Fakultät für Mathematik und Informatik
der FernUniversität in Hagen

Masterarbeit

im Lehrgebiet Stochastik und Mathematische Physik

1D Rényi Entanglement Entropy of Free Relativistic Fermions

von

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Juli 2022

Prüfer: Univ.-Prof. Dr. Wolfgang Spitzer

To Laura
To my family

Acknowledgements

I would like to thank Prof. Dr. Spitzer for his always friendly and supportive supervision, for many constructive discussions especially regarding the entanglement coefficient, for the proof of Theorem 3.8.2 and for suggesting several generalizations and refinements of the results established in this Thesis.

Furthermore, I would like to express my gratitude to Prof. Giancarlo Maero (Università degli Studi di Milano, Italy) who found the time to critically review my manuscript with unbiased mind and provided me with valuable feedback, especially regarding the physics content. And, of course, for the good old times.

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Chapter 1

Introduction

The first theoretical concept of correlation as a property that uniquely characterizes quantum-mechanical systems was exemplified as a thought experiment by the famous Einstein-Podolsky-Rosen paradox [EPR35]. In response to this, Schrödinger recognized that there exist global states of a composite system that cannot be written as a product of the states of individual subsystems, even though the interaction among them has completely ceased [Sch35], and he introduced the term entanglement to describe this phenomenon. The first quantitative approach to entanglement was provided by the Bell inequalities [Bel64].

More recently, entanglement became a theory of enormous success, and this progress was especially driven by the research in quantum information, communication and cryptography (cf. e.g. Ref. [Lie14]), although the concept of entanglement is ubiquitous in modern Physics, and it also applies e.g. to quantum field theories [Wit18], condensed matter [Laf16], quantum gravity [KTPP20], black hole theory [BKLS86] just to mention a few research areas. Quantum entanglement even became eventually accessible to experiments, which confirmed the theoretical predictions (cf. e.g. the review paper [HHHH09] for a discussion of experimental works on the subject).

Because of its profound theoretical and practical significance, a rigorous mathematical treatment of the entanglement of systems of physical interest is essential to gain deeper insight into this complex and elusive concept.

Longo and Xu [LX17], for instance, provided the first mathematically rigorous computation of the mutual information of a system of free fermions, and they proved that this quantity is finite. Their approach lies on information-theoretical foundations and they exploit an integral representation of the Shannon entropy,

$$H_1(t) := -t\ln t - (1-t)\ln(1-t) = -\int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda \left(\left(\lambda - \frac{1}{2}\right)(R_t(\lambda) - R_t(-\lambda)) - \frac{2\lambda}{\lambda + \frac{1}{2}} \right), \tag{1.1}$$

valid for $t \in (0,1)$, where $R_t(\pm\lambda) := \frac{1}{t-\frac{1}{2}\pm\lambda}$. Eq. 1.1 had already been previously proposed in Ref. [CH09b]. The definition domain of H_1 is usually extended by continuity to the closed interval $[0,1]$, setting $H_1(0) = H_1(1) = 0$.

In a quantum-mechanical picture, the correlations of a relativistic system of quasi-free fermions are described by a suitable one-particle density operator $0 \leq D \leq 1$ [BR02]. Employing the Spectral Theorem of linear self-adjoint operators, operator D may be inserted into Eq. 1.1, and this yields the von Neumann entropy $S_1(D) := \operatorname{tr} H_1(D)$ [Neu28], that quantifies the degree of information contained in the quantum state D, in the language of information theory.

The entanglement entropy is a measure of quantum entanglement. Among several possible definitions (cf. e.g. the review [AF09, Nis18]), we take here the mutual entropy, in agreement with Longo and Xu. Splitting a quantum mechanical system of N free fermions described by one-particle density D into two subsystems of $n_1 < N$ and $n_2 = N - n_1$ fermions (with $n_1 \neq 0$) described by one-particle density operators D_1 and D_2 respectively, we define the bipartite entanglement entropy as the number

$$S_1(D_1) + S_1(D_2) - S_1(D) \tag{1.2}$$

that is always non-negative as may be deduced from the strong subadditivity property of the von Neumann entropy S_1 [CC09]. The mutual entropy quantifies the information about subsystem 2 that may be obtained from subsystem 1.

In this framework, the terms $R_D(\pm\lambda)$ in Eq. 1.1 represent by definition the resolvent of the density operator D evaluated in the points $\frac{1}{2} \mp \lambda$. Therefore, a central problem in the present treatment is the determination of the resolvent of D, and this depends in general on the choice of the system's definition domain. We choose a quantum mechanical system of free relativistic fermions distributed either on a finite number of bounded intervals in $\mathbb{R}$ or on finitely many intervals stretched on a Jordan curve of constant curvature in the plane $\mathbb{R}^2$ since in both cases an explicit expression for the resolvent R_D follows from classical results from the theory of singular integrals [Mus53, Mik64].

In the present Thesis, we draw inspiration from Longo and Xu's work, and we aim at a generalization of their results. From an information-theoretical standpoint, we assume that the underlying system is described by the Rényi entropy [Rén61]

$$H_\alpha : [0,1] \to \mathbb{R}^+, \qquad t \mapsto \frac{1}{1-\alpha} \ln(t^\alpha + (1-t)^\alpha) \tag{1.3}$$

with $\alpha \in (0,1)$. One of the reasons for the interest in Eq. 1.3 is that, apart from the well-known Shannon entropy, the Rényi entropy is the only alternative entropy form that satisfies the additivity property.

We define the Rényi entanglement entropy again as a mutual entropy, analogously to Eq. 1.2, replacing $S_1(D)$ by $S_\alpha(D) := \operatorname{tr} H_\alpha(D)$, with the help of the Spectral Theorem. Although it was pointed out that the Rényi mutual entropy may become negative for some values of the index α [AGS12, Nis18], we prove that for $\alpha \in (0,1)$ it is always non-negative, and it may be therefore employed as a legitimate measure of entanglement. Moreover, the Rényi mutual entropy is known to satisfy the area law, even at finite temperature [CC09], which is an important scaling property of the entanglement entropy [ECP10]. This fact corroborates our choice of the mutual entropy.

The central idea in this Thesis is to provide a suitable integral representation of the Rényi entropy that is qualitatively similar to Eq. 1.1. Especially, we must be careful that, even in this more complicated case, the resolvent R_D of the density operator appears in linear terms only. Obviously, the simple linear factor $\lambda - \frac{1}{2}$ in Eq. 1.1 is replaced by a far more complicated function of λ, but apart from this, the original Longo and Xu's method still works here.

To this aim, we employ the Nevanlinna-Herglotz canonical integral representation of the Rényi function 1.3 extended by analytic continuation to a suitable subset of the complex plane. The Nevanlinna-Herglotz theory (cf. e.g. Refs. [Ges17, Don74]) applies to analytic self-maps on the upper, or equivalently on the lower complex half-plane. We shall see that the complex Rényi entropy function can be written in terms of Nevanlinna-Herglotz functions, at least for Rényi indices restricted to the interval $\alpha \in (0,1)$.

The $\alpha \in (0,1)$ interval upon which we mainly focus in this Thesis is interesting, since it contains the $\alpha = \frