglement entropy without breaking the continuous symmetry of space, in chapter 5 we consider a generic class of quantum field theories defined in three-dimensional Euclidean space. We show that the area law is equivalent to a property of the entropy known as strong additivity. The strong additivity property has a natural information-theoretic interpretation in terms of conditional independence which we relate to the theory of quantum Markov networks. Our hope is that this characterization of the area law will help to define a continuous theory in which the entanglement entropy is finite.

We conclude in chapter 6 with several proposed directions for future work.

# Chapter 2

## Quantum field theory

A natural setting in which to study the properties of entanglement entropy is quantum field theory in a fixed background spacetime. In this theory, gravity is treated according to classical general relativity, but all other fields are quantized. One therefore constructs a classical background as a solution to Einstein's equations, and then studies quantum fields that propagate on this classical background. This theory has been successfully used to calculate radiation from a black hole, so it is natural to seek the entropy within this theory as well.

In this chapter we will consider quantum field theory in flat Minkowski space. There are several reasons for this choice, mostly due to difficulties that arise in more general curved backgrounds. The first difficulty is the ambiguity in the choice of vacuum state. We would like to identify the entropy of a horizon with the vacuum entanglement entropy, but general spacetimes do not admit a unique choice of vacuum state. At best we could hope to compute the entanglement entropy in one of the cases where there is a physically motivated choice of vacuum state.

The most pressing difficulty is the challenge of regularizing the theory in the presence of curvature. As we will see, the entanglement entropy diverges because of the inclusion of modes of arbitrarily small wavelength. This ultraviolet divergence must be regulated by introducing a distance scale  $\epsilon$  and ignoring modes with wavelengths smaller than  $\epsilon$ . Even in flat space, this is difficult to do without violating Lorentz invariance. In curved space this process is even further complicated due to the presence of curvature.

The entanglement entropy is equally well defined in flat space, so as a first step we can study its properties there. Although Minkowski space has no horizon, we can instead consider entanglement entropy for an arbitrary set  $\Omega \subset \mathbb{R}^3$ . In fact, we can expect flat space calculations to be a good approximation to those in curved space. This is because the entanglement entropy is primarily a UV phenomenon, and for non-microscopic black holes the horizon is approximately flat, so that Minkowski space is a good approximation of the near-horizon geometry.

Consider a classical scalar field  $\phi$  in flat space with conjugate momentum  $\pi$ .



The simplest case is the Klein-Gordon scalar field which has the Hamiltonian

$$H(\phi, \pi) = \frac{1}{2} \int_{\mathcal{B}} [\pi(x, t)^2 + |\nabla \phi(x, t)|^2 + m^2 \phi(x, t)^2] d^3x$$

To simplify quantization we have confined the system to a box  $\mathcal{B} = [-L/2, L/2]^3$ . We can then consider the Fourier modes of the field

$$\begin{aligned} \phi_k &= L^{-3/2} \int_{\mathcal{B}} \phi(x) \exp\left(i \frac{2\pi k x}{L}\right) d^3x & k \in \frac{2\pi}{L} \mathbb{Z}^3 \\ \pi_k &= L^{-3/2} \int_{\mathcal{B}} \pi(x) \exp\left(i \frac{2\pi k x}{L}\right) d^3x \end{aligned}$$

In terms of the modes, the Hamiltonian simplifies to

$$H(\phi, \pi) = \frac{1}{2} \sum_k [|\pi_k|^2 + |k|^2 |\phi_k|^2 + m^2 |\phi_k|^2]$$

which reduces the quantum field to a collection of independent harmonic oscillators, one for each mode  $k$ . It is important to note that these are complex-valued harmonic oscillators; these can either be quantized directly or by making a change of variables to real-valued oscillators. The angular frequency of mode  $k$  is given by

$$\omega_k = \sqrt{|k|^2 + m^2}$$

In this case we can define the *vacuum state*  $|0\rangle$  to be the state of least energy. It can be written explicitly as the product of ground states of oscillators with frequencies  $\omega_k$

$$\langle 0|\phi\rangle = \prod_k \sqrt{\frac{\omega_k}{\pi}} \exp\left(-\frac{1}{2}\omega_k |\phi_k|^2\right)$$

We can now take the limit of this expression as  $L \rightarrow \infty$ , replacing the discrete index  $k$  with a continuous parameter also denoted  $k$

$$\langle 0|\phi\rangle \propto \exp\left(-\frac{1}{2} \int \omega_k |\phi_k|^2 d^3k\right)$$

This can be interpreted as the probability amplitude for measuring the field configuration  $\phi$  when the field is in its ground state. Because this integral includes both arbitrarily short and long wavelengths, there are infrared and ultraviolet divergences which lead to ill-defined expressions for certain physical quantities. A regularization must be applied in order to extract physical predictions.

Given an arbitrary region of space  $\Omega$ , we can write  $\phi = (\phi_\Omega, \phi_{\bar{\Omega}})$  where  $\bar{\Omega}$  denotes the set-theoretic complement of  $\Omega$ . In general, there do not exist states  $|0_\Omega\rangle$  and  $|0_{\bar{\Omega}}\rangle$  such that

$$\langle 0|\phi\rangle = \langle 0_\Omega|\phi_\Omega\rangle \langle 0_{\bar{\Omega}}|\phi_{\bar{\Omega}}\rangle$$

Thus the vacuum state  $|0\rangle$  is entangled. In order to calculate the entanglement entropy, we will have to introduce a regularization.

## 2.1 The Hamiltonian approach

The Klein-Gordon quantum field theory considered above can be thought of as a theory of a continuous family of harmonic oscillators, with one oscillator at each point in space. A natural way to regularize the theory is to replace the continuum of harmonic oscillators with a finite lattice of harmonic oscillators. To recover continuum results, we take the limit in which the density and number of oscillators increases to fill all of space.

We will therefore consider the entanglement entropy of a finite collection of coupled harmonic oscillators [17, 18]. If the displacement of the oscillators is given by  $q = (q_1, \dots, q_N)$  with conjugate momenta  $p = (p_1, \dots, p_n)$ . The Hamiltonian is

$$H(q, p) = \frac{1}{2} \left( \sum_{i=1}^N p_i^2 + \sum_{i,j=1}^N K_{ij} q_i q_j \right) = \frac{1}{2} (p^T p + q^T K q)$$

By choosing a basis which diagonalizes the matrix  $K$ , we can express this as a theory of uncoupled harmonic oscillators. It is useful to introduce the matrix  $W = \sqrt{K}$ , whose diagonal elements are the angular frequencies of the uncoupled modes. The ground state density matrix  $\rho$  therefore has the Gaussian form

$$\langle q | \rho | q' \rangle = \sqrt{\det \frac{W}{\pi}} e^{-\frac{1}{2} q^T W q} e^{-\frac{1}{2} q'^T W q'}$$

Let  $n < N$  be the set of oscillators within a region  $\Omega$ . Because of the Gaussian form of  $\rho$ , we can explicitly perform the partial trace over the oscillators  $n+1, \dots, N$  using the identity

$$\int \exp(-x^T A x + b^T x) d^n x = \sqrt{\frac{\pi^n}{\det(A)}} \exp\left(\frac{b^T A^{-1} b}{4}\right) \quad (2.1)$$

We can express  $q = (q_i, q_o)$  in terms of “inside” and “outside” oscillators, and  $W$  in block form as

$$W = \begin{bmatrix} W_i & W_b \\ W_b^T & W_o \end{bmatrix}$$

The outside density matrix is obtained by integrating over the inside oscillators

$$\langle q_o | \rho_o | q_o \rangle = \sqrt{\det \frac{W}{\pi}} \left( \int e^{-q_i^T W_i q_i - (q_o + q'_o)^T W_b q_i} d^n q_i \right) e^{-\frac{1}{2} q_o^T W_o q_o} e^{-\frac{1}{2} q'_o{}^T W_o q'_o}$$

Using (2.1), this becomes

$$\langle q_o | \rho_o | q_o \rangle = \frac{\sqrt{\det \frac{W}{\pi}}}{\sqrt{\det \frac{W_i}{\pi}}} e^{-\frac{1}{4} (q_o + q'_o)^T W_b^T W_i^{-1} W_b (q_o + q'_o)} e^{-\frac{1}{2} q_o^T W_o q_o} e^{-\frac{1}{2} q'_o{}^T W_o q'_o}$$

This is most conveniently expressed by introducing variables

$$x = \sqrt{W_o} q_o$$

$$\Lambda = W_o^{-1/2} W_b^T W_i^{-1} W_b W_o^{-1/2}$$

and using the identity for the determinant of a block matrix

$$\begin{aligned} \det W &= \det W_i \det W_o \det(I - W_o^{-1} W_b^T W_i^{-1} W_b) \\ &= \det W_i \det W_o \det(I - \Lambda) \end{aligned}$$

With these substitutions, the outside density matrix is

$$\langle x | \rho_o | x' \rangle = \sqrt{\det \frac{I - \Lambda}{\pi}} e^{-\frac{1}{2} x^T x} e^{-\frac{1}{2} x'^T x'} e^{-\frac{1}{4} (x+x')^T \Lambda (x+x')}$$

By diagonalizing the matrix  $\Lambda$  into eigenvalues  $\{\lambda_j\}_{j=1}^n$ , the matrix  $\rho_o$  can be expressed as a product of density matrices  $\rho_j$  where

$$\langle x | \rho_j | x' \rangle = \sqrt{\frac{1 - \lambda_j}{\pi}} e^{-\frac{1}{2} (x^2 + x'^2)} e^{-\frac{1}{4} \lambda_j (x+x')^2}$$

To compute the entropy of the density matrix  $\rho_j$  we introduce new variables  $\omega_j$  and  $\xi_j$  such that

$$\omega_j = \frac{(1 - \xi_j^2)}{(1 + \xi_j)^2} \quad \text{and} \quad \lambda_j = \frac{4\xi_j}{(1 - \xi_j)^2}$$

The density matrix  $\rho_j$  is diagonal in the energy eigenbasis for the harmonic oscillator with angular frequency  $\omega_j$ , and can be written as

$$\rho_j = (1 - \xi_j) \sum_{n=1}^{\infty} \xi_j^n |n\rangle \langle n|$$

The entropy of the  $j^{\text{th}}$  oscillator can be written either in terms of  $\xi_j$  or  $\lambda_j$ ,

$$\begin{aligned} S_j &= -\log(1 - \xi_j) - \frac{\xi_j}{1 - \xi_j} \log \xi_j \\ &= \log \frac{1}{2} \sqrt{\lambda_j} + \sqrt{1 + \lambda_j} \log \left( \sqrt{1 + \frac{1}{\lambda_j}} + \frac{1}{\sqrt{\lambda_j}} \right) \end{aligned} \quad (2.2)$$

Thus the entanglement entropy is given by the sum

$$S = \sum_{j=1}^n S_j$$

It is possible to express the eigenvalues of  $\Lambda$  directly in terms of the operator  $W$  using the expression for the inverse of a  $2 \times 2$  block matrix

$$W^{-1} = \begin{bmatrix} (W_i - W_b W_o^{-1} W_b^T)^{-1} & -(W_i - W_b W_o^{-1} W_b^T)^{-1} W_b W_o^{-1} \\ -W_o^{-1} W_b^T (W_i - W_b W_o^{-1} W_b^T)^{-1} & W_o^{-1} + W_o^{-1} W_b^T (W_i - W_b W_o^{-1} W_b^T)^{-1} W_b W_o^{-1} \end{bmatrix}$$

If we now let  $P$  be the projector onto the interior degrees of freedom, then

$$PW(I - P)W^{-1} = \begin{bmatrix} -W_b W_o^{-1} W_b^T (W_i - W_b W_o^{-1} W_b^T)^{-1} & 0 \\ 0 & 0 \end{bmatrix}$$

Up to additional zero eigenvalues which do not contribute to the entropy, this is equivalent to the operator

$$\Lambda' = (I - W_b W_o^{-1} W_b^T W_i^{-1})^{-1}$$

whose non-zero spectrum is the same as the operator  $(I - \Lambda)^{-1}$ . Thus to find the entropy it is sufficient to compute the eigenvalues of  $\Lambda'$ .

We can now remove the cutoff and take the continuum limit of this expression, by making the following substitutions. Let  $K$  be the operator  $-\nabla^2 + m^2$ ,  $W = \sqrt{K}$  and  $P$  be the projector onto the subspace  $L^2(\Omega)$ . The compact operator  $\Lambda'$  has a non-zero spectrum given by an infinite sequence  $\{\lambda_n\}_{n=1}^{\infty}$  such that  $\lim_{n \rightarrow \infty} \lambda_n = 0$ . The entanglement is now given as a sum over the spectrum

$$S(\Omega) = \sum_{j=1}^{\infty} S_j \tag{2.3}$$

Where  $S_j$  is given by (2.2). The problem of computing the entanglement entropy of a vacuum state has been reduced to finding the spectrum of the integral operator  $\Lambda'$ .

## 2.2 The Euclidean approach

The Hamiltonian approach allows the entanglement entropy to be expressed in terms of the spectrum of an integral operator. This expression is divergent, and its dependence on the geometry of  $\Omega$  is difficult to calculate except in special cases or by numerical methods. We therefore present an alternative derivation of the entanglement entropy in terms of the Euclidean path integral. As we will see, the expressions are still divergent, but the relation between the entanglement entropy and the geometry of the region  $\Omega$  is much clearer.

In the Schrödinger picture, the state  $|\psi(t)\rangle$  evolves according to the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle$$

Thus given an initial state  $|\psi(0)\rangle$ , the state at a later time  $t$  is given by

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle \quad \text{where} \quad U(t) = e^{-itH}$$

The path integral formalism is a method for expressing the matrix elements of  $U(t)$ . In particular if  $f$  is a field configuration at time 0 and  $g$  is a field configuration at time  $t$ , then the probability amplitude for a process in which the field evolves from  $f$  to  $g$  in time  $t$  is

$$\langle g | e^{-itH} | f \rangle = \int_{\phi(x,0)=f(x)}^{\phi(x,t)=g(x)} e^{iS(\phi)} \mathcal{D}\phi \quad (2.4)$$

Where  $S$  is the action for the Klein-Gordon field

$$S(\phi) = \frac{1}{2} \int \left( \frac{\partial\phi}{\partial t} \right)^2 - |\nabla\phi(x)|^2 - m^2\phi^2 d^4x$$

The path integral is generally ill-defined analytically, but is a useful computational tool.

We can also express the vacuum state  $|0\rangle$  using the path integral formalism. To do this, we perform a *Wick rotation* which entails a change of variables to the *imaginary time*  $\tau = it$ . Performing this substitution in equation (2.4) we find a path integral representation of the operator  $e^{-\beta H}$

$$\langle g | e^{-\beta H} | f \rangle = \int_{\phi(x,0)=f(x)}^{\phi(x,\beta)=g(x)} e^{-S_E(\phi)} \mathcal{D}\phi$$

Where  $S_E$  is the Euclidean action

$$S_E(\phi) = \frac{1}{2} \int \left( \frac{\partial\phi}{\partial t} \right)^2 + |\nabla\phi(x)|^2 + m^2\phi^2 d^4x$$

The substitution  $\tau = it$  has two effects on this expression. It causes the time derivative  $\frac{\partial}{\partial t}$  to change signature, and also appears in the integration  $d^4x$ , resulting in a factor of  $i$  that multiplies with the factor of  $i$  in  $e^{iS(\phi)}$  to give  $e^{-S_E(\phi)}$ . Up to a normalization factor, this is a thermal state at temperature  $T = \beta^{-1}$ , which is given by  $Z(\beta)^{-1} e^{-\beta H}$  where  $Z(\beta)$  is the *partition function*

$$Z(\beta) = \text{Tr} e^{-\beta H}$$

The vacuum state density matrix  $\rho = |0\rangle\langle 0|$  is the low-temperature limit of the thermal state  $Z(\beta)^{-1} e^{-\beta H}$ . As  $\beta$  becomes large, any states with energy larger than the ground state energy by an amount  $\Delta E$  are suppressed by a factor  $e^{-\beta\Delta E}$ <sup>1</sup>

$$\lim_{\beta \rightarrow \infty} Z(\beta)^{-1} e^{-\beta H} = |0\rangle\langle 0|$$

---

<sup>1</sup>This assumes there is a unique ground state separated by a finite energy gap from the first excited state. For the scalar field theory considered in this chapter it is sufficient to put the system in a box so that the Laplacian operator has discrete spectrum.

This means that  $\rho |g\rangle \propto |0\rangle$  independently of  $g$

$$\begin{aligned}\langle f|0\rangle &\propto \lim_{\beta \rightarrow \infty} \int_{\phi(x,0)=f(x)}^{\phi(x,\beta)=g(x)} e^{-S_E(\phi)} \mathcal{D}\phi \\ &= \int_{\phi(x,0)=f(x)} e^{-S_E(\phi)} \mathcal{D}\phi\end{aligned}$$

Therefore the vacuum state is obtained by a Euclidean path integral over the whole region  $\tau > 0$ .

The vacuum state density matrix can therefore naturally be expressed by combining two vacuum state path integrals: one for  $\tau \in [0, \infty)$  and one for  $\tau \in (-\infty, 0]$  as follows

$$\begin{aligned}\langle g|\rho|f\rangle &= \langle g|0\rangle \langle 0|f\rangle \\ &= \int_{\phi(x,0^+)=f(x)}^{\phi(x,0^-)=g(x)} e^{-S_E(\phi)} \mathcal{D}\phi\end{aligned}$$

Here the integral is taken over all fields on  $\mathbb{R}^4$  with boundary conditions such that

$$\lim_{\tau \rightarrow 0^+} \phi(x, \tau) = f(x) \quad \lim_{\tau \rightarrow 0^-} \phi(x, \tau) = g(x)$$

Given a region  $\Omega \subseteq \Sigma$  a classical field  $f$  can be written as  $|f\rangle = |f_\Omega\rangle \otimes |f_{\bar{\Omega}}\rangle$ . The reduced density matrix is obtained from the density matrix by a partial trace

$$\langle f_\Omega|\rho_\Omega|g_\Omega\rangle = \int \langle f_\Omega| \otimes \langle f_{\bar{\Omega}}|\rho|g_\Omega\rangle \otimes |f_{\bar{\Omega}}\rangle \mathcal{D}f_{\bar{\Omega}}$$

This is naturally expressed in the path integral formalism since it amounts to replacing the condition on the path integral

$$\phi(x, 0^+) = f(x) \quad \phi(x, 0^-) = g(x) \quad x \in \bar{\Omega}$$

with the continuity condition

$$\phi(x, 0^+) = \phi(x, 0^-) \quad x \in \bar{\Omega}$$

Yielding

$$\langle g|\rho_\Omega|f\rangle = \int_{\phi(x,0^+)=f(x), x \in \Omega}^{\phi(x,0^-)=g(x), x \in \Omega} e^{-S_E(\phi)} \mathcal{D}\phi \quad (2.5)$$

To see how this expression is useful for studying the entropy, we consider an important special case in which  $\Omega$  is a half-space.

### 2.2.1 Rindler space and the Unruh effect

The Unruh effect is the prediction that in quantum field theory a uniformly accelerated detector will respond as if exposed to a thermal state at the Unruh temperature

$$T_U = \frac{a}{2\pi}$$

There are a number of ways to derive the Unruh effect. Unruh's original derivation describes the response of an accelerating detector coupled to the field [13]. We will present a derivation of the Unruh effect using the Euclidean path integral [21]. This approach is much more abstract than Unruh's derivation, which directly describes the behaviour of detectors. Moreover the Euclidean approach only applies to the uniformly accelerating detector, while Unruh's method can be used to describe detectors moving along arbitrary trajectories. The utility of the path integral derivation is that it illustrates how the Euclidean path integral is related to entanglement entropy.

The *Rindler wedge* is the wedge-shaped region of Minkowski space

$$\{(x, y, z, t) | x > |t|\}$$

The Rindler coordinates are  $(r, \eta, y, z)$  where

$$\begin{aligned} r &= \sqrt{x^2 - t^2} & t &= r \sinh \eta \\ \eta &= \tanh^{-1} \left( \frac{t}{x} \right) & x &= r \cosh \eta \end{aligned}$$

In terms of these coordinates, the Minkowski metric is

$$ds^2 = -r^2 d\eta^2 + dr^2 + dy^2 + dz^2$$

A uniformly accelerating observer with proper acceleration  $a$  in the  $+x$  direction is described by the world-line in terms of proper time  $\chi^2$

$$\begin{aligned} x(\chi) &= \frac{1}{a} \cosh(a\chi) & r(\chi) &= \frac{1}{a} \\ t(\chi) &= \frac{1}{a} \sinh(a\chi) & \eta(\chi) &= a\chi \end{aligned}$$

The *Rindler Hamiltonian* is defined as the generator of translations in the  $\eta$  direction, just as the Hamiltonian generates translations in the  $t$  direction. After Wick rotation,  $t = i\tau$  and  $\theta = i\eta$ , and the spacetime has the Euclidean signature  $ds^2 = d\tau^2 + dx^2 + dy^2 + dz^2$ . We then have

$$\begin{aligned} \tau &= it = ir \sinh(\eta) = ir \sinh(-i\theta) = r \sin \theta \\ x &= r \cosh \theta = r \cosh(-i\theta) = r \cos \theta \end{aligned}$$

---

<sup>2</sup>We denote proper time as  $\chi$  to avoid confusion with the imaginary time  $\tau$ .

Thus  $(r, \theta, y, z)$  are cylindrical coordinates for the Euclidean spacetime.

Just as the operator  $e^{-\beta H}$  can be obtained by the Euclidean path integral for  $\tau \in [0, \beta]$ , the operator  $e^{-\beta H_R}$  is obtained by a Euclidean path integral for  $\theta \in [0, \beta]$ .

$$\langle g | e^{-\beta H_R} | f \rangle = \int_{\phi(r,0)=f(r)}^{\phi(r,\beta)=g(r)} e^{-S_E(\phi)} \mathcal{D}\phi$$

This corresponds to a path integral over a wedge in the  $(x, y, z, t)$  coordinates.

For  $\beta = 2\pi$  the wedge covers the entire Euclidean spacetime, so we have

$$\langle g | e^{-2\pi H_R} | f \rangle = \int_{\phi(x,0^+)=f(x),x \geq 0}^{\phi(x,0^-)=g(x),x \geq 0} e^{-S_E(\phi)} \mathcal{D}\phi$$

This is identical to the expression (2.5) for the reduced density matrix  $\rho_\Omega$  where  $\Omega = \{(x, y, z) | x \geq 0\}$  is the half-space. It follows that the reduced density matrix  $\rho_\Omega$  is a thermal state

$$\rho_\Omega = Z^{-1} e^{-2\pi H_R} \quad (2.6)$$

Note that the temperature  $\frac{1}{2\pi}$  is a temperature relative to the observer whose clock measures the coordinate time  $\eta$ . The accelerating observer's proper time is related to  $\eta$  by  $\chi = \frac{1}{a}\eta$  so the temperature is given by  $\frac{a}{2\pi}$  which is the Unruh temperature.

It follows that the entanglement entropy  $S(\rho_\Omega)$  is the entropy of a thermal state (2.6). For states of this form, the entropy can be written entirely in terms of the partition function  $Z(\beta)$

$$\begin{aligned} S_{\text{Therm}} &= \left(1 - \beta \frac{\partial}{\partial \beta}\right) \log Z \\ &= \log Z - \beta Z^{-1} \frac{\partial}{\partial \beta} \text{Tr} (e^{-\beta H}) \\ &= \log Z + \beta Z^{-1} \text{Tr} (H e^{-\beta H}) \\ &= \log Z + \beta \langle H \rangle \end{aligned} \quad (2.7)$$

This coincides with the von Neumann entropy

$$\begin{aligned} S(\rho) &= -\text{Tr}(\rho \log \rho) \\ &= -\text{Tr}(\rho \log (Z^{-1} e^{-\beta H})) \\ &= -\text{Tr}(\rho (-\log Z + \log e^{-\beta H})) \\ &= \log Z + \beta \langle H \rangle \end{aligned}$$

Note that for  $\beta \neq 2\pi$ ,  $Z(\beta)$  requires doing a path integral over a geometry with a conical singularity.



## 2.2.2 The deficit angle method

If  $\Omega$  is a general region of space, the previous argument that relied on polar coordinates is not applicable. However we will see that it is still possible to express the entropy in terms of the partition function in the Euclidean spacetime.

As a first step toward computing  $S(\rho_\Omega)$ , we can express the quantity  $\text{Tr}(\rho_\Omega^n)$  as a path integral on a new manifold  $\mathcal{M}_n$ <sup>3</sup>. Recall that  $\langle f | \rho_\Omega | g \rangle$  is expressed as a path integral with fields having boundary conditions  $\lim_{\tau \rightarrow 0^+} \phi(x, \tau) = f(x)$  and  $\lim_{\tau \rightarrow 0^-} \phi(x, \tau) = g(x)$  for all  $x \in \Omega$ . The manifold  $\mathcal{M}_n$  is obtained by taking  $n$  copies of  $\mathbb{R}^4$ , and gluing the  $\tau < 0$  side of  $\Omega \times \{0\}$  of the  $n^{\text{th}}$  copy of  $\mathbb{R}^4$  to the  $\tau > 0$  side of  $\Omega \times \{0\}$  of the  $(n+1)^{\text{th}}$  copy of  $\mathbb{R}^4$ . Then  $\text{Tr}(\rho^n)$  may be expressed directly as a path integral over  $\mathcal{M}_n$

$$\text{Tr}(\rho^n) = \int e^{-S_E(\phi)} \mathcal{D}\phi$$

This new manifold  $\mathcal{M}_n$  is flat everywhere except for the 2-dimensional surface  $\partial\Omega$  which is a conical singularity. A polygon that does not encircle  $\partial\Omega$  will have exterior angles summing to  $2\pi$ , but a polygon that encircles  $\partial\Omega$  will have exterior angles summing to  $2\pi n$ . This conical singularity is described by a *deficit angle*  $\delta = 2\pi - \beta$  where  $\beta = 2\pi n$  is the sum of the exterior angles of a polygon that encircles the conical singularity.

In order to compute the von Neumann entropy  $S(\rho)$  from  $\text{Tr}(\rho^n)$ , it is useful to introduce the *Rényi  $\alpha$ -entropy*

$$S_\alpha(\rho) = \frac{\log \text{Tr} \rho^\alpha}{\alpha - 1}$$

which is defined for all  $\alpha \geq 0$  except for  $\alpha = 1$ . The Rényi  $\alpha$ -entropy shares some useful properties of the von Neumann entropy. In particular they are additive across tensor products, and the maximally mixed state of dimension  $d$  has  $\alpha$ -entropy

$$S_\alpha(I/d) = \frac{\log \text{Tr}(I/d^\alpha)}{1 - \alpha} = \frac{\log(d^{1-\alpha})}{1 - \alpha} = \log d$$

In the limit  $\alpha \rightarrow 1$  we have

$$\lim_{\alpha \rightarrow 1} S_\alpha(\rho) = \lim_{\alpha \rightarrow 1} \frac{\log \text{Tr} \rho^\alpha - \log \text{Tr} \rho}{1 - \alpha} = -\frac{d}{d\alpha} \log \text{Tr}(\rho^\alpha) \Big|_{\alpha=1} = S(\rho) \quad (2.8)$$

So the von Neumann entropy can be recovered as the  $\alpha \rightarrow 1$  limit of the Rényi entropy.

We can express the formula (2.8) for the von Neumann entropy in a form that does not require  $\rho$  to be normalized [19]

$$S(\rho) = \left(1 - \frac{d}{d\alpha}\right) \log \text{Tr}(\rho^\alpha) \Big|_{\alpha=1}$$

---

<sup>3</sup> $\mathcal{M}_n$  is actually a conifold, and not a manifold, since it contains a conical singularity.

This reduces to the original expression when  $\text{Tr}(\rho) = 1$ , and is invariant under rescaling of  $\rho$ , since for any scalar  $a > 0$ ,

$$\begin{aligned} \left(1 - \frac{d}{d\alpha}\right) \log \text{Tr}((a\rho)^\alpha) \Big|_{\alpha=1} &= \left(1 - \frac{d}{d\alpha}\right) (\log \text{Tr}(\rho^\alpha) + \alpha \log a) \Big|_{\alpha=1} \\ &= S(\rho) + (\log a - \log a) = S(\rho) \end{aligned}$$

We observe that for integer  $\alpha = n$ , the Rényi entropy can be expressed in terms of the Euclidean path integral on the manifold  $\mathcal{M}_n$ , which is flat everywhere except for a conical singularity of  $\beta = 2\pi n$  at the surface  $\partial\Omega$ . To evaluate the Shannon entropy, we need the Rényi entropy as  $\alpha \rightarrow 1$ . This suggests that we define  $Z(\beta)$  as the partition function of a manifold which is flat everywhere with a conical singularity of conical angle  $\beta$ . Letting  $\beta = 2\pi\alpha$ , we have

$$\begin{aligned} S &= \left(1 - \frac{\partial}{\partial\alpha}\right) \log \text{Tr}\rho^\alpha \Big|_{\alpha=1} \\ &= \left(1 - \beta \frac{\partial}{\partial\beta}\right) \log Z(\beta) \Big|_{\beta=2\pi} \end{aligned} \tag{2.9}$$

Note that in the Rindler spacetime, this expression is equivalent to the expression (2.7) for the entropy in terms of the partition function. The great advantage of this expression is that  $Z(\beta)$  can be computed in terms of the geometry of the surface  $\partial\Omega$ .

### 2.2.3 Heat kernel and effective action

What makes the Euclidean framework so powerful is that it allows the entropy of entanglement to be understood in terms of the partition function  $Z(\beta)$  on a manifold with a conical singularity. In particular, the entropy depends only on the *Euclidean effective action*

$$W(\beta) = -\log Z(\beta)$$

The effective action can then be expressed in terms of properties of the Laplacian operator on the manifold  $\mathcal{M}_\beta$ .

To give an expression for the effective action, we first diagonalize the positive operator  $-\nabla^2$ . By putting the system in a box, this operator has a discrete spectrum and can be diagonalized in terms of positive eigenvalues  $\lambda_n$  and eigenfunctions  $\phi_n(x)$  so that

$$-\nabla^2 \phi_n(x) = \lambda_n \phi_n(x)$$

These eigenfunctions form a complete orthogonal basis, so that any field  $\phi(x)$  can be written as

$$\phi(x) = \sum_n c_n \phi_n(x)$$

Then the Euclidean action is

$$S_E(\phi) = \frac{1}{2} \int \phi(x)(m^2 - \nabla^2)\phi(x)d^4x = \frac{1}{2} \sum_n (\lambda_n + m^2)c_n^2$$

We can then express the partition function as

$$\begin{aligned} Z &= \int \exp\left(-\frac{1}{2} \sum_n (\lambda_n + m^2)c_n^2\right) \mathcal{D}\phi \\ &= \prod_n \int \exp\left(-\frac{1}{2}(\lambda_n + m^2)x^2\right) dx \\ &= \prod_n (\lambda_n + m^2)^{-1/2} \\ &= \det(m^2 - \nabla^2)^{-1/2} \end{aligned}$$

So that the Euclidean effective action is given by the functional determinant

$$W = -\log Z = \frac{1}{2} \log \det(m^2 - \nabla^2)$$

To study the behaviour of this operator we introduce the *trace of the heat kernel*

$$\zeta_{\mathcal{M}}(t) = \text{Tre}^{t\nabla^2} = \sum_n e^{-t\lambda_n}$$

The trace of the heat kernel has been studied in the case of manifolds with conical singularities [22]. In particular, it has a well-studied asymptotic expansion in the limit  $t \rightarrow 0$  in terms of geometric invariants of the underlying manifold. To understand how  $W$  relates to the geometry of the underlying manifold, we express it in terms of the trace of the heat kernel.

Let  $\epsilon$  be a small cutoff scale with dimensions of length. We consider the following expression in terms of the heat kernel

$$\begin{aligned} -\int_{\epsilon^2}^{\infty} \frac{1}{t} \zeta(t) e^{-m^2 t} dt &= -\sum_n \int_{\epsilon^2}^{\infty} \frac{1}{t} e^{-(\lambda_n + m^2)t} dt \\ &= -\sum_n E_1(\epsilon^2(\lambda_n + m^2)) \end{aligned}$$

Where we have introduced the *exponential integral* function

$$E_1(z) = \int_1^{\infty} \frac{1}{t} e^{-zt} dt$$

For small  $z$ , we have the identity

$$E_1(z) = -\gamma - \log z - \sum_{n=1}^{\infty} \frac{(-1)^n z^n}{nn!} \approx -\gamma - \log z$$

where  $\gamma$  is Euler's constant. Thus for small  $\epsilon$

$$E_1(\epsilon^2(\lambda_n + m^2)) \approx \gamma + \log \epsilon^2(\lambda_n + m^2) = -\gamma - 2 \log \epsilon - \log(\lambda_n + m^2)$$

We will ignore the additive constant, since we are not interested in the exact value of this expression, only the way it changes when  $\lambda_n$  is varied. Thus we have for small  $\epsilon$

$$-\int_{\epsilon^2}^{\infty} \frac{1}{t} \zeta(t) e^{-m^2 t} dt \approx \sum_n \log(\lambda_n + m^2) = \log \det(m^2 - \nabla^2)$$

Combining this expression for  $Z(\beta)$  with the expression for the entropy (2.9), we have

$$\begin{aligned} S(\rho_\Omega) &= \left(1 - \beta \frac{\partial}{\partial \beta}\right) \log Z(\beta) \Big|_{\beta=2\pi} \\ &= -\frac{1}{2} \left(1 - \beta \frac{\partial}{\partial \beta}\right) \log \det(m^2 - \nabla^2) \Big|_{\beta=2\pi} \\ &= \frac{1}{2} \int_{\epsilon^2}^{\infty} \frac{e^{-m^2 t}}{t} \left(1 - \beta \frac{\partial}{\partial \beta}\right) \zeta_{\mathcal{M}_\beta}(t) dt \Big|_{\beta=2\pi} \end{aligned}$$

The presence of the term  $\frac{e^{-m^2 t}}{t}$  ensures that this expression only depends on the behaviour of  $\zeta_{\mathcal{M}_\beta}(t)$  for small values of  $t$ .

For small  $t$  the heat kernel has an asymptotic expansion [22]

$$\zeta_{\mathcal{M}}(t) = \sum_{k \geq 0} t^{(k-n)/2} a_k(\mathcal{M})$$

The coefficients  $a_k$  can be expressed in terms of the geometry of the manifold  $\mathcal{M}$ . The leading term always depends on the volume. The odd terms are integrals over the boundary, which will be neglected because we consider manifolds without boundary

$$\begin{aligned} a_0(\mathcal{M}) &= \frac{\text{Vol}(\mathcal{M})}{4\pi} \\ a_1(\mathcal{M}) &= a_3(\mathcal{M}) = \dots = 0 \end{aligned}$$

The manifolds we will consider have conical singularities, which affect  $a_2$ . Letting  $C_\beta$  denote a cone of angle  $\beta$  this term is [22]

$$a_2(C_\beta) = \frac{4\pi^2 - \beta^2}{24\pi\beta^2} = \frac{1}{12} \left( \frac{2\pi}{\beta} - \frac{\beta}{2\pi} \right)$$

Consider the example of the Rindler spacetime. The geometry is a product of an infinite cone  $C_\beta$  in the  $(x, t)$  plane with a 2-dimensional plane in the  $(y, z)$  coordinates

$$\mathcal{M}_\beta = C_\beta \times R^2$$

In order to eliminate the infrared divergence due to infinite volume, we make the  $y$  and  $z$  coordinates periodic with period  $L$ . Similarly, we allow the radial coordinate  $r$  to run to a maximum radius  $R$ . We will neglect contributions to the heat kernel coefficients from the boundary  $r = R$ . Thus we consider the manifold

$$\mathcal{M}_\beta = C_\beta \times S_L^1 \times S_L^1$$

where  $S_L^1$  is the circle of circumference  $L$ .

The trace of the heat kernel on a product of manifolds is simply the product of the traces of heat kernels

$$\zeta_{\mathcal{M} \times \mathcal{N}}(t) = \zeta_{\mathcal{M}}(t) \zeta_{\mathcal{N}}(t)$$

The heat kernel for  $C_\beta$  has two contributions: one from the total volume and one from the conical singularity

$$\begin{aligned} \zeta_{C_\beta}(t) &= a_0(C_\beta) \frac{1}{t} + a_2(C_\beta) \\ &= \frac{\beta R^2}{4\pi} \frac{1}{t} + \frac{1}{12} \left( \frac{2\pi}{\beta} - \frac{\beta}{2\pi} \right) \end{aligned}$$

The heat kernel for the remaining part is

$$\zeta_{S_L^1}(t) = \frac{L}{\sqrt{4\pi t}}$$

The relevant terms in the heat kernel are proportional to  $\beta$  or  $\beta^{-1}$ . For the terms which are linearly proportional to  $\beta$ ,

$$\left( 1 - \beta \frac{\partial}{\partial \beta} \right) \beta = \beta - \beta = 0$$

Whereas for the terms proportional to  $\beta^{-1}$ ,

$$\left( 1 - \beta \frac{\partial}{\partial \beta} \right) \beta^{-1} = \beta^{-1} + \beta^{-1} = 2\beta^{-1}$$

Thus the terms proportional to  $\beta$  do not contribute to the entropy, and the remaining term is simply

$$\left( 1 - \beta \frac{\partial}{\partial \beta} \right) \zeta_{C_\beta}(t) \Big|_{\beta=2\pi} = \frac{1}{6} \frac{2\pi}{\beta} \Big|_{\beta=2\pi} = \frac{1}{6}$$

This simplifies the expression for the entanglement entropy, which becomes

$$\begin{aligned} S(\Omega) &= \frac{1}{2} \int_{\epsilon^2}^{\infty} \frac{e^{-m^2 t}}{t} \zeta_{S_L^1}(t)^2 \frac{1}{6} dt \\ &= \frac{L^2}{48\pi} \int_{\epsilon^2}^{\infty} \frac{e^{-m^2 t}}{t^2} dt \end{aligned}$$

This is proportional to the horizon area  $A = L^2$ .

The remaining term is an exponential integral

$$\begin{aligned} \int_{\epsilon^2}^{\infty} \frac{e^{-m^2 t}}{t^2} dt &= \int_1^{\infty} \frac{e^{-m^2 \epsilon^2 u}}{\epsilon^4 u^2} \epsilon^2 du \\ &= \frac{1}{\epsilon^2} E_2(m^2 \epsilon^2) \end{aligned}$$

Where we have the exponential integral function

$$E_2(z) = \int_1^{\infty} \frac{e^{-zt}}{t^2} dt$$

We assume that  $m^2 \epsilon^2$  will be small, so that the Compton wavelength is much larger than the cutoff scale. Then for small  $z$  we have  $E_2(z) \approx E_2(0) = \frac{1}{2}$ . This gives the final answer

$$S(\Omega) = \frac{A}{96\pi\epsilon^2}$$

This is proportional to the area, and diverges quadratically with the cutoff scale. The constant  $96\pi$  is just an artifact of the particular regularization method we used to remove the ultraviolet divergence. It has no particular significance, and different methods of regularization lead to different constants, but the qualitative behaviour is the same.

An important aspect of this derivation is that the terms in the heat kernel that are integrals over  $\mathcal{M}_\beta$  do not contribute to the entropy. The remaining terms are all integrals over  $\partial\Omega$ , which implies the *strong additivity property* [23]

$$S(\Omega_1) + S(\Omega_2) = S(\Omega_1 \cup \Omega_2) + S(\Omega_1 \cap \Omega_2)$$

This property is discussed in more detail in chapter 5.

## 2.3 The species problem

An objection to the identification of entanglement entropy with black hole entropy first pointed out by Sorkin, is the observation that the entanglement entropy  $S(\Omega)$  depends on the number of quantum fields, whereas  $S_{\text{BH}}$  is given by the Bekenstein-Hawking formula and depends only on the constants  $\hbar$ ,  $c$  and  $G$  [7].

The solution to this problem arises when we consider that the gravitational constant  $G$  undergoes a renormalization that depends on the matter fields present [24, 25]. We must make a distinction between the bare gravitational constant  $G_0$  which appears in the classical action, and the renormalized gravitational constant  $G_R$  which appears in the effective action.

The entropy can be expressed in terms of the effective action  $W = -\log Z$ . If we expand  $W$  as a power series in curvature [25]

$$\begin{aligned} W &= \int (a_0 + a_1 R + O(R^2)) \sqrt{g} d^4x \\ &= \frac{-1}{16\pi G_R} \int (2\Lambda_R + R + O(R^2)) \sqrt{g} d^4x \end{aligned}$$

Comparing these equations, the renormalized gravitational constant is related to  $a_1$  by

$$a_1 = \frac{-1}{16\pi G_R}$$

We now return to the Rindler spacetime with deficit angle  $2\pi - \beta$ . The entropy is given by

$$S = - \left( 1 - \beta \frac{\partial}{\partial \beta} \right) W \Big|_{\beta=2\pi}$$

There are three classes of terms that arise in  $W$  [24]:

- The cosmological constant term  $a_0$ . Being constant, its integral is proportional to the volume of space, which depends linearly on  $\beta$ . Thus this term does not contribute to the entropy.
- The Einstein-Hilbert term  $a_1 R$ . The only contribution from the curvature is at the singularity, so that

$$\int R \sqrt{g} d^4x = 2A(2\pi - \beta)$$

This term gives a contribution to the entropy of

$$\begin{aligned} \left( 1 - \beta \frac{\partial}{\partial \beta} \right) \int a_1 R \sqrt{g} d^4x \Big|_{\beta=2\pi} &= \left( 1 - \beta \frac{\partial}{\partial \beta} \right) 2a_1 A(2\pi - \beta) \Big|_{\beta=2\pi} \\ &= 4\pi a_1 A \end{aligned} \tag{2.10}$$

- Higher-order terms in  $R$ . These all contribute with a  $\beta$  dependence given by  $(2\pi - \beta)^n$  for  $n \geq 2$ . It follows that when  $\beta$  is set to  $2\pi$ , these terms vanish.

It follows that only the Einstein-Hilbert term contributes to the entropy, with a contribution given by equation (2.10). Using the definition of  $a_1$  in terms of the renormalized gravitational constant, we see that

$$S = 4\pi A a_1 = \frac{A}{4G_R} \tag{2.11}$$

Thus the species problem is completely avoided once the renormalization of  $G$  is taken into account.

A consequence of equation (2.11) is that the divergence in the entanglement entropy is directly related to the non-renormalizability of gravity. This suggests the need for a physical cutoff on degrees of freedom near the Planck scale. In the next chapter we will consider a proposal for such a theory.

# Chapter 3

## Loop quantum gravity

While the entanglement entropy is a promising candidate for the microscopic origin of black hole entropy, an issue we must face is the fact that the former is ultraviolet divergent and non-renormalizable. Since the divergence of the entanglement entropy is intimately related to the non-renormalizability of gravity, it is necessary to consider a model of quantum gravity which is ultraviolet-finite. One such theory, which we will now consider is loop quantum gravity [26]. The calculation of entanglement entropy which we will present in this chapter is an extended version of previous work by the author [27].

The starting point of loop quantum gravity is the Hamiltonian formulation of general relativity in Ashtekar variables. We begin with a manifold  $\mathcal{M} = \mathbb{R} \times \Sigma$  where  $\mathbb{R}$  represents time and  $\Sigma$  represents space. The Ashtekar variables are an  $SU(2)$  connection  $A_a^i$  and a densitized inverse triad  $E_i^a$  on  $\Sigma$ . They are related to the 3-metric  $q_{ab}$  and extrinsic curvature tensor  $K_{ab}$  by

$$\begin{aligned} A_a^i &= \Gamma_a^i + \gamma \sqrt{\det q} K_{ab} E_i^b \\ (\det q) q_{ab} &= E_i^a E_j^b \delta_{ij} \end{aligned}$$

where  $\Gamma_a^i$  is the spin connection associated to the triad [28]. The variable  $\gamma$  is the Barbero-Immirzi parameter, which is a free dimensionless parameter of loop quantum gravity. As we will see  $\gamma$  plays an important role in the relationship between entropy and area.

The dynamics in the Ashtekar formulation of general relativity is given entirely in terms of constraints, each of which generates a different type of gauge transformation. If a state is in the kernel of the constraint, this is equivalent to the state being invariant under the corresponding gauge transformation. The constraints are:

- the Gauss' law constraint, that generates  $SU(2)$  gauge transformations,
- the diffeomorphism constraint, that generates diffeomorphisms of  $\Sigma$ , and
- the Hamiltonian constraint, that generates diffeomorphisms of  $\mathcal{M}$  in the time direction.



The strategy employed in loop quantum gravity is to first quantize, then to solve the constraints. This means first constructing a Hilbert space containing a unitary representation of the  $SU(2)$  gauge transformations and the diffeomorphism group of  $\Sigma$ . This is the *Kinematical Hilbert space* which we will denote  $\mathcal{K}$ . The quotient of  $\mathcal{K}$  with the group of  $SU(2)$  gauge transformations is the gauge-invariant Hilbert space  $\mathcal{K}_0$ . The quotient of  $\mathcal{K}_0$  with the diffeomorphism group<sup>1</sup> is the diffeomorphism-invariant Hilbert space  $\mathcal{K}_{\text{diff}}$ . Finally, the kernel of the Hamiltonian constraint operator  $H$  is the physical Hilbert space  $\mathcal{H}$ .

The relation between these Hilbert spaces can be illustrated schematically as follows:

$$\mathcal{K} \xrightarrow{SU(2)} \mathcal{K}_0 \xrightarrow{\text{Diff}^*} \mathcal{K}_{\text{diff}} \xrightarrow{H} \mathcal{H}$$

For the purposes of this derivation, only  $\mathcal{K}$  and  $\mathcal{K}_0$  are directly relevant, although the construction of  $\mathcal{K}_{\text{diff}}$  is very briefly sketched. The true physical states of the theory are those in the dynamical Hilbert space  $\mathcal{H}$ . Although there exist candidates for the Hamiltonian constraint operator, construction of a Hilbert space of solutions to the Hamiltonian constraint is still an open problem [29]. The considerations in this chapter are therefore purely kinematical, as has been the case for all previous investigations of black hole entropy in loop quantum gravity.

An important feature of the Ashtekar variables is that the connection and the densitized triad are canonically conjugate

$$\{A_a^i(x), E_j^b(y)\} = (8\pi\gamma G)\delta_a^b\delta_j^i\delta^3(x, y)$$

In particular we can treat the connection  $A$  as the configuration variable analogous to position in the Schrödinger picture of quantum mechanics. The states in the quantum theory are then described by wave functionals on the space of  $SU(2)$  connections. In this representation the connection  $A$  is promoted to a multiplication operator  $\hat{A}$  and the triad  $E$  becomes a differential operator  $\hat{E}_i^a = -i\hbar\frac{\delta}{\delta A_a^i}$ .

For a suitable definition of the Hilbert space of functionals, the gauge and diffeomorphism constraints can be explicitly solved. The resulting Hilbert space is separable and has a basis labelled by knotted  $SU(2)$  spin networks [30]. The spin networks are abstract graphs whose edges are labelled by half-integers  $j$  which represent irreducible representations of  $SU(2)$ . The vertices are labelled by intertwining operators which are rules for mapping the representations on the incident vertices into the trivial representation  $j = 0$ . The geometry of the manifold  $\Sigma$  is therefore replaced by a discrete combinatorial structure. This suggests that loop quantum gravity provides the ultraviolet finiteness required to remove the divergence of the entanglement entropy.

Loop quantum gravity is a background-independent theory; the manifold  $\Sigma$  is not equipped with a classical metric, so that all information about the geometry of  $\Sigma$  is encoded in the quantum state. In order to recover a notion of geometry for the spin network states it is necessary to define geometric operators for the quantities

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<sup>1</sup>Technically, it is a larger group of extended diffeomorphisms  $\text{Diff}^*(\Sigma)$  [26].

of interest. These are obtained by constructing expressions for these quantities in terms of the connection  $A_a^i$  and the densitized triad  $E_i^a$ , and then substituting the operators  $\hat{A}_a^i$  and  $\hat{E}_i^a$ .

The simplest geometric operator is the area operator, associated with a 2-dimensional surface  $\sigma$  embedded in  $\Sigma$ . The geometry of  $\Sigma$  is described completely by a spin network  $S$ . Suppose for simplicity that no vertices of the spin network  $S$  lie on  $\sigma$ . In general there will be  $P$  ‘‘punctures’’ where the spin network  $S$  intersects with  $\sigma$ , and we can let  $\tilde{j}_p$  denote the spin of the edge intersecting at the  $p^{\text{th}}$  puncture. Then the area operator  $\mathbf{A}(\sigma)$  acts on the spin network state  $|S\rangle$  as

$$\mathbf{A}(\sigma) |S\rangle = 8\pi G\gamma \sum_{p=1}^P \sqrt{\tilde{j}_p(\tilde{j}_p + 1)} |S\rangle \quad (3.1)$$

There are several things to note about this equation. The spin network states are eigenvectors of the area operator, and therefore represent states of minimum area uncertainty. The corresponding eigenvalues take the form of a sum over punctures where the spin network intersects the surface. Note also that the Barbero-Immirzi parameter  $\gamma$  appears in the spectrum of the area operator. It does not appear in the definition of the spin network states, and therefore will not appear in the calculation of the entanglement entropy. The Barbero-Immirzi parameter therefore controls the coefficient of proportionality between entropy and area. It has been suggested that the value of the Barbero-Immirzi parameter could be fixed by requiring consistency with the Bekenstein-Hawking formula.

Equation (3.1) describes what is called the non-degenerate part of the area spectrum, since it does not apply in the ‘‘degenerate’’ case in which a vertex of the spin network lies on the surface  $\sigma$ . The full spectrum of the area operator must include the case where one or more vertices intersect the surface [31]. In this case the eigenvalue to the area operator is still expressed as a sum over the points where the spin network intersects the surface. Where one or more vertices intersect  $\sigma$ , the action of the area operator may be computed using SU(2) recoupling theory. The recoupling theory is described in section 3.3.3.

It should be noted that there is also a volume operator  $V(\Omega)$  for each 3-dimensional region  $\Omega \subset \Sigma$ . This operator is also diagonal in the spin network basis, and its eigenvalue is a sum over all vertices in  $\Omega$  of degree at least four. Its construction is more complicated than the area operator and the details are not relevant for this discussion. We refer the reader to the book of Rovelli [26].

Note that all of these operators are defined on the kinematical Hilbert space  $\mathcal{K}$ . The calculation of entanglement entropy will also be carried out in the kinematical Hilbert space. This is analogous to performing calculations in a fixed gauge or in a fixed coordinate system. Working in  $\mathcal{K}$  does not affect the results of the calculations, which are independent of the choice of coordinate system and are therefore well-defined also in  $\mathcal{K}_{\text{diff}}$ .

### 3.1 Black hole entropy in loop quantum gravity

The dominant view in loop quantum gravity is that black hole entropy arises as ignorance about the state of the black hole horizon geometry. This point of view has been advocated by Krasnov and Rovelli [32, 33]. In this approach the state of a black hole is treated as an ensemble of indistinguishable configurations with a single relevant macroscopic parameter being the area of the event horizon. It is argued that the black hole entropy should be given by

$$S = \log N(A)$$

where  $N(A)$  is the number of horizon geometries of area  $A$ . The entropy is therefore given as a function of area, which may be studied in the asymptotic limit of large area. For certain choices of ensemble this yields  $S \propto A$  in the asymptotic limit  $A \rightarrow \infty$ .

This approach to black hole entropy introduces the issue of which statistical ensemble should be used. Rovelli and Krasnov each arrived at different numerical values of the entropy by considering different statistical ensembles. The entropy further depends on which configurations are considered distinct, and whether the degenerate spectrum of the area operator is included. These ambiguities affect not only the numerical coefficient in front of the area, but also affect the form of sub-leading order corrections to the entropy.

A key issue with the state counting approach is the assumption that the horizon area is the only relevant macroscopic parameter. This assumption is based on the classical area theorem of Hawking, which states that horizon area is non-decreasing as a function of time. It is therefore argued that area is a conserved quantity for a black hole in equilibrium. This result depends on the specific dynamics of general relativity; in a more general theory we know that the entropy has a more general form as a function of horizon shape [34]. The state-counting approach can only lead to an entropy that is a function of the area alone, and therefore cannot explain corrections to the black hole entropy.

While corrections to the area law have been studied in loop quantum gravity, they are necessarily of the form  $f(A)$  where  $f$  is a function such that  $f(A)/A \rightarrow 0$  as  $A \rightarrow \infty$ . They have typically taken the form of a logarithmic correction to the entropy [35, 36]. These corrections are not of the same form as those that arise from modified gravity, and are small enough to be negligible for black holes of larger than Planckian size. The physical meaning of these logarithmic corrections is therefore unclear, since for all but the smallest microscopic black holes they will be negligibly small.

An alternative to the state counting approach is to treat a horizon as a boundary of space, and construct a theory of quantum gravity on the exterior region [37]. Boundary conditions must be introduced and the gravitational action acquires an additional term that depend on the boundary geometry. This term can be used to define a theory on the boundary, which can then be quantized. This resolves

the ambiguity in choosing an ensemble of states, since the quantity  $N(A)$  can be defined as the dimension of the space of eigenvectors to the area operator in the boundary Hilbert space with fixed area eigenvalue  $A$ .

One such theory was explicitly constructed by Smolin for self-dual boundary conditions, resulting in an  $SU(2)$  Chern-Simons theory on the boundary surface [37]. This program was extended by Ashtekar et. al. to the isolated horizon boundary conditions [6, 38, 39]. The relation between this model and the entanglement entropy is explored more thoroughly in section 3.4.

Entanglement entropy has previously been studied in loop quantum gravity by Dasgupta[40]. Instead of using spin network states, a new kind of coherent states were introduced. These coherent states are defined over a web-like graph, which contains two classes of edges: those which emanate radially from a central point, and those which run along trajectories of constant distance from the central point. The coherent states are elements of  $L^2(SU(2))$  labelled by elements of  $SL(2, \mathbb{C})$ , since  $SU(2)$  is a real form of  $SL(2, \mathbb{C})$ . This is analogous to the case of the harmonic oscillator, in which the coherent states are elements of  $L^2(\mathbb{R})$  labelled by complex numbers  $x + ip$ .

A horizon is introduced as a fixed radius where the apparent horizon condition is imposed on edges inside and outside the horizon. The apparent horizon condition introduces correlations between the state inside the horizon and the state outside the horizon which are responsible for the entanglement entropy. We note that unlike the work of Dasgupta, our result applies to arbitrary graph topologies and does not require the imposition of apparent horizon boundary conditions.

Terno and Livine also considered entanglement of spin network states but used a very different definition of a black hole [41, 42]. Rather than tracing over the black hole interior, they treat a black hole as a single spin network vertex. The former corresponds to the case where the holonomies inside the black hole are unknown; the latter corresponds to the case where all holonomies are known and trivial. The single-vertex black hole is labelled with an intertwiner between all the representations of edges intersecting the horizon. The number of possible intertwiners is taken to be the dominant source of black hole entropy. The entanglement corresponding to a division of the horizon punctures into two sets is interpreted as a logarithmic correction to the black hole entropy. This is in contrast with the present approach, in which the entire black hole entropy is naturally attributed to entanglement.

## 3.2 Kinematical Hilbert space

The strategy pursued by loop quantum gravity is to first quantize, then apply constraints. To do this we first construct the *kinematical Hilbert space* as a space of wave functionals on connections with a unitary representation of the diffeomorphism group of  $\Sigma$  and of local  $SU(2)$  gauge transformations. A motivation for the

definition of the kinematical Hilbert space is the idea that a connection is determined by the holonomy along every smooth curve. To make this idea concrete it is necessary to introduce generalized  $SU(2)$  connections and generalized  $SU(2)$  gauge transformations. Our definitions follow the work of Ashtekar and Lewandowski [43].

Let  $\gamma_1$  and  $\gamma_2$  be analytic curves such that the endpoint of  $\gamma_1$  coincides with the beginning of  $\gamma_2$ . The *composition*  $\gamma_1 \circ \gamma_2$  is the curve obtained by the union of  $\gamma_1$  and  $\gamma_2$ . The *inverse*  $\gamma^{-1}$  is the curve  $\gamma$  with its orientation reversed. A *generalized  $SU(2)$  connection* on  $\Sigma$  is a function  $A$  that maps every analytic curve  $\gamma$  in  $\Sigma$  to an element  $A(\gamma) \in SU(2)$  in a way that preserves composition and inverses

$$\begin{aligned} A(\gamma_1 \circ \gamma_2) &= A(\gamma_1) \circ A(\gamma_2) \\ A(\gamma^{-1}) &= A(\gamma)^{-1} \end{aligned}$$

The set of generalized connections is denoted  $\overline{\mathcal{A}}$ . These conditions are satisfied by the holonomy of an  $SU(2)$  connection  $A_\mu$  given by

$$A(\gamma) = \mathcal{P} \exp \left( \int_\gamma A_\mu dx^\mu \right)$$

As the name implies, a generalized connection need not arise from a connection  $A_\mu$  in this way.

A *generalized gauge transformation* is a map  $g : \Sigma \rightarrow SU(2)$ . Unlike the usual gauge transformations, a generalized gauge transformation need not be continuous. The gauge transformation  $g$  acts on a generalized connection as

$$(gA)(\gamma) = g(\gamma(0))A(\gamma)g(\gamma(1)) \tag{3.2}$$

The action of a generalized connection  $A$  is defined to match the action of a gauge transformation on a holonomy.

A *graph*  $\Gamma$  is a finite set of piecewise analytic curves  $\gamma : [0, 1] \rightarrow \Sigma$  that intersect each other only at their endpoints. The curves are called the *edges* of  $\Gamma$  and their endpoints are called *vertices*<sup>2</sup>.

Let  $\Gamma$  be a graph with edges  $\gamma_1, \dots, \gamma_L$  and let  $f \in L^2(SU(2)^L, \mu)$  where  $\mu$  is the Haar measure on  $SU(2)$ . We can define a functional on the space of generalized connections  $\overline{\mathcal{A}} \rightarrow \mathbb{C}$  by

$$\psi_{\Gamma, f}(A) = f(A(\gamma_1), \dots, A(\gamma_L))$$

For fixed  $\Gamma$ , the image of the map  $f \mapsto \psi_{\Gamma, f}$  is the *graph subspace* denoted  $\mathcal{K}_\Gamma$ .

We would like to define  $\mathcal{K}$  as a space which contains every  $\mathcal{K}_\Gamma$  as a subspace. A natural choice is the direct sum  $\bigoplus_\Gamma \mathcal{K}_\Gamma$ , but this does not give the desired Hilbert

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<sup>2</sup>In the loop quantum gravity literature edges are sometimes called *links* and the vertices are sometimes called *nodes*.

space. This is because the representation in terms of graph states contains some redundancy; it is possible to define states supported in different graph subspaces which define the same function of the connection  $A$ , as in the following example. Let  $\Gamma$  and  $\Gamma'$  be two graphs such that every edge  $\gamma_1, \dots, \gamma_L$  of  $\Gamma$  can be written as a composition of edges in  $\Gamma'$  and their inverses. If this is the case we write  $\Gamma \subseteq \Gamma'$ . In particular, we have that for every  $\ell = 1, \dots, L$  there is a function  $m_\ell$  such that  $\gamma_\ell = m_\ell(\gamma'_1, \dots, \gamma'_{L'})$ . Let  $\psi_{\Gamma, f} \in \mathcal{K}_\Gamma$ , and define

$$f'(\gamma'_1, \dots, \gamma'_{L'}) = f(m_1(\gamma'_1, \dots, \gamma'_L), \dots, m_L(\gamma'_1, \dots, \gamma'_L))$$

Clearly the states  $\psi_{\Gamma, f}$  and  $\psi_{\Gamma', f'}$  define the same functional on the space of generalized connections, so we would like to identify them in the kinematical Hilbert space. We therefore define the operator  $T_{\Gamma, \Gamma'} : \mathcal{K}_\Gamma \rightarrow \mathcal{K}_{\Gamma'}$  by  $T\psi_{\Gamma, f} = \psi_{\Gamma', f'}$ .

Whenever  $\Gamma \subseteq \Gamma'$ ,  $T_{\Gamma, \Gamma'}$  is an isometry. This fact depends crucially on the group invariance of the Haar measure. In particular, the functions  $i(g) = g^{-1}$  and  $m(g, h) = gh$  satisfy

$$\begin{aligned} \mu(i^{-1}(X)) &= \mu(X) \\ (\mu \times \mu)(m^{-1}(X)) &= \mu(X) \end{aligned}$$

where  $X$  is any subset of  $SU(2)$  and  $\mu$  is the Haar measure. For a detailed construction of the isometry operator  $T_{\Gamma, \Gamma'}$ , see [44].

If  $\Gamma \subseteq \Gamma' \subseteq \Gamma''$  then the corresponding isometries satisfy the compatibility condition

$$T_{\Gamma, \Gamma'} T_{\Gamma', \Gamma''} = T_{\Gamma, \Gamma''}$$

We can therefore define the kinematical Hilbert space  $\mathcal{K}$  as the *direct limit* of the spaces  $\mathcal{K}_\Gamma$  [45]. This Hilbert space is defined such that there exist isometries  $U_\Gamma : \mathcal{K}_\Gamma \rightarrow \mathcal{K}$  where  $U_\Gamma \circ T_{\Gamma, \Gamma'} = U_{\Gamma'}$ . It further satisfies a universal property making it the unique smallest Hilbert space such that the isometries  $U_\Gamma$  exist, up to unitary equivalence. Thus we have constructed  $\mathcal{K}$  as the smallest Hilbert space containing all the graph subspaces  $\mathcal{K}_\Gamma$ . Note that because there are an uncountable number of graphs,  $\mathcal{K}$  is non-separable.

This completes the definition of the kinematical Hilbert space  $\mathcal{K}$ . It contains a representation of the group of generalized  $SU(2)$  gauge transformations defined by the action of the  $SU(2)$  gauge transformations on the generalized connections (3.2). This representation is unitary as a consequence of the group invariance of the Haar measure. We can similarly find a unitary representation of the diffeomorphism group  $\text{Diff}(\Sigma)$  by the action of the diffeomorphism group on each graph  $\Gamma$ .

In order to define the entropy of entanglement for a region  $\Omega \subseteq \Sigma$  we need to define a tensor product decomposition of the Hilbert space  $\mathcal{K}$  corresponding to the decomposition  $\Sigma = \Omega \cup \bar{\Omega}$ . To do this we define this decomposition for the graph spaces. Let  $\Gamma$  be a graph in  $\Sigma$ , and  $\Omega \subset \Sigma$  any region whose boundary intersects  $\Gamma$  in a finite number of points. We can then define the graph  $\Gamma_\Omega$  to consist of the portions of edges of  $\Gamma$  that lie in  $\Omega$ . The graph  $\Gamma_{\bar{\Omega}}$  is defined analogously. Note

that  $\Gamma_\Omega$  may have more edges than  $\Gamma$  if some edges of  $\Gamma$  intersect the boundary of  $\Omega$  multiple times.

We can then define a graph  $\Gamma' = \Gamma_\Omega \cup \Gamma_{\bar{\Omega}}$  whose edge set consists of the union of all edges from  $\Gamma_\Omega$  and all edges from  $\Gamma_{\bar{\Omega}}$ . Because every edge of  $\Gamma$  can be expressed as a composition of edges in  $\Gamma_\Omega$  and  $\Gamma_{\bar{\Omega}}$  we have  $\Gamma \subseteq \Gamma'$ . We also have the natural identification

$$\mathcal{K}_{\Gamma'} = \mathcal{K}_{\Gamma_\Omega} \otimes \mathcal{K}_{\Gamma_{\bar{\Omega}}}$$

Therefore for any state in  $\mathcal{K}_\Gamma$  can be identified as a state of  $\mathcal{K}_{\Gamma_\Omega} \otimes \mathcal{K}_{\Gamma_{\bar{\Omega}}}$ . This gives a natural tensor product decomposition for which we can compute the entanglement entropy of any state.

### 3.2.1 Spin network states

We now construct a basis of  $\mathcal{K}_\Gamma$  consisting of extended spin network states [43]. While there are of course many possible choices of basis, the extended spin network states are useful because of their simple transformation properties under generalized gauge transformations. In particular, the extended spin network basis contains as a subset the spin network basis of the gauge-invariant Hilbert space  $\mathcal{K}_0$ .

To construct a basis of  $\mathcal{K}_\Gamma$  we first construct a basis for  $L^2(\text{SU}(2))$  since

$$\mathcal{K}_\Gamma \cong L^2(\text{SU}(2)^L) \cong L^2(\text{SU}(2))^{\otimes L}$$

A basis of  $L^2(\text{SU}(2))$  can be constructed using the Peter-Weyl theorem, which gives a unitary equivalence

$$L^2(\text{SU}(2)) \cong \bigoplus_{j=0, \frac{1}{2}, 1, \dots} V_j \otimes V_j^* \quad (3.3)$$

where the half-integer spin  $j$  indexes all irreducible representations of  $\text{SU}(2)$ . The space  $V_j = \mathbb{C}^{2j+1}$  is the vector space for the spin- $j$  representation  $R^j : \text{SU}(2) \rightarrow U(2j+1)$ .

By applying the decomposition (3.3) to each edge of a graph  $\Gamma$  we have the unitary equivalence

$$\begin{aligned} \mathcal{K}_\Gamma &\cong \bigotimes_{\ell=1}^L \bigoplus_{j_\ell=0, \frac{1}{2}, 1, \dots} V_{j_\ell} \otimes V_{j_\ell}^* \\ &\cong \bigoplus_{\vec{j}} \bigotimes_{\ell=1}^L V_{j_\ell} \otimes V_{j_\ell}^* \end{aligned}$$

Where  $\vec{j} = (j_1, \dots, j_L)$  and the direct sum over  $\vec{j}$  is shorthand for the sum  $j_\ell = 0, \frac{1}{2}, 1, \dots$  for all  $\ell = 1, \dots, L$ . We therefore have a direct sum decomposition of  $\mathcal{K}_\Gamma$

$$\mathcal{K}_\Gamma = \bigoplus_{\vec{j}} \mathcal{K}_{\Gamma, \vec{j}} \quad \mathcal{K}_{\Gamma, \vec{j}} \equiv \bigotimes_{\ell=1}^L V_{j_\ell} \otimes V_{j_\ell}^*$$

The action of the generalized gauge transformations on the Hilbert space  $\mathcal{K}_{\Gamma, \vec{j}}$  has a rather simple form. For a fixed vertex  $v_n$ , the state transforms by  $g(v_n)$  in the following representation

$$\left( \begin{array}{c} \otimes \\ \{\ell: \gamma_\ell(0)=v_n\} \end{array} R^{j_\ell} \right) \otimes \left( \begin{array}{c} \otimes \\ \{\ell: \gamma_\ell(1)=v_n\} \end{array} R^{j_\ell^*} \right)$$

We can express this representation as a direct sum of irreducible representations  $J_n$ . For each  $J_n$  we can introduce an *intertwining operator*

$$i_n : \left( \begin{array}{c} \otimes \\ \{\ell: \gamma_\ell(0)=v_n\} \end{array} V_{j_\ell} \right) \otimes \left( \begin{array}{c} \otimes \\ \{\ell: \gamma_\ell(1)=v_n\} \end{array} V_{j_\ell^*} \right) \rightarrow V_{J_n} \quad (3.4)$$

that commutes with the action of  $g(v_n)$ . Upon fixing an intertwining operator for each vertex, we have a Hilbert space  $\mathcal{K}_{\Gamma, \vec{j}, \vec{J}, \vec{i}}$  where  $\vec{i} = (i_1, \dots, i_N)$  specifies an intertwining operator for each node.

The intertwiners form a vector space, which becomes an inner product space using the inner product

$$\langle i_1 | i_2 \rangle = \text{Tr}(i_1 i_2^*)$$

This gives a further decomposition of the Hilbert space  $\mathcal{K}_\Gamma$

$$\mathcal{K}_\Gamma \cong \bigoplus_{\vec{j}} \bigoplus_{\vec{J}} \bigoplus_{\vec{i}} \bigotimes_{n=1}^N V_{J_n}$$

Where the sum over  $\vec{i}$  is a sum over an orthogonal basis of the intertwiner space in equation (3.4). The gauge transformation  $g(v_n)$  acts on this space in the representation  $R^{J_n}$ . To specify a state in  $\mathcal{K}_{\Gamma, \vec{j}, \vec{J}, \vec{i}}$  we need only specify a set of vectors  $\vec{m} = (m_1, \dots, m_N)$  where  $m_n \in V_{J_n}$  for  $n = 1, \dots, N$ . This motivates the following definition:

An *extended spin network* is a tuple  $S = (\Gamma, \vec{j}, \vec{J}, \vec{i}, \vec{m})$  where

- $\Gamma$  is a graph in  $\Sigma$  consisting of vertices  $v_1, \dots, v_N$  and edges  $\gamma_1, \dots, \gamma_L$ ,
- $\vec{j} = (j_1, \dots, j_L)$  where  $j_\ell \in \{\frac{1}{2}, 1, \frac{3}{2}, \dots\}$  labels each edge with a non-trivial irreducible representation of  $\text{SU}(2)$ ,
- $\vec{J} = (J_1, \dots, J_N)$  where  $J_n \in \{0, \frac{1}{2}, 1, \frac{3}{2}, \dots\}$  labels each vertex with a possibly trivial irreducible representation of  $\text{SU}(2)$ ,
- $\vec{i} = (i_1, \dots, i_N)$  where  $i_n$  is an intertwining operator from the representations of all incoming edges and the duals of all outgoing edges to the spin  $J_n$  representation, and
- $\vec{m} = (m_1, \dots, m_N)$  where  $m_n \in V_{J_n}$  is a vector in the spin  $J_n$  representation space.



The *extended spin network state*  $|S\rangle$  is defined as a functional acting on a generalized connection  $A \in \overline{\mathcal{A}}$  as follows

$$\langle A|S\rangle = \left( \bigotimes_{n=1}^N m_n^* \right) \circ \left( \bigotimes_{n=1}^N i_n \right) \circ \left( \bigotimes_{\ell=1}^L R^{j_\ell}(A(\gamma_\ell)) \right)$$

In this expression, for each  $\ell$  the expression  $R^{j_\ell}(A(\gamma_\ell))$  defines a matrix in  $U(2j_\ell+1)$  which may be viewed as an element of  $V_{j_\ell} \otimes V_{j_\ell}^*$ . Thus the rightmost part of this expression has a tensor factor corresponding to  $V_{j_\ell}$  at the endpoint of every edge and one corresponding to  $V_{j_\ell}^*$  at the beginning of each edge. The intertwiner  $\bigotimes i_n$  maps this to a vector in the space  $\bigotimes J_n$ , which can be contracted with  $\bigotimes m_n^*$  yielding a complex number.

A generalized gauge transformation acts on the extended spin network state by transforming the vector  $m_n$  in the spin- $J_n$  representation of  $g(v_n)$ . Thus the gauge invariant sector of the Hilbert space is simply the space spanned by extended spin network states with  $J_n = 0$  and  $m_n = 1$  for  $n = 1, \dots, N$ . In this case the extended spin network state reduces to a *spin network state*. We will write  $S = (\Gamma, \vec{j}, \vec{i})$  for a spin network state, with  $J_n = 0$  and  $m_n = 1$  implied.

An important property of these states that we will use is their orthogonality. We first assume that all intertwiners  $i_n$  are normalized so that  $\text{Tr}(i_n^* i_n) = 1$ . We can do this without loss of generality because scaling  $i_n$  has the same effect as scaling  $m_n$  in the definition of the extended spin network state (3.2.1). Now suppose that  $S = (\Gamma, \vec{j}, \vec{J}, \vec{i}, \vec{m})$  and  $S' = (\Gamma, \vec{j}, \vec{J}, \vec{i}, \vec{m}')$  so that  $S$  and  $S'$  differ only by their set of vectors. Then

$$\langle S|S'\rangle = \prod_{n=1}^N \frac{\langle m_n | m'_n \rangle}{2J_n + 1} \quad (3.5)$$

Thus the extended spin network state is normalized when the vectors  $m_n$  are normalized so that  $\|m_n\| = \sqrt{2J_n + 1}$ .

### 3.3 Entanglement entropy of spin network states

Having defined the tensor product decomposition of the Hilbert space  $\mathcal{K}_\Gamma$  and with the definition of the spin network states, we can now compute the entanglement entropy of the spin network states. Before computing the entropy of entanglement for an arbitrary spin network it is useful to consider the simpler case of the Wilson loop states.

#### 3.3.1 Wilson loop states

Let  $\gamma$  be a curve in  $\Sigma$  such that  $\gamma(0) = \gamma(1)$  and  $j \in \{\frac{1}{2}, 1, \frac{3}{2}, \dots\}$ . The *Wilson loop state* is the state  $|\gamma, j\rangle$  defined by

$$\langle A|\gamma, j\rangle = \text{Tr}(R^j A(\gamma))$$

The Wilson loops are the simplest possible examples of spin network states, where the graph  $\Gamma$  consists of a single curve  $\gamma$  labelled by spin  $j$  and a single vertex with intertwiner  $i_n$  given by the normalized identity map  $i_n = \frac{I_j}{\sqrt{2j+1}}$  where  $I_j$  is the identity map  $I_j : V_j \rightarrow V_j$ .

The *Wilson line state*  $|\gamma, j, a, b\rangle$  is defined similarly as the matrix element of the representation of the holonomy along  $\gamma$

$$\langle A|\gamma, j, a, b\rangle = \sqrt{2j+1} [R^j A(\gamma)]_{a,b}$$

In terms of these states the Wilson loop state can be written as

$$|\gamma, j\rangle = \sum_a [R^j A(\gamma)]_{a,a} = \frac{1}{\sqrt{2j+1}} \sum_a |\gamma, j, a, a\rangle$$

We can check that the Wilson lines are orthonormal using the following fact from representation theory. Let  $x, y, z, w \in V_j$  then

$$\int_{\text{SU}(2)} \langle R^j(g)x|y\rangle \langle R^j(g^{-1})z|w\rangle dg = \frac{1}{2j+1} \langle z|y\rangle \langle x|w\rangle$$

Then letting  $\{e_i\}_{i=1}^{2j+1}$  denote an orthonormal basis of  $V_j$ ,

$$\begin{aligned} \langle \gamma, j, a, b|\gamma, j, c, d\rangle &= (2j+1) \int_{\text{SU}(2)} [R^j(g)]_{a,b} [R^j(g)]_{c,d}^* dg \\ &= (2j+1) \int_{\text{SU}(2)} \langle R^j(g)e_b|e_a\rangle \langle R^j(g^{-1})e_c|e_d\rangle dg \\ &= (2j+1) \frac{1}{2j+1} \langle e_a|e_c\rangle \langle e_b|e_d\rangle \\ &= \delta_{ac}\delta_{bd} \end{aligned} \tag{3.6}$$

We can then verify the normalization of the Wilson loop state

$$\begin{aligned} \langle \gamma, j|\gamma, j\rangle &= \frac{1}{2j+1} \sum_{a,b=1}^{2j+1} \langle \gamma, j, a, a|\gamma, j, b, b\rangle \\ &= \frac{1}{2j+1} \sum_{a,b=1}^{2j+1} \delta_{a,b}\delta_{a,b} \\ &= 1 \end{aligned}$$

For a single curve  $\gamma = \gamma_1 \circ \gamma_2$  we have an identification  $\mathcal{K}_\gamma \subseteq \mathcal{K}_{\gamma_1} \otimes \mathcal{K}_{\gamma_2}$ . In order to express the state  $|\gamma, j, a, b\rangle$  in this decomposition, we introduce a resolution of

the identity

$$\begin{aligned}
\langle A|\gamma_1 \circ \gamma_2, j, a, b\rangle &= \sqrt{2j+1} [R^j A(\gamma_1 \circ \gamma_2)]_{a,b} \\
&= \sqrt{2j+1} \sum_{c=1}^{2j+1} [R^j A(\gamma_1)]_{a,c} [R^j A(\gamma_2)]_{c,b} \\
&= \frac{1}{\sqrt{2j+1}} \sum_{c=1}^{2j+1} \langle A|\gamma_1, j, a, c\rangle \langle A|\gamma_2, j, c, b\rangle
\end{aligned}$$

This gives the following decomposition of the Wilson loop state

$$|\gamma_1 \circ \gamma_2, j, a, b\rangle = \frac{1}{\sqrt{2j+1}} \sum_{c=1}^{2j+1} |\gamma_1, j, a, c\rangle \otimes |\gamma_2, j, c, b\rangle \quad (3.7)$$

In fact, this equation is a Schmidt decomposition of the state  $|\gamma_1 \circ \gamma_2, j, a, b\rangle$ , which follows from the orthogonality of the Wilson line states (3.6).

This identity can be iterated to give a Schmidt decomposition of an arbitrary Wilson loop state. Let  $\Omega$  be a subset of  $\Sigma$  for which we will calculate the entanglement entropy. In general the curve  $\gamma$  intersects  $\partial\Omega$  at  $n$  points. We can decompose the curve as  $\gamma = \gamma_1 \circ \dots \circ \gamma_n$  where  $\gamma_1, \gamma_3, \dots, \gamma_{n-1} \subset \Omega$  and  $\gamma_2, \gamma_4, \dots, \gamma_n \subset \bar{\Omega}$ . Then applying equation (3.7) at all intersection points

$$\begin{aligned}
|\gamma, j\rangle &= \frac{1}{\sqrt{2j+1}^n} \sum_{a_1, \dots, a_n=1}^{2j+1} \bigotimes_{i=1}^n |\gamma_i, j, a_i, a_{i+1}\rangle \\
&= \frac{1}{\sqrt{2j+1}^n} \sum_{a_1, \dots, a_n=1}^{2j+1} \left( \bigotimes_{i=1,3,\dots}^{n-1} |\gamma_i, j, a_i, a_{i+1}\rangle \right) \otimes \left( \bigotimes_{i=2,4,\dots}^n |\gamma_i, j, a_i, a_{i+1}\rangle \right) \quad (3.8)
\end{aligned}$$

The states on the left of this tensor product are in the Hilbert space

$$\mathcal{K}_{\gamma_1} \otimes \mathcal{K}_{\gamma_3} \otimes \dots \otimes \mathcal{K}_{\gamma_{n-1}} = \mathcal{K}_{\gamma \cap \Omega}$$

Similarly, the right side of the tensor product is in  $\mathcal{K}_{\gamma \cap \bar{\Omega}}$ .

Equation (3.8) is a Schmidt decomposition of the Wilson loop state  $|\gamma, j\rangle$ . The Schmidt rank is  $(2j+1)^n$  and each Schmidt coefficient equals  $(2j+1)^{-n/2}$ . Each reduced density matrix is therefore proportional to a rank- $(2j+1)^n$  projection operator. The entanglement entropy of the Wilson loop state  $|\gamma, j\rangle$  can be determined directly from the Schmidt decomposition

$$S(\Omega) = \log(2j+1)^n = n \log(2j+1)$$

This equation depends linearly on the linking number of  $\gamma$  with  $\partial\Omega$ , just as the area operator

$$A(\partial\Omega) \propto n\sqrt{j(j+1)}$$

### 3.3.2 Spin network states

The formula for entanglement entropy of a Wilson loop state extends naturally to the extended spin network states. We first give a formula that is a direct analogue of the formula for inserting a resolution identity into the Wilson line state (3.7).

Let  $S$  be an extended spin network, and  $v$  a point on an edge  $\gamma_\ell$  at which we will insert a vertex. We can then write  $\gamma_\ell$  as a composition of two curves meeting at  $v$ ,  $\gamma_\ell = \gamma'_\ell \circ \gamma''_\ell$  so that  $\gamma'_\ell(1) = \gamma''_\ell(0) = v$ . We construct an equivalent spin network  $S'$  as follows. Let  $S' = (\Gamma', \vec{j}', \vec{J}', \vec{v}', \vec{m}')$ .

- $\Gamma'$  is the graph with edges

$$\gamma_1, \dots, \gamma_{\ell-1}, \gamma'_\ell, \gamma''_\ell, \gamma_{\ell+1}, \dots, \gamma_L$$

and vertices  $v_1, \dots, v_N, v$ ,

- The new edges are assigned the same representations as the subdivided edge  $\vec{j}' = (j_1, \dots, j_{\ell-1}, j_\ell, j_\ell, \dots, j_L)$ ,
- The intertwiner assigned to the new node is proportional to the identity intertwiner  $\vec{v}' = (i_1, \dots, i_n, \frac{1}{\sqrt{2j+1}}I)$ ,
- The representation attached to the inserted node is trivial  $\vec{J}' = (J_1, \dots, J_n, 0)$  and  $\vec{m}' = (m_1, \dots, m_n, 1)$ .

Then the extended spin networks  $S$  and  $S'$  define the same state  $|S'\rangle = |S\rangle$ .

Suppose now that  $\Omega$  is a subset of  $\Sigma$  for which we will consider the reduced density matrix of a spin network state  $|S\rangle$ . For the moment we will assume that no vertices of  $\Gamma$  lie exactly on the boundary  $\partial\Omega$ . By applying the previous construction repeatedly we may assume without loss of generality that all edges of  $S$  intersect the boundary  $\partial\Omega$  at vertices. Let  $P$  be the number of points where  $\Gamma$  intersects  $\partial\Omega$ ,  $N_\Omega$  the number of vertices of  $\Gamma$  in  $\Omega$ , and  $N_{\bar{\Omega}}$  the number of vertices in  $\bar{\Omega}$ . We can then partition the vertices  $v_1, \dots, v_N$  into three classes

- vertices that lie on the boundary,  $v_n \in \partial\Omega$  for  $n = 1, \dots, P$ ,
- vertices in  $\Omega$ ,  $v_n \in \Omega$  for  $n = P + 1, \dots, P + N_\Omega$ , and
- vertices in  $\bar{\Omega}$ ,  $v_n \in \bar{\Omega}$  for  $n = P + N_\Omega + 1, \dots, N$ .

Similarly, the edges  $\gamma_1, \dots, \gamma_L$  can be partitioned so that  $\gamma_\ell \subset \Omega$  for  $\ell = 1, \dots, L_\Omega$  and  $\gamma_\ell \subset \bar{\Omega}$  for  $\ell = L_\Omega + 1, \dots, L$ .

By assumption all the vertices on the boundary arose from the construction for inserting a vertex. This means that  $S$  has  $i_p = \frac{1}{\sqrt{2j_p+1}}I$  for  $p = 1, \dots, P$  where  $\tilde{j}_p$

denotes the spin of the edge that was subdivided to produce the vertex  $v_p$ . Each of these intertwiners  $i_p$  may be expanded in an orthogonal basis of  $V_{\tilde{j}_p}$ ,

$$i_p = \frac{1}{\sqrt{2\tilde{j}_p + 1}} \sum_{a_p=1}^{2\tilde{j}_p+1} |e_{a_p}\rangle\langle e_{a_p}| \quad (3.9)$$

Given a vector  $\vec{a} = (a_1, \dots, a_P)$  we define the extended spin network state  $|S_\Omega, \vec{a}\rangle$  as follows:

- the graph  $\Gamma_\Omega$  consisting of edges  $\gamma_1, \dots, \gamma_{L_\Omega}$  and vertices  $v_1, \dots, v_{P+N_\Omega}$ ,
- the labels on the edges are unchanged,  $j'_\ell = j_\ell$  for  $\ell = 1, \dots, L_\Omega$ ,
- the existing nodes are also unchanged  $J'_n = J_n$ ,  $i'_n = i_n$  and  $m'_n = m_n$  for  $n = P + 1, \dots, P + N_\Omega$ , and
- the vertices on the boundary have for  $p = 1, \dots, P$ .

$$\begin{aligned} J'_p &= \tilde{j}_p \\ i'_p &= \frac{1}{\sqrt{2\tilde{j}_p + 1}} I \\ m'_p &= \sqrt{2\tilde{j}_p + 1} e_{a_p} \end{aligned}$$

The state  $|S_\Omega, \vec{a}\rangle$  is defined analogously.

We can then apply the resolution of the identity (3.9) at each intertwiner of  $S$  on the boundary, giving

$$|S\rangle = \left( \prod_{p=1}^P \frac{1}{\sqrt{2\tilde{j}_p + 1}} \right) \sum_{\vec{a}} |S_\Omega, \vec{a}\rangle \otimes |S_{\bar{\Omega}}, \vec{a}\rangle \quad (3.10)$$

where the sum over  $\vec{a}$  denotes a sum over all n-tuples  $(a_1, \dots, a_P)$  with  $a_p = 1, \dots, 2\tilde{j}_p + 1$ .

By the orthogonality relation (3.5), the set  $\{|S_\Omega, \vec{a}\rangle\}_{\vec{a}}$  is orthonormal. Therefore (3.10) is a Schmidt decomposition of  $|S\rangle$ . The Schmidt rank is

$$N = \prod_{p=1}^P (2\tilde{j}_p + 1) \quad (3.11)$$

The entanglement entropy of  $|S\rangle$  is therefore

$$S(\Omega) = \sum_{p=1}^P \log(2\tilde{j}_p + 1) \quad (3.12)$$

The Schmidt decomposition also allows us to compute the reduced density matrix for the region  $\Omega$ ,

$$\rho(\Omega) = \frac{1}{N} \sum_{\vec{a}} |S_{\Omega}, \vec{a}\rangle \langle S_{\Omega}, \vec{a}| \quad (3.13)$$

Note that although the individual states  $|S_{\Omega}, \vec{a}\rangle$  transform non-trivially under a gauge transformation, the linear combination (3.13) is gauge-invariant.

This is not surprising, since the proper graph subspace  $\mathcal{K}_{\Gamma_{\Omega}}$  does not contain any gauge-invariant pure states except in the trivial case where  $\Gamma$  does not intersect the boundary. This is a result of *Schur's lemma*, which states that any intertwining operator  $V_j \rightarrow V_{j'}$  is either proportional to the identity if  $j = j'$  or zero if  $j \neq j'$ . If the graph  $\Gamma \cap \Omega$  contains vertices of degree one on the boundary, a gauge invariant pure state would need to have an intertwining operator  $V_j \rightarrow V_0$ , which is impossible. However it *is* possible to have a gauge invariant mixed state, which is a density matrix  $V_j \rightarrow V_j$ . By Schur's lemma there is exactly one such state, which is proportional to the identity. It is the maximally mixed state  $\frac{1}{2j+1}I$ , whose entropy is  $\log(2j+1)$ .

The similarity between the entanglement entropy and the area operator is apparent. The entanglement entropy is a sum over intersections of the spin network with the surface  $\partial\Omega$ , much like the eigenvalue to the area operator  $\hat{A}(\partial\Omega)$ . However they are not linearly related for any choice of the Immirzi parameter. Possible physical implications of this fact are discussed in section 3.5.

Spin networks therefore give a rather literal realization of the holographic picture of 't Hooft in terms of entanglement [2]. The bits on the boundary do not encode possible states of the interior, rather they represent entangled bits or “ebits” shared by the region  $\Omega$  and its complement. Any surface, including a black hole horizon is divided into elementary cells, each labelled by a spin  $j$ . Each of these cells carries one ebit for  $j = \frac{1}{2}$ , one ebit for  $j = 1$ , etc. The entanglement is a direct consequence of how gauge transformations act at points on the boundary, and in this sense the degrees of freedom responsible for the entanglement entropy are entirely local to the boundary.

### 3.3.3 Degenerate spin network states

In the previous section, we derived a general expression for the entanglement entropy  $S(\Omega)$  of a spin network state  $|S\rangle$  when no vertices of  $S$  intersect the boundary of the region  $\Omega$ . This expression (3.12) is analogous to the non-degenerate part of the area spectrum (3.1). We know however that the spectrum of the area operator also has a degenerate part, corresponding to the case in which a vertex of the graph  $\Gamma$  lies on the boundary. In this section we consider the entanglement entropy of these degenerate spin networks.

First, we have the technical subtlety that it is in general possible to have edges of  $\Gamma$  that lie exactly on the boundary of  $\Omega$ . In this case we must be careful,

since these could behave differently from edges which only touch the boundary at isolated points. For example, the degenerate spectrum of the area operator changes depending on whether incident edges are tangent to the surface. For the purposes of the entanglement entropy the tensor product decomposition requires that the edges on the boundary must be part of  $\Omega$  or  $\bar{\Omega}$ . This means we must specify whether  $\Omega$  is topologically open or closed. We could also choose  $\Omega$  to be neither open nor closed, in which case a boundary edge could lie partly in  $\Omega$  and partly in  $\bar{\Omega}$ . For the calculation of entropy, it will not matter whether edges lie on the boundary or not, but only whether they lie in  $\Omega$  or  $\bar{\Omega}$ . This is to be expected; the fact that the area operator acts differently on tangential edges results from a particular choice of regularization. In fact it is possible to construct regularizations with no dependence on tangential edges. This ambiguity is not present in the calculation of entanglement entropy, since no regularization is required. For definiteness we will consider  $\Omega$  to be an open set, so that  $\partial\Omega \subset \bar{\Omega}$ . This choice is based on the interpretation of  $\Omega$  as a black hole exterior region, which is always an open set.

In the case of a spin network state which may have vertices lying on the boundary, we may still construct the reduced spin network states  $|S_\Omega, \vec{a}\rangle$ . Because there now exist intertwiners on the boundary which are not proportional to the identity, we do not have the Schmidt decomposition (3.10). In general we have the following decomposition (which is *not* a Schmidt decomposition)

$$|S\rangle = \sum_{\vec{a}, \vec{a}'} \lambda_{\vec{a}, \vec{a}'} |S_\Omega, \vec{a}\rangle \otimes |S_{\bar{\Omega}}, \vec{a}'\rangle$$

We will find it convenient to work with the operator  $\hat{S}$  defined by the partial transpose

$$\hat{S} = \sum_{\vec{a}, \vec{a}'} \lambda_{\vec{a}, \vec{a}'} |S_\Omega, \vec{a}\rangle \langle S_{\bar{\Omega}}, \vec{a}'|$$

The partial transpose is a bijection, so all the information about  $|S\rangle$  is encoded in  $\hat{S}$ . In particular, the Schmidt decomposition of  $|S\rangle$  corresponds to a singular value decomposition of  $\hat{S}$ .

The support of this operator is confined to the subspace spanned by the vectors  $\{|S_\Omega, \vec{a}\rangle\}$ . This is a subspace of dimension  $\prod_{p=1}^P (2j_p + 1)$ , so there is unitary equivalence

$$\text{span}\{|S_\Omega, \vec{a}\rangle\} \cong \bigotimes_{p=1}^P V_{j_p} \tag{3.14}$$

Associated to each vertex  $v_n$  on the boundary is an intertwining operator  $i_n$  between the tensor products of all edges incident to  $v_n$ . Let  $j_1, \dots, j_P$  be the spins associated to edges incident to  $v_n$  from  $\Omega$  and  $j'_1, \dots, j'_{P'}$  be those associated to edges incident to  $v_n$  from  $\bar{\Omega}$ . The intertwiner can then be naturally described as an operator

$$i_n : \bigotimes_{i=1}^P V_{j_i} \rightarrow \bigotimes_{i=1}^{P'} V_{j'_i}$$

Using the unitary equivalence between Hilbert spaces (3.14) we have the unitary equivalence between operators

$$\hat{S} \cong i_{\partial\Omega} := \bigotimes_{\{n:v_n \in \partial\Omega\}} i_n$$

By the equivalence between the singular value decomposition of  $\hat{S}$  and the Schmidt decomposition of  $|S\rangle$  the entanglement entropy can be expressed in terms of  $\hat{S}$

$$S(\Omega) = S(\hat{S}\hat{S}^*)$$

Which in turn allows us to express the entropy in terms of  $i_{\partial\Omega}$

$$S(\hat{S}\hat{S}^*) = S(i_{\partial\Omega}i_{\partial\Omega}^*) = S\left(\bigotimes_{n:v_n \in \partial\Omega} i_n i_n^*\right) = \sum_{n:v_n \in \partial\Omega} S(i_n i_n^*) \quad (3.15)$$

In the last line, we used the additivity of the von Neumann entropy across tensor products. Thus the entanglement entropy can be expressed as a sum of terms of the form  $S(i_n i_n^*)$  which we recognize as the entanglement entropy of an intertwining operator. In the next section we will compute the entanglement entropy of these intertwining operators.

Note that the formula for the entropy of the non-degenerate spin network (3.12) is a special case of this formula. In the non-degenerate case we view each point where a spin- $j$  edge crosses the boundary as a bivalent intertwiner  $i_n : V_j \rightarrow V_j$ . Each intertwiner on the boundary has the form  $i_n = \frac{1}{\sqrt{2j+1}} I_j$ ; this fact can be seen directly from the formula for inserting vertices on the boundary, and is a direct consequence of Schur's lemma combined with the normalization of  $i_n$ . It follows that the entanglement entropy of  $i_n$  is

$$S(i_n^* i_n) = S\left(\frac{1}{2j+1} I_j\right) = \log(2j+1)$$

Since the entanglement entropy of the spin network is just a sum of terms of this form (3.15), we arrive at the formula for the entanglement entropy (3.12).

### 3.3.4 Graphical calculus and intertwiners

We now consider the problem of finding the entanglement entropy of an intertwining operator. Initially one would not expect to find a general expression for the entanglement entropy; this requires diagonalization of a density matrix, for which there is generally no explicit formula. Here the group invariance plays an important role since it restricts the possible operators that may appear. For example, we know there is no general formula for the spectrum of a general map  $V_j \rightarrow V_j$ <sup>3</sup>. If the map

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<sup>3</sup>In principle this is only true for  $j \geq 2$ . The reason is that finding the spectrum of a matrix is equivalent to finding the zeroes of its characteristic polynomial. The characteristic polynomial has degree  $2j+1$ , and therefore there is no explicit expression for the roots when  $2j+1 \geq 5$ , or  $j \geq 2$ .



is required to be an intertwiner, Schur's lemma allows us to compute the entropy explicitly. Although we will not provide a formula for the entanglement entropy of a general intertwining operator, we can give an explicit formula in certain special cases which happen to be of physical interest.

Calculations involving intertwiners are most easily expressed using a graphical calculus originally developed by Penrose [30]. This graphical calculus has been generalized to Temperley-Lieb recoupling theory, which may be viewed as a  $q$ -deformed version of spin network theory [46]. For a discussion of how recoupling theory applies to loop quantum gravity and a translation between Temperley-Lieb recoupling theory and spin network notation see the book by Rovelli ([26], appendix A). For a thorough introduction to spin networks and their graphical calculus see the course notes of Baez [47]. We will give a short introduction to the graphical calculus. This introduction is not meant to be complete, and results will be introduced as needed for the calculation of entanglement entropy.

An intertwining operator  $T : V_{j_1} \otimes \cdots \otimes V_{j_n} \rightarrow V_{j'_1} \otimes \cdots \otimes V_{j'_m}$  is represented as a box with lines  $n$  entering from the top and  $m$  lines exiting from the bottom

$$T = \begin{array}{|c|} \hline \cdots \\ \hline T \\ \hline \cdots \\ \hline \end{array}$$

A special case is the identity operator  $I_j : V_j \rightarrow V_j$ , which is represented as a single vertical line

$$I_j = \begin{array}{|c|} \hline \\ \hline j \\ \hline \end{array}$$

Composition of two intertwiners  $T$  and  $S$  is represented as vertical concatenation of boxes

$$ST = \begin{array}{|c|} \hline \cdots \\ \hline T \\ \hline \cdots \\ \hline S \\ \hline \cdots \\ \hline \end{array}$$

Horizontal concatenation of boxes represents the tensor product

$$T \otimes S = \begin{array}{|c|} \hline \cdots \\ \hline T \\ \hline \cdots \\ \hline \end{array} \begin{array}{|c|} \hline \cdots \\ \hline S \\ \hline \cdots \\ \hline \end{array}$$

The 1-dimensional vector space  $V_0 = \mathbb{C}$  is denoted by no lines. There is a unique intertwining operator  $\text{cup}_j : V_j \otimes V_j \rightarrow \mathbb{C}$ . This map has two incoming lines of spin  $j$  and no outgoing lines, and is denoted

$$\text{cup}_j = \begin{array}{c} \cup \\ j \end{array}$$

Its dual is the map  $\text{cap}_j : \mathbb{C} \rightarrow V_j \otimes V_j$  denoted

$$\text{cap}_j = \begin{array}{c} \cap \\ j \end{array}$$

With these definitions the graphical calculus is topologically invariant, so that any planar deformation of a diagram represents the same intertwiner.

A network with no inputs and no outputs represents a linear map  $\mathbb{C} \rightarrow \mathbb{C}$ , which is just a complex number. For any network  $T$  we can define a complex number by connecting all inputs to outputs using  $\text{cup}_j$  and  $\text{cap}_j$ . This gives a multiple of the trace of an operator:

$$\text{Tr}(T) \propto \text{cap}_j \left( \begin{array}{c} \dots \\ \boxed{T} \\ \dots \end{array} \right) \text{cup}_j$$

We can apply this to the identity operator, getting a circle of spin  $j$

$$\Delta_j = \text{cap}_j \circ \text{cup}_j = (-1)^{2j} \text{Tr}(I_j) = (-1)^{2j} (2j + 1)$$

There is a unique intertwiner between three spins  $a, b, c$  providing they satisfy the Clebsch-Gordan condition:

$$a + b + c \in \mathbb{Z} \quad \text{and} \quad |a - b| \leq c \leq a + b$$

This intertwiner is denoted by a 3-vertex



By attaching two 3-vertices together we construct the  $\theta$ -net

$$\theta(a, b, c) = \text{cap}_j \left( \begin{array}{c} a \\ \boxed{b} \\ c \end{array} \right) \text{cup}_j$$

It is possible to give an explicit combinatorial formula for  $\theta(a, b, c)$  [46, 26].

We now express some basic properties of the von Neumann entropy in terms of these diagrams

$$S \left( \begin{array}{c} \dots \\ \boxed{S} \\ \dots \\ \dots \\ \boxed{T} \\ \dots \end{array} \right) = S \left( \begin{array}{c} \dots \\ \boxed{T} \\ \dots \\ \dots \\ \boxed{S} \\ \dots \end{array} \right) \quad (3.16)$$

$$S \left( \begin{array}{c} \dots \\ \boxed{S} \\ \dots \end{array} \otimes \begin{array}{c} \dots \\ \boxed{T} \\ \dots \end{array} \right) = S \left( \begin{array}{c} \dots \\ \boxed{S} \\ \dots \end{array} \right) + S \left( \begin{array}{c} \dots \\ \boxed{T} \\ \dots \end{array} \right) \quad (3.17)$$

$$S \left( \frac{(-1)^{2j}}{\Delta_j} \middle| j \right) = \log(2j + 1) \quad (3.18)$$

The first property (3.16) follows from the fact that the von Neumann entropy depends only on the non-zero spectrum of the operator, and the following property of the spectrum

$$\sigma(ST) \setminus \{0\} = \sigma(TS) \setminus \{0\}$$

Property (3.17) expresses the additivity of the von Neumann entropy across tensor products. The last property (3.18) is the von Neumann entropy of the maximally mixed state on a vector space of dimension  $2j + 1$ .

An important fact that we will use is Schur's lemma. It states that if  $T$  is an intertwining operator  $V_i \rightarrow V_j$  then either  $i \neq j$  and  $T$  is zero, or  $i = j$  and  $T$  is a scalar multiple of the identity. It can be expressed concisely in graphical form

$$\begin{array}{c} | \\ \boxed{T} \\ | \end{array} \begin{array}{c} i \\ \\ j \end{array} = \frac{\boxed{T}^j}{\Delta_j} \delta_{ij} \begin{array}{c} | \\ \\ j \end{array} \quad (3.19)$$

As we will see this formula combined with the properties of the von Neumann entropy is what makes it possible to compute the entanglement entropy of intertwining operators.

Suppose that our intertwiner  $I$  is of the following form:

$$\begin{array}{c} | \dots | \\ \boxed{I} \\ | \dots | \end{array} = \begin{array}{c} | \dots | \\ \boxed{S} \\ | \\ j \\ | \\ \boxed{T} \\ | \dots | \end{array} \quad (3.20)$$

Here the single edge of spin  $j$  is called the *principal link*. Intertwiners of this form have a physical interpretation. Suppose a surface  $\sigma$  intersects a vertex  $v$ , the eigenvalue to the area operator  $\hat{A}(\sigma)$  depends on the intertwiner at  $v$ . The superposition of two intertwiners corresponding to different eigenvalues is again an intertwiner, but is not an eigenvalue of the area operator  $\hat{A}(\sigma)$ . Therefore for a given surface only certain intertwiners diagonalize the area operator. The intertwiners of the form (3.20) are precisely the intertwiners that diagonalize the area operator  $\hat{A}(\partial\Omega)$  [31].

The entanglement entropy of  $I$  is the von Neumann entropy  $S(II^*)$ , which can be evaluated using the properties of  $S$  along with Schur's lemma:

$$S \left( \begin{array}{c} | \dots | \\ \boxed{S} \\ | \\ j \\ | \\ \boxed{T} \\ | \dots | \\ \boxed{T} \\ | \\ j \\ | \\ \boxed{S} \\ | \dots | \end{array} \right) = S \left( \begin{array}{c} | j \\ \boxed{T} \\ | \dots | \\ \boxed{T} \\ | \\ j \\ | \dots | \\ \boxed{S} \\ | \dots | \\ \boxed{S} \\ | j \end{array} \right) = S \left( \begin{array}{c} \boxed{T} \\ | \dots | \\ \boxed{T} \\ | \\ j \\ | \dots | \\ \boxed{S} \\ | \dots | \\ \boxed{S} \end{array} \right) \begin{array}{c} j \\ \frac{1}{\Delta_j} \\ | \\ j \end{array} = \log(2j + 1)$$

The diagram in the second last step represents  $\text{Tr}(II^*)$ , which is equal to 1 by the normalization of the intertwiner.

With some effort we can generalize this to intertwiners with two principal links. To do this we use the following identity, which is a graphical version of the Clebsch-Gordan rule [47]

$$a \otimes b = |a - b| \oplus \dots \oplus (a + b)$$

$$a \left| \begin{array}{c} | \\ \\ b \end{array} \right| = \sum_{i=|a-b|}^{a+b} \frac{\Delta_i}{\theta(a, b, i)} \begin{array}{c} a \\ \diagdown \\ i \\ \diagup \\ b \end{array} \quad (3.21)$$

Let  $P_i$  denote the  $i^{\text{th}}$  term in the sum above. Then we can check that  $\{P_i\}_{i=|a-b|}^{a+b}$  is an orthogonal set of projectors

$$P_i P_j = \frac{\Delta_i \Delta_j}{\theta(a, b, i) \theta(a, b, j)} \begin{array}{c} a \searrow j \\ \bigcirc \\ a \nearrow i \\ b \end{array} = \frac{\Delta_i \Delta_j}{\theta(a, b, i) \theta(a, b, j)} \left( \delta_{ij} \frac{\theta(a, b, i)}{\Delta_i} \begin{array}{c} a \searrow b \\ i \\ a \nearrow b \end{array} \right) = \delta_{ij} P_i$$

Equation (3.21) is a resolution of the identity on  $V_a \otimes V_b$  into projectors. Note that this is not a complete resolution of the identity into rank-1 projectors, since

$$\text{Tr} P_i = (-1)^{2a+2b} \frac{\Delta_i}{\theta(a, b, i)} \text{Tr} \left( \begin{array}{c} a \searrow b \\ i \\ a \nearrow b \end{array} \right) = (-1)^{2i} \Delta_i = 2i + 1$$

We can use this resolution of the identity to express any intertwining operator  $S$  as follows

$$\begin{aligned} \begin{array}{c} a \searrow b \\ \boxed{S} \\ a \nearrow b \end{array} &= \sum_{i,j} \frac{\Delta_i \Delta_j}{\theta(a, b, i) \theta(a, b, j)} \begin{array}{c} a \searrow j \\ \boxed{S} \\ a \nearrow i \\ b \end{array} \\ &= \sum_{i,j} \frac{\Delta_i \Delta_j}{\theta(a, b, i) \theta(a, b, j)} \frac{1}{\Delta_i} \begin{array}{c} a \searrow b \\ \boxed{S} \\ a \nearrow b \end{array} \delta_{ij} \begin{array}{c} a \searrow b \\ i \\ a \nearrow b \end{array} \\ &= \sum_i \left( \frac{1}{\theta(a, b, i)} \begin{array}{c} a \searrow b \\ \boxed{S} \\ a \nearrow b \end{array} \right) \left( \frac{\Delta_i}{\theta(a, b, i)} \begin{array}{c} a \searrow b \\ i \\ a \nearrow b \end{array} \right) \\ &= \sum_i \lambda_i P_i \end{aligned}$$

Where we have defined the constant  $\lambda_i$  as

$$\lambda_i = \frac{1}{\theta(a, b, i)} \begin{array}{c} a \searrow b \\ \boxed{S} \\ a \nearrow b \end{array} \begin{array}{c} a \searrow b \\ i \\ a \nearrow b \end{array} \quad (3.22)$$

We therefore have a formula for diagonalizing an arbitrary intertwining operator on  $V_a \otimes V_b$ . If a reduced density matrix  $\rho$  is expressed as  $\sum_i \lambda_i P_i$ , we can compute its von Neumann entropy

$$S \left( \sum_i \lambda_i P_i \right) = -\text{Tr} \left( \sum_i \lambda_i \log \lambda_i P_i \right) = -\sum_i (2i + 1) \lambda_i \log \lambda_i$$

Where the eigenvalues  $\lambda_i$  may be computed from (3.22) using the rules of the graphical calculus.

Now suppose that we have an intertwiner  $I$  with two principal links:

$$I = \begin{array}{c} \dots \\ \boxed{S} \\ \dots \\ a \quad b \\ \dots \\ \boxed{T} \\ \dots \end{array}$$

Then the entanglement entropy of  $I$  is

$$S \left( \begin{array}{c} \dots \\ \boxed{S} \\ \dots \\ a \quad b \\ \dots \\ \boxed{T} \\ \dots \\ \boxed{T} \\ \dots \\ a \quad b \\ \dots \\ \boxed{S} \\ \dots \end{array} \right) = S \left( \begin{array}{c} a \quad b \\ \boxed{T} \\ \dots \\ \boxed{T} \\ \dots \\ a \quad b \\ \dots \\ \boxed{S} \\ \dots \\ \boxed{S} \\ \dots \\ a \quad b \end{array} \right) = S \left( \sum_i \lambda_i P_i \right)$$

Where the coefficients  $\lambda_i$  are given by

$$\lambda_i = \frac{1}{\theta(a, b, i)} \left( \begin{array}{c} a \quad b \\ \boxed{T} \\ \dots \\ \boxed{T} \\ \dots \\ a \quad b \\ \dots \\ \boxed{S} \\ \dots \\ \boxed{S} \\ \dots \\ a \quad b \end{array} \right)_i = \frac{1}{\theta(a, b, i)^2} \left( \begin{array}{c} a \quad b \\ \boxed{T} \\ \dots \\ \boxed{T} \\ \dots \\ a \quad b \end{array} \right)_i \left( \begin{array}{c} a \quad b \\ \boxed{S} \\ \dots \\ \boxed{S} \\ \dots \\ a \quad b \end{array} \right)_i$$

Once again these coefficients can be computed using the graphical calculus, giving an explicit form for the entropy of an intertwiner with two principal links.

### 3.4 Isolated horizons

For non-degenerate spin networks, the reduced density matrix (3.13) is of a very special form. All of its eigenvalues are equal, so that the reduced density matrix is proportional to a projector onto a subspace of dimension

$$N = \prod_{p=1}^P (2\tilde{j}_p + 1) \tag{3.23}$$

This subspace depends only on the intersection of the spin network with the boundary, and its dimension grows with the area of the boundary. This suggests that there is a Hilbert space associated to the boundary whose dimension is  $N$ , and which would be sufficient to completely encode all observables relevant for an outside observer's description of the black hole.

In fact, exactly such a Hilbert space has been constructed in the isolated horizon framework for loop quantum gravity. In the isolated horizon framework, one

considers a spacetime  $\Omega \times \mathbb{R}$  where  $\mathbb{R}$  is time, and  $\Omega$  has a boundary  $\partial\Omega$ . Here  $\Omega$  represents the exterior region of a black hole and  $\partial\Omega$  represents the horizon. The classical theory is given in terms of an action  $S(A, E)$  which is a function of the Ashtekar variables. To get the equations of motion one must vary the action, and then integrate by parts. In the presence of a boundary, the integration by parts gives a term proportional to the variation  $\delta A$  on the boundary. There are several ways to remedy this situation. One may simply require  $\delta A = 0$  on the boundary, so that only a limited class of variations are considered. The alternative pursued in the isolated horizon program is to add an additional boundary term to the action that cancels the extra term in  $\delta A$  on the boundary. This yields additional equations of motion that must be satisfied on the boundary.

This procedure was originally carried out by Smolin using the Capovilla-Dell-Jacobson action for general relativity [37]. In this case the boundary action is the action for  $SU(2)$  Chern-Simons theory and the boundary conditions are known as the self-dual boundary conditions. This analysis was extended by Ashtekar et. al. to the isolated horizon boundary conditions [6, 39]. The isolated horizon boundary conditions give a set of conditions describing a spherical black hole whose area is constant in time [48]. The boundary action in this model is described by a  $U(1)$  Chern-Simons theory. In this section we will consider the isolated horizon boundary conditions, but similar considerations apply to the self-dual boundary conditions.

The classical theory described above may be quantized using the techniques of loop quantum gravity. The resulting kinematical Hilbert space has the form

$$\mathcal{K} = \mathcal{K}_{\partial\Omega} \otimes \mathcal{K}_{\Omega}$$

Where the *bulk space*  $\mathcal{K}_{\Omega}$  is the kinematical Hilbert space described in section 3.2. The *boundary space*  $\mathcal{K}_{\partial\Omega}$  is a direct sum of Chern-Simons Hilbert spaces

$$\mathcal{K}_{\partial\Omega} = \bigoplus_{\mathcal{P}} \mathcal{K}_{\partial\Omega}^{\mathcal{P}}$$

Here the sum over  $\mathcal{P}$  runs over all vectors  $\mathcal{P} = (x_1, \dots, x_P, j_1, \dots, j_P)$  where  $\{x_p\}_{p=1}^P$  are points in  $\partial\Omega$  called *punctures* and  $(j_1, \dots, j_P)$  is a labelling of the punctures with spins. The vector space  $\mathcal{K}_{\partial\Omega}^{\mathcal{P}}$  is the Hilbert space of Chern-Simons theory on  $\partial\Omega$  with the labelled punctures  $\mathcal{P}$ . Chern-Simons theory is topological, meaning that there are no local degrees of freedom: the connection on  $\partial\Omega$  is flat except at the punctures. It follows that the only degrees of freedom in  $\mathcal{K}_{\partial\Omega}^{\mathcal{P}}$  are the holonomies of curves with non-trivial winding numbers around the punctures.

From the kinematical Hilbert space one must pass to the gauge-invariant Hilbert space  $\mathcal{K}_0$ . The gauge transformations on  $\mathcal{K}_{\Omega}$  act the same way as in the theory without boundary, and the action of the gauge transformations on  $\mathcal{K}_{\partial\Omega}$  is determined by the boundary conditions. We can then form the quotient with these gauge transformations, giving the gauge-invariant Hilbert space

$$\mathcal{K}_0 = \bigoplus_{\mathcal{P}} \frac{\mathcal{K}_{\Omega}^{\mathcal{P}} \otimes \mathcal{K}_{\partial\Omega}^{\mathcal{P}}}{\mathcal{G}} \quad (3.24)$$

The space  $\mathcal{K}_\Omega^{\mathcal{P}}$  is spanned by the extended spin network states  $|S_\Omega, \vec{a}\rangle$  with spin networks  $S$  whose edges meet  $\partial\Omega$  at the points  $x_1, \dots, x_p$  with spins  $j_1, \dots, j_p$ . The quotient with  $\mathcal{G}$  indicates that we still have to take the quotient with gauge transformations that act on the boundary punctures. These act on the the extended spin networks as well as on the states of the Chern-Simons theory.

Given any gauge-invariant state in  $\mathcal{K}_\Omega^{\mathcal{P}} \otimes \mathcal{K}_{\partial\Omega}^{\mathcal{P}}$ , we can take the partial trace yielding a mixed state on  $\mathcal{K}_{\partial\Omega}^{\mathcal{P}}$ . In fact, because of the way gauge transformations act, it is the maximally mixed state on  $\mathcal{K}_{\partial\Omega}^{\mathcal{P}}$ . The entropy of entanglement is therefore given by  $\log \dim \mathcal{K}_{\partial\Omega}^{\mathcal{P}}$ , where  $\dim \mathcal{K}_{\partial\Omega}^{\mathcal{P}}$  is given in the limit of large numbers of punctures  $P \rightarrow \infty$  as

$$\dim \mathcal{K}_{\partial\Omega}^{\mathcal{P}} \sim \prod_{p=1}^P (2\tilde{j}_p + 1) \quad (3.25)$$

Therefore the dimension of the boundary theory approaches the Schmidt rank of the spin network state intersecting the boundary  $\partial\Omega$  in the punctures  $\mathcal{P}$ .

It is not hard to see why the dimension of the boundary Hilbert space should be the same as the Schmidt rank. For any state in  $\mathcal{K}_\Omega^{\mathcal{P}} \otimes \mathcal{K}_{\partial\Omega}^{\mathcal{P}}$ , its restriction to the space  $\mathcal{K}_\Omega$  is a gauge invariant mixed state with support on an extended spin network with endpoints coinciding with the punctures  $\mathcal{P}$ . There is exactly one such mixed state; it is the mixed spin network state given by equation (3.13). It follows from the Schmidt decomposition that the reduced density matrix on  $\mathcal{K}_{\partial\Omega}^{\mathcal{P}}$  must have the same spectrum, making it a maximally mixed state whose rank is  $\prod (2\tilde{j}_p + 1)$ .

However the dimension of the boundary Hilbert space (3.25) and the Schmidt rank  $N$  of the spin network state (3.11) are not exactly equal. In fact the dimension of the boundary Hilbert space is slightly smaller than  $N$ . the reason for this difference comes from what would appear to be the most innocuous of the isolated horizon boundary conditions: the restriction to spherical topology.

On a punctured sphere, the product of the holonomies around any set of points is trivial. This gives a restriction on the surface degrees of freedom [49]. In particular, we saw that the range of the reduced density matrix is isomorphic to a product of representation spaces

$$N = \dim \left( \bigotimes_{p=1}^P V_{\tilde{j}_p} \right)$$

The Hilbert space  $\mathcal{K}_{\partial\Omega}^{\mathcal{P}}$  is instead isomorphic to a quotient of this space with the diagonal action of  $\text{SU}(2)$

$$\dim \mathcal{K}_{\partial\Omega}^{\mathcal{P}} = \dim \left( \frac{\bigotimes_{p=1}^P V_{\tilde{j}_p}}{\text{SU}(2)} \right)$$

Equivalently, this is the number of intertwiners  $\bigotimes V_{\tilde{j}_p} \rightarrow \mathbb{C}$ .

In fact, this difference has caused some confusion in the derivation of the black hole entropy. The Schmidt rank  $N$  is the number of sequences  $\{a_p\}_{p=1}^P$  satisfying  $a_p \in \{-\tilde{j}_p, -\tilde{j}_p + 1, \dots, \tilde{j}_p\}$ . The dimension of the boundary Hilbert space is

equal to the number of such sequences that satisfy the additional *spin projection constraint*

$$\sum_{p=1}^P a_p = 0 \tag{3.26}$$

The spin projection constraint was not taken into account in the original counting of black hole entropy [6]. It was subsequently corrected, leading to a modification of the logarithmic correction to the entropy [35, 36].

We have shown that the dimension of the boundary Hilbert space agrees with the result computed purely from considering the Schmidt decomposition of a spin network state. The latter calculation is completely independent of the complex apparatus of the isolated horizon framework, yet yields an almost identical state counting. The only modification from the isolated horizon framework is the introduction of the spin projection constraint, whose origin is purely topological and which is so small that it is unlikely to have any physical implications.

The fact that the state counting in the isolated horizon approach is independent of boundary conditions was already suggested by Husain [50]. He illustrated this with a model having the same kinematics as the isolated horizon framework, but with a degenerate metric so that the boundary does not define a horizon. It was shown explicitly that the constraint requiring  $\partial\Omega$  to be an apparent horizon does not enter into the calculations. It was further conjectured that the boundary entropy does not depend on the choice of boundary action, and that any other topological theory such as BF theory could replace Chern-Simons theory on the boundary. The arguments of this section strongly support this conclusion, by giving an account for black hole entropy without introducing any boundary conditions at all.

The same considerations would appear to apply to the boundary theory of Smolin [37]. His construction is similar, but requires a formulation of loop quantum gravity with a positive cosmological constant [51]. In this theory the  $SU(2)$  spin networks are replaced with quantum-deformed  $SU(2)_q$  spin networks and the boundary theory is an  $SU(2)_q$  Chern-Simons theory where  $q = e^{\frac{2\pi i}{k+2}}$ . In the limit  $k \rightarrow \infty$ , the dimension of the boundary state space coincides with the Schmidt rank. Interestingly, this is the limit in which the cosmological constant approaches zero. To make the correspondence between the entanglement entropy and Smolin's boundary theory precise, one would need to compute the Schmidt decomposition of the  $SU(2)_q$  spin network states.

### 3.5 Corrections to the area law

We have already noted the similarity between the entanglement entropy (3.12) of a general region  $\Omega$  in terms of a spin network intersecting  $\partial\Omega$  and the eigenvalue of



the area operator (3.1), given by these two expressions

$$S(\Omega) = \sum_{p=1}^P \log(2\tilde{j}_p + 1) \quad (3.27)$$

$$A(\partial\Omega) = 8\pi G\gamma \sum_{p=1}^P \sqrt{\tilde{j}_p(\tilde{j}_p + 1)} \quad (3.28)$$

These quantities do not have a linear relationship, suggesting the possibility of corrections to the Bekenstein-Hawking formula.

One of the motivations for studying corrections to the black hole entropy formula is that these corrections could indicate deviations from Einstein gravity. In a theory with a diffeomorphism-invariant gravitational action, Wald [34] has shown that for a black hole with bifurcate Killing horizons, the entropy is of the form

$$S = 2\pi \oint_{\partial\Omega} Q$$

where  $Q$  is the Noether charge depending on the Lagrangian. This suggests that corrections to black hole entropy encode corrections to the gravitational action.

The formal similarity between the entropy formula (3.12) and the area operator (3.28) suggests that the entanglement entropy may be expressed as the integral of a local density over the horizon. This suggests that we define the horizon entropy density  $Q$  as the geometric quantity such that

$$\left( \widehat{2\pi \oint_{\partial\Omega} Q} \right) |S\rangle = \sum_{p \in \mathcal{P}} \log(2j_p + 1) |S\rangle \quad (3.29)$$

Usually in loop quantum gravity, we start with a geometric expression in terms of the Ashtekar variables  $A$  and  $E$  and apply a quantization procedure to produce an operator. Here we have the inverse problem: we have defined an operator and want to know whether it corresponds to a geometric expression. So far it is not clear whether such a geometric quantity  $Q$  exists, or what its form could be.

## 3.6 Weave states

One possibility for relating the entanglement entropy to the classical geometry of a manifold  $\Sigma$  is to construct a spin network state approximating the geometry, known as a weave state [52]. A weave state is a spin network state such that the eigenvalues of the area and volume operators approximate the classical volumes and areas of the associated surfaces. Although the original weave states were later found to have zero spatial volume, it was subsequently shown that it is possible to construct weave states for which both the area and volume operators approximate their classical values [53].

One procedure for constructing a random weave state in flat space is to randomly sprinkle points in  $\mathbb{R}^3$  at a fixed density  $\rho$  [54]. These points are taken to be the vertices of a graph  $\Gamma$ , and the edges of  $\Gamma$  correspond to the Delauney triangulation of the set of points. In a fixed region  $\Omega$  the expected number of points, and hence the expected quantum volume of the region, is proportional to the classical volume of  $\Omega$ . Similarly the number of intersections with a 2-dimensional surface  $\sigma$ , and hence the eigenvalue to the area operator, grows linearly with the area of  $\sigma$ .

For the statistical weave state the expected entanglement entropy is proportional to the number of intersections of the spin network with  $\partial\Omega$ , and hence proportional to the classical area of  $\partial\Omega$ . As we will see in chapter 5 this is a consequence of a general theorem of geometric probability theory.

# Chapter 4

## The second law

Any microscopic description of the Bekenstein-Hawking entropy should be able to account for the laws of black hole thermodynamics. In this chapter we will consider the analogue of the second law of thermodynamics for the entanglement entropy. Specifically, we will investigate conditions under which the entanglement entropy is non-decreasing in time.

We will consider the proposal due to Rafael Sorkin that increase of entanglement entropy is a consequence of the fact that a black hole horizon is a causal barrier [20]. An important defining feature of a black hole event horizon is that the evolution of the black hole exterior is independent of the state of the interior. Evolution maps of this form are called semicausal [55].

Let  $A$  and  $B$  be Hilbert spaces, and  $U$  be a unitary map  $U : A \otimes B \rightarrow A \otimes B$ . Let  $\mathcal{E}$  be the trace-preserving completely positive map  $\mathcal{E}(\rho) = U\rho U^*$ . The map  $\mathcal{E}$  is *semicausal*  $A \rightarrow B$  if there exists a trace-preserving completely positive map  $\mathcal{E}|_A$  such that

$$\mathrm{Tr}_B \circ \mathcal{E} = \mathcal{E}|_A \circ \mathrm{Tr}_B \quad (4.1)$$

This definition says that system  $A$  evolves autonomously from system  $B$ . Equivalently, it says that there is no signalling from  $B$  to  $A$ . We can think of system  $A$  as analogous to the black hole exterior, and system  $B$  as the black hole interior.

Sorkin's proposed proof of entropy increase rests on the following result due to Lindblad [56]. Let  $\mathcal{E}$  be any channel, and let  $\rho$  be a density matrix. Then

$$S(\mathcal{E}(\rho) \parallel \mathcal{E}(\sigma)) \leq S(\rho \parallel \sigma)$$

The quantity  $S(\rho \parallel \sigma)$  is the *quantum relative entropy of  $\rho$  with respect to  $\sigma$* , defined for  $\sigma > 0$  as

$$S(\rho \parallel \sigma) = \mathrm{Tr}(\rho[\log(\rho) - \log(\sigma)])$$

When  $\sigma$  does not have full support, the operator  $\log \sigma$  is not well defined. In this case it is still possible to define  $S(\rho \parallel \sigma)$  as a limit which diverges when  $\mathrm{supp}(\sigma) \cap \mathrm{supp}(\rho) \neq \{0\}$  [56].

In order to see how this leads to a condition for entropy increase, let  $\sigma$  be the maximally mixed state  $\sigma = \frac{1}{n}I$  so that

$$S(\rho||\sigma) = \text{Tr}\rho \log \rho - \text{Tr}\rho \log \frac{1}{n} = -S(\rho) + \log n$$

Now suppose the channel  $\mathcal{E}$  is *unital*, so that  $\mathcal{E}(I) = I$ . Then by Lindblad's theorem, we have

$$\begin{aligned} S(\mathcal{E}(\rho)||\mathcal{E}(\sigma)) &\leq S(\rho||\sigma) \\ -S(\mathcal{E}(\rho)) + \log n &\leq -S(\rho) + \log n \\ S(\mathcal{E}(\rho)) &\geq S(\rho) \end{aligned}$$

Therefore a channel  $\mathcal{E}$  leads to an increase of entropy for all initial states if and only if  $\mathcal{E}$  is unital.

The entropy of entanglement of the system  $AB$  is the von Neumann entropy of system  $A$ , so increase of entanglement entropy is equivalent to increase of entropy for system  $A$ . By the previous result, this is equivalent to the statement that  $\mathcal{E}|_A$  is unital. To see that this is the case, we simply apply the definition of the semicausal map  $\mathcal{E}$  (4.1) to the maximally mixed state on  $A \otimes B$ :

$$\begin{aligned} \mathcal{E}|_A \circ \text{Tr}_B \left( \frac{1}{n_A n_B} I_A \otimes I_B \right) &= \text{Tr}_B \circ \mathcal{E} \left( \frac{1}{n_A n_B} I_A \otimes I_B \right) \\ \mathcal{E}|_A \left( \frac{1}{n_A} I_A \right) &= \text{Tr}_B \left( \frac{1}{n_A n_B} I_A \otimes I_B \right) \\ \mathcal{E}|_A \left( \frac{1}{n_A} I_A \right) &= \frac{1}{n_A} I_A \end{aligned}$$

It follows that if  $U$  is a finite-dimensional unitary matrix such that its associated channel  $\mathcal{E}$  is semicausal, then the entanglement entropy of any pure state of  $AB$  is non-decreasing under the action of  $U$ .

In finite dimensional Hilbert spaces, the above argument in fact holds trivially. This is because in finite dimensions all unitary semicausal maps  $A \rightarrow B$  are also semicausal  $B \rightarrow A$  ([55], theorem 7). Such a unitary operator is called fully causal. Any fully causal unitary map  $U$  factors as  $U = U_A \otimes U_B$ . It follows that the entropy of entanglement neither increases nor decreases, but is exactly preserved by the evolution.

In the next section we consider the case where  $A$  and  $B$  are infinite dimensional separable Hilbert spaces. Specifically we will determine whether the two results above - that all unitary semicausal operators are fully causal, and that entanglement entropy increases under semicausal evolution - continue to hold in the infinite-dimensional setting.

## 4.1 Infinite dimensions

To understand why semicausal operations do not exist in finite dimensional Hilbert spaces, we can appeal to a classification of semicausal maps for tripartite finite dimensional systems [57]. In this model we consider operations on a system  $ABC$  which do not allow signalling from  $B$  to  $A$ . All of these maps may be described by an interaction of  $A$  with  $C$  followed by an interaction of  $C$  with  $B$ . In other words, Alice prepares a qubit, sends the qubit to Bob, who then interacts with it. Maps of this form are called semilocalizable.

To see why the bipartite case cannot be semicausal, we see that in order to send a single qubit, a piece of system  $A$  must be transferred to  $B$ . For this to happen  $\dim A$  must decrease by a factor of two, and  $\dim B$  must increase by a factor of two. In an infinite dimensional Hilbert space it is possible to double the dimension without changing the dimension of the Hilbert space. This is the subject of the famous Hilbert's hotel paradox, whose content is that an infinite set can be put in bijection with two copies of itself. This idea motivates the construction of the following unitary semicausal map.

Let  $A = \ell^2(\mathbb{N})$  and  $B = \ell^2(\mathbb{N})$  and define  $U$  by

$$U = \sum_{m,n=0}^{\infty} (|m\rangle|2n\rangle\langle 2m| \langle n| + |m\rangle|2n+1\rangle\langle 2m+1| \langle n|)$$

It can be easily verified that  $U$  is semicausal  $A \rightarrow B$ .

The channel  $\mathcal{E}|_A$  is described in terms of Kraus operators as

$$\mathcal{E}|_A(\rho) = E_0^\dagger \rho E_0 + E_1^\dagger \rho E_1$$

where

$$E_0 = \sum_{n=0}^{\infty} |2n\rangle\langle n|$$

$$E_1 = \sum_{n=0}^{\infty} |2n+1\rangle\langle n|$$

Thus we have shown that unlike the finite-dimensional case, it is possible to have a unitary causal map that is not fully causal. However, the increase of entropy no longer holds, which can be easily seen for the state  $\rho = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$

$$\mathcal{E}|_A(\rho) = |0\rangle\langle 0|$$

Thus the theorem that entropy is increasing in finite dimensional spaces does not hold for infinite-dimensional ones.

The reason entropy can decrease is that in this case the operator  $\mathcal{E}|_A$  is not unital

$$\mathcal{E}|_A(I_A) = E_0^\dagger E_0 + E_1^\dagger E_1 = I_A + I_A = 2I_A$$

Lindblad's theorem therefore gives the weaker inequality

$$\begin{aligned} S(\mathcal{E}(\rho) \parallel \mathcal{E}(I)) &\leq S(\rho \parallel I) \\ -S(\mathcal{E}(\rho)) - \log 2 &\leq -S(\rho) \\ S(\mathcal{E}(\rho)) &\geq S(\rho) - \log 2 \end{aligned}$$

Thus the entropy may decrease by at most one bit. For the map  $U$ , this inequality is saturated for the state  $\rho = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$ .

We have considered Sorkin's argument in two cases. In the case where the systems  $A$  and  $B$  are described by finite dimensional Hilbert spaces, the theorem holds trivially. When  $A$  and  $B$  are described by infinite-dimensional Hilbert spaces, the theorem no longer holds because there is no analogue of the maximally mixed state.

In the finite-dimensional case, the algebra of observables of system  $A$  is the algebra of all  $n \times n$  matrices, which is a von Neumann factor of type  $I_n$  [58]. In the infinite case, the algebra of observables is the algebra  $\mathcal{B}(\mathcal{H})$  of bounded operators on a separable Hilbert space  $\mathcal{H}$ , which is a von Neumann factor of type  $I_\infty$ . We could equally consider the case where the algebra of observables on the exterior of a black hole is a von Neumann factor of type II or III <sup>1</sup>.

Of particular interest is the type-II<sub>1</sub> factor, which in a sense is an intermediate case between a factor of type  $I_n$  and a factor of type  $I_\infty$ . An important property of II<sub>1</sub> factors is the existence of a unique maximally mixed state, a property which is important in the proof of entropy increase. The problem of formulating Sorkin's conjecture in the framework of more general von Neumann algebras is left as an area for future work.

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<sup>1</sup>The suggestion that Sorkin's conjecture may hold for type II von Neumann factors is due to Aron Wall, and was pointed out to me by Ted Jacobson.

# Chapter 5

## The area law

In many cases of physical interest, the entanglement entropy of the region  $\Omega$  is known to scale with the surface area of the boundary  $\partial\Omega$ . This empirical fact is sometimes called the area law for entanglement entropy. We have shown that the area law holds both for the vacuum state of a quantum field and for spin network states in loop quantum gravity. In this chapter we will investigate the conditions under which the area law holds exactly.

We will assume a quantum field theory on Euclidean space  $\Sigma = \mathbb{R}^3$  with a preferred state  $|\psi\rangle$  that is Euclidean invariant. For each  $\Omega \subset \Sigma$ , there is an associated entropy  $S(\Omega)$ . We wish to find necessary and sufficient conditions that

$$S(\Omega) = A(\partial\Omega) \quad \text{for all } \Omega \subset \Sigma$$

### 5.1 Valuations and intrinsic volumes

In order to understand when the entanglement entropy is proportional to area, it is useful to develop a characterization of area as a function of subsets of  $\mathbb{R}^3$ . For example, it is known that the volume is characterized as the unique Euclidean-invariant measure on  $\mathbb{R}^3$ . We will use a similar characterization of the area from the theory of geometric probability [59].

Let  $L$  be a collection of subsets of  $\Sigma$ . We say that  $L$  is a *lattice* if for every pair of subsets  $A, B \in L$  we also have  $A \cup B \in L$  and  $A \cap B \in L$ .

A function  $f : L \rightarrow \mathbb{R}$  is a *valuation* if it is zero on the empty set

$$f(\emptyset) = 0$$

and is *strongly additive*

$$f(A \cup B) = f(A) + f(B) - f(A \cap B) \tag{5.1}$$

This identity is also known as the inclusion-exclusion principle, and has a natural interpretation in terms of counting. Suppose we wish to count the elements of  $A \cup B$ . We can begin by adding the number of elements in  $A$  and the number of elements in  $B$ . The elements of  $A \cap B$  will have been counted twice, so we subtract this from the total. It is natural to think of a valuation as a continuous notion of cardinality.

The strong additivity condition is similar to the Carathéodory condition on a measure, which states that if  $B$  is a measurable set then

$$\mu(A) = \mu(A \cap B) + \mu(A \setminus B)$$

In fact the Carathéodory condition implies the valuation condition

$$\begin{aligned} \mu(A \cup B) &= \mu((A \cup B) \cap B) + \mu((A \cup B) \setminus B) \\ &= \mu(B) + \mu(A \setminus B) \\ &= \mu(B) + \mu(A) - \mu(A \cap B) \end{aligned}$$

Thus a signed measure is a special case of a valuation. As we will see, the converse is not true; there exist valuations which are not measures.

Let  $\mathcal{K}$  denote the lattice of *polyconvex* sets, consisting of all finite unions of compact, convex sets. The set  $\mathcal{K}$  is clearly a lattice, since it is closed under union and intersection. It is also metric space with the Hausdorff distance

$$\begin{aligned} d(A, B) &= \max \left( \sup_{a \in A} d(a, B), \sup_{a \in A} d(b, A) \right) \\ d(a, B) &= \inf_{b \in B} d(a, b) \end{aligned}$$

Two sets  $A$  and  $B$  are close in the Hausdorff distance if every point of  $A$  is close to a point of  $B$  and vice versa. We will say that a valuation is *continuous* if it is continuous in the topology induced by the Hausdorff metric.

A valuation  $f$  is *Euclidean-invariant* if  $f(A) = f(TA)$  for every Euclidean transformation  $T \in E(n)$  and  $A \in \mathcal{K}$ . An important theorem of measure theory is the characterization of the Lebesgue measure as the unique Euclidean-invariant measure on  $\mathbb{R}^n$ . The analogue of this theorem for valuations is *Hadwiger's theorem*:

The vector space of Euclidean-invariant continuous valuations on  $\mathcal{K}$  is  $n + 1$ -dimensional, and has a basis consisting of the *intrinsic volumes*  $\mu_0, \dots, \mu_n$ . The intrinsic volume  $\mu_k$  is homogeneous of degree  $k$ , meaning for every  $a > 0$ ,

$$\mu_k(a\Omega) = a^k \mu_k(\Omega) \tag{5.2}$$

Thus in three dimensions,  $\mu_3$  has the dimensions of volume,  $\mu_2$  has the dimensions of area,  $\mu_1$  has the dimensions of length and  $\mu_0$  is dimensionless. The proof of Hadwiger's theorem is elementary, but beyond the scope of this chapter [59, 60, 61].

In  $\mathbb{R}^3$ , the intrinsic volumes are as follows:



- $\mu_3(\Omega) = V(\Omega)$  is the volume of  $\Omega$ .
- $\mu_2(\Omega) = A(\partial\Omega)$  is the surface area of the boundary of  $\Omega$
- $\mu_1(\Omega)$  is the mean width of  $\Omega$ , defined as follows.

For a compact convex set  $\Omega$  containing the origin, define the *support function*

$$h_\Omega(v) = \max \{x \cdot v | x \in \Omega\}$$

For a unit vector  $v$ , this represents the distance from the origin to the closest plane which is orthogonal to  $v$  and tangent to  $\Omega$ . This gives the interpretation that for each unit vector  $v$  the quantity

$$h_\Omega(v) + h_\Omega(-v)$$

gives the width of the set  $\Omega$  as measured parallel to  $v$ . The *mean width* is obtained by averaging the width over all directions

$$B(\Omega) = \frac{1}{2\pi} \int_{S^2} h_k(v) dv$$

While the above definition applies only to convex sets, it can be shown that  $B = \frac{1}{2\pi}M$  where  $M$  is the integral mean curvature  $H$  of the boundary

$$B(\Omega) = \frac{1}{2\pi} \int_{\partial\Omega} H dA$$

This latter definition extends to all polyconvex sets.

- $\mu_0(\Omega) = \chi(\Omega)$  is the Euler characteristic. The Euler characteristic depends on the topology of  $\Omega$ , and is given by  $\chi = 2 - 2g$  where  $g$  is the topological genus of  $\Omega$ . By the Gauss-Bonnet theorem the Euler characteristic is proportional to the integral of the Gauss curvature  $K$  over the boundary.

$$\chi(\Omega) = \frac{1}{2\pi} \int_{\partial\Omega} K dA$$

Hadwiger's theorem establishes that a necessary condition for the area law is that the function  $S(\Omega)$  be a continuous Euclidean-invariant valuation. Before giving an interpretation of this condition, we will show that the valuation condition is also a sufficient condition for the area law.

Suppose that we consider a purely classical statistical field theory for which the Shannon entropy  $H(\Omega)$  satisfies the conditions of Hadwiger's theorem. Then it follows that the entropy must be proportional to the volume. This is because the Shannon entropy is *monotone*

$$\Omega \subseteq \Omega' \Rightarrow H(\Omega) \leq H(\Omega') \tag{5.3}$$

Since volume is the only monotone valuation, the Shannon entropy must be proportional to volume ([59], theorem 8.1.1). This leads to the usual volume scaling law for the entropy in classical thermodynamics.

In the case of a pure quantum state, the situation is quite different from the classical case. The quantum entropy does not satisfy the above monotonicity property (5.3). It does however satisfy the symmetry property

$$S(\Omega) = S(\overline{\Omega}) \tag{5.4}$$

Thus suppose  $S$  is a continuous Euclidean-invariant valuation. Then by Hadwiger's theorem  $S$  is of the form

$$S(\Omega) = \sum_{i=0}^3 \alpha_i \mu_i(\Omega) \tag{5.5}$$

Clearly the volume does not satisfy the symmetry property (5.4). Because the functions  $\{\mu_i\}_{i=0}^n$  are linearly independent,  $\alpha_3 = 0$ .

We will now show that properties of the entanglement entropy imply the only non-zero term in equation (5.5) is proportional to the area. To do this we appeal to another property of the entropy, the *positivity*

$$S(\Omega) \geq 0$$

Suppose that  $\alpha_0 < 0$ . Fix  $\Omega$  to be a surface of positive Euler characteristic, such as a sphere ( $\chi = 2$ ). Then for such a surface we can use the homogeneity property (5.2) to show that

$$\begin{aligned} \lim_{a \rightarrow 0} S(a\Omega) &= \lim_{a \rightarrow 0} \sum_{i=0}^3 \alpha_i \mu_i(a\Omega) \\ &= \lim_{a \rightarrow 0} \sum_{i=0}^3 \alpha_i a^i \mu_i(\Omega) \\ &= \alpha_0 \mu_0(\Omega) < 0 \end{aligned}$$

By continuity, there exists some  $a > 0$  for which  $S(a\Omega)$  is negative. This contradicts positivity, so we must have  $\alpha_0 \geq 0$ . Repeating this argument for a surface of negative Euler characteristic such as a double torus ( $\chi = -2$ ) yields  $\alpha_0 \leq 0$ . Combining these two properties, we see that  $\alpha_0 = 0$ . Repeating this argument for two surfaces of positive and negative total mean curvature,  $\alpha_1 = 0$ .

We therefore have the following result:

The area law in 3-dimensional Euclidean space holds for every convex set if and only if  $S$  is a Euclidean-invariant continuous convex valuation.

What remains to be understood is under which conditions will the entropy define a continuous valuation.

## 5.2 Strong additivity and the Markov property

Suppose we have a Euclidean-invariant state  $|\psi\rangle$ . We will assume that the entanglement entropy has been regulated so that  $S(\Omega)$  is finite and continuous. It is always the case that  $S(\emptyset) = 0$ , so the only condition requiring interpretation is the strong additivity condition (5.1).

Given two overlapping sets  $A$  and  $B$ , we can divide the Hilbert space of their union as

$$\begin{aligned}\mathcal{H}_{A \cup B} &= \mathcal{H}_X \otimes \mathcal{H}_Y \otimes \mathcal{H}_Z \\ X &= A \setminus B \quad Y = A \cap B \quad Z = B \setminus A\end{aligned}$$

We will use a notation in which concatenation of symbols corresponds to union of subsystems, so that we have the identifications  $XY = A$ ,  $YZ = B$  and  $XYZ = A \cup B$ .

The *conditional entropy* is defined as the quantity

$$S(X|Y) = S(XY) - S(Y)$$

The *conditional mutual information* is

$$\begin{aligned}I(X : Z|Y) &= S(X|Y) - S(X|YZ) \\ &= S(XY) - S(Y) - S(XYZ) + S(YZ) \\ &= S(A) + S(B) - S(A \cap B) - S(A \cup B)\end{aligned}$$

The *strong subadditivity* inequality states that the conditional mutual information is non-negative, which is equivalent to [62]

$$S(A \cup B) \leq S(A) + S(B) - S(A \cap B)$$

The strong additivity condition holds exactly when this inequality is saturated. The strong additivity condition is therefore equivalent to the vanishing of the conditional mutual information

$$I(X : Z|Y) = 0 \quad \text{for all } A, B \in \mathcal{K} \tag{5.6}$$

This equation says that conditioned on the state of  $A \cap B$ , the state of  $A \setminus B$  is independent of the state of  $B \setminus A$ .

This condition is analogous to the classical Markov property for random variables  $X, Y, Z$ , given by

$$p(X|YZ) = p(X|Y) \tag{5.7}$$

There is no object analogous to the conditional probability  $p(X|Y)$  for quantum systems. However the following are all equivalent:

$$\begin{aligned}p(X|YZ) &= p(X|Y) \\ H(X|YZ) &= H(X|Y) \\ H(XYZ) - H(YZ) &= H(XY) - H(Y)\end{aligned}$$

This last condition is analogous to the condition (5.6) with Shannon entropy in place of von Neumann entropy.

There are a number of equivalent characterizations of the Markov property. Ruskai showed that the Markov property is equivalent to the operator equation [63]

$$\log \rho_Y + \log \rho_{XYZ} = \log \rho_{XY} + \log \rho_{YZ} \quad (5.8)$$

Note that this has a similar form to the classical Markov property, since the following are equivalent

$$\begin{aligned} p(X|YZ) &= p(X|Y) \\ \log p(X|YZ) &= \log p(X|Y) \\ \log p(XYZ) - \log p(YZ) &= \log p(XY) - \log p(Y) \end{aligned}$$

Which resembles (5.8), with  $p(X)$  in place of  $\rho_X$ .

### 5.3 Quantum Markov networks

The quantum Markov property is a mathematical statement of conditional independence for a set of three systems. The strong additivity condition holds for all pairs of sets in  $\mathcal{K}$ , and describes a much more complex set of independence relations for a large number of quantum systems. To study systems of this kind, Leifer and Poulin introduced quantum Markov networks [64]. Quantum Markov networks allow conditional independence of systems to be represented in a graphical way.

A *quantum Markov network* is pair  $(G, \rho)$  where  $G = (V, E)$  is an abstract graph with vertices labelled by Hilbert spaces  $\mathcal{H}_v$ , and  $\rho$  is a state in  $\otimes_{v \in V} \mathcal{H}_v$  such that for every vertex  $v$

$$I(\{v\} : V - n(v) - \{v\} | n(v)) = 0$$

Where  $n(v)$  is the set of neighbours of  $v$ .

As a simple example, consider a triple of systems  $X, Y, Z$  such that  $I(X : Z|Y) = 0$  as in the previous section. This is represented by a graph with vertices  $(X, Y, Z)$  and edges  $(X, Y)$  and  $(Y, Z)$ .

The lattice  $\mathcal{K}$  is infinite, but we can consider a finite sublattice by decomposing  $\Sigma$  into a finite number of closed tetrahedra. Let  $\mathcal{T}$  be the collection of all tetrahedra, their closed faces, edges and vertices and arbitrary unions of these. Then  $\mathcal{T}$  is closed under union and intersection and hence forms a finite sublattice of  $\mathcal{K}$ .

We can now consider the entropy function  $S$  defined on the lattice  $\mathcal{T}$ . An initial problem is that  $S$  is only defined for tetrahedra, and unions of tetrahedra. In order to define  $S$  for a face  $F$  that is the intersection of tetrahedra  $T_1$  and  $T_2$ , we define

$$S(F) = S(T_1) + S(T_2) - S(T_1 \cup T_2)$$

In other words, whenever  $S$  is not defined, we define it by the requirement of strong additivity. We can then appeal to Groemer's integral theorem, which ensures that the valuation  $S$  defined only on tetrahedra extends uniquely to a valuation on the lattice  $\mathcal{T}$  [59].

For each such decomposition of  $\Sigma$  into tetrahedra, there is an associated graph dual  $G_{\mathcal{T}}$ . We define the vertex set  $V(G_{\mathcal{T}})$  to be the set of all tetrahedra in  $\mathcal{T}$ . The edge set  $E(G_{\mathcal{T}})$  is defined as the set of all pairs  $(T_1, T_2)$  such that  $T_1$  and  $T_2$  share a common face. To each vertex  $v$  of  $G_{\mathcal{T}}$  we can define the Hilbert space  $\mathcal{H}_v$  to be the Hilbert space  $\mathcal{H}_T$  of the corresponding tetrahedron  $T$ . Because the tetrahedra cover all of  $\Sigma$  and the intersection of any two tetrahedra has measure zero, we have the identification

$$\mathcal{H}_{\Sigma} = \bigotimes_T \mathcal{H}_T = \bigotimes_v \mathcal{H}_v$$

Thus given a decomposition  $\mathcal{T}$  of the manifold  $\Sigma$  with a state  $\rho \in \mathcal{H}_{\Sigma}$ , there is a natural choice of graph  $G_{\mathcal{T}}$  and a state  $\rho \in \bigotimes_v \mathcal{H}_v$ .

We can now show that if  $\rho$  satisfies strong additivity, then  $(G, \rho)$  is a quantum Markov network.

$$\begin{aligned} I(\{x\} : V - n(x) - \{x\} | n(x)) &= S(V - n(x) - \{x\} | n) - S(V - n(x) - \{x\} | \{x\} \cup n(x)) \\ &= S(V - \{x\}) - S(n(x)) - S(V) + S(\{x\} \cup n(x)) \\ &= S(A) - S(A \cap B) - S(A \cup B) + S(B) \\ &= 0 \end{aligned}$$

Where we have defined  $A = \{x\} \cup n(x)$  and  $B = V - \{x\}$ .

We leave for future work the question of whether the converse also holds. That is, whether  $G_{\mathcal{T}}$  being a quantum Markov network implies that the entropy function extends uniquely to a valuation on the lattice  $\mathcal{T}$ .

## 5.4 Examples

We have constructed a number of states satisfying some of the conditions required for an exact area law: continuity, strong additivity, and Euclidean invariance. As we saw in chapter 2, the vacuum state of a quantum scalar field in flat space satisfies the strong additivity and is Euclidean invariant. However it does not satisfy the continuity condition, because the entropy is divergent.

In chapter 3, we showed that when  $|\psi\rangle$  is a spin network state the entropy  $S(\Omega)$  is a sum of intersections between the spin network and the boundary  $\partial\Omega$ . It therefore satisfies the strong additivity condition, and is finite. Because the spin networks are discrete, the entropy is not continuous or Euclidean invariant. It is possible to define a statistical weave state as a Euclidean-invariant ensemble of

spin network states, as described in section 3.6. In this case the expectation value of the entanglement entropy satisfies all the conditions for a Euclidean-invariant valuation, and therefore satisfies the area law.

In the one dimensional case we can define a state whose entropy satisfies all conditions of Hadwiger's theorem. In the one-dimensional Euclidean space  $\mathbb{R}$ , polyconvex sets consist of unions of closed intervals. Let  $\Omega$  be a polyconvex set,

$$\Omega = [a_1, b_1] \cup \dots \cup [a_n, b_n]$$

There are only two continuous translation-invariant valuations on the real line, the number of connected components and the total length

$$\begin{aligned} \mu_0(\Omega) &= n \\ \mu_1(\Omega) &= \sum_{i=1}^n b_i - a_i \end{aligned}$$

Since  $\mu_1$  does not satisfy the symmetry property, the entropy of a state satisfying strong additivity must be proportional to  $\mu_0$ .

We will consider the Hilbert space of generalized connections on the real line, as described in chapter 3. A natural choice of state is the Wilson loop state

$$\psi(A) = \text{Tr} \mathcal{P} \exp \left( \int_{-\infty}^{\infty} A(x) dx \right)$$

As we showed in chapter 3, the entanglement entropy is exactly one bit for every endpoint, which is two bits for each connected component

$$S(\Omega) = 2 \log 2 \mu_0(\Omega)$$

Thus we have an exact area law, where in one dimension the boundary of a polyconvex set is a finite number of points, and the area is simply the number of boundary points.

We have given several examples of states satisfying some of the conditions required for an exact area law. In the 1-dimensional real line, we have constructed a state satisfying all three conditions, so that the area law is exactly satisfied. It is not known whether it is possible to construct a state satisfying all three conditions in two or more dimensions. We consider this an important problem for future work.

# Chapter 6

## Conclusion and future work

The entanglement entropy provides a compelling solution to the problem of giving a microscopic derivation of the Bekenstein-Hawking entropy. A priori, the entanglement entropy would seem to have no relation to gravitational physics. Remarkably, when quantum effects are taken into account the entanglement entropy is found to obey exactly the Bekenstein-Hawking area law in terms of the renormalized gravitational constant  $G_R$ ,

$$S = \frac{A}{4} \frac{c^3}{\hbar G_R}$$

It follows that in order to describe a universe with a finite gravitational constant  $G$ , the entanglement entropy between two regions must be finite. This reinforces both the necessity of a physical ultraviolet cutoff in nature, and the importance of information theory as a tool for understanding this cutoff.

In loop quantum gravity the continuum spacetime of general relativity is replaced with a discrete spin network, which has a finite entanglement entropy. Each edge of the spin network acts like a maximally entangled state, carrying an entanglement entropy equal to the logarithm of the dimension of its associated representation. The standard approach to black hole entropy in loop quantum gravity, based on counting states of isolated horizons, emerges as a special case of our entanglement entropy calculation. The latter calculation has many advantages; it is simpler, applies to all types of horizons and can be extended to the more general class of degenerate spin network states.

Although the entanglement entropy in loop quantum gravity is finite, the continuous spacetime manifold is replaced by a discrete structure. An important question about the entanglement entropy is its relation to the geometry of space in the continuum limit. This is related to the general problem in loop quantum gravity of understanding how continuum physics arises from a discrete structure. Despite its fundamental importance, little progress has been made on this difficult issue.

An important area for future work is to realize Sorkin's proposal for a proof of the increase of entanglement entropy as a consequence of causality. We have shown that the conjecture is either trivial or false when the algebra of operators

on the black hole exterior is described by a von Neumann factor of type I. It may however be possible to find an analogue of the conjecture for a factor of type II or III. In particular the type  $II_1$  factor has several properties that make it a promising candidate.

Our hope is that it will be possible to define a continuous theory for which the entanglement entropy satisfies the Bekenstein-Hawking area law exactly. To this end we have considered a model of quantum theory in Euclidean space and studied properties that lead to an exact area law. The area law is found to be equivalent to strong additivity of the entropy, which has a straightforward information-theoretic interpretation in terms of conditional independence of subsystems. As a next step we would like to use this characterization to define a theory satisfying the exact area law.



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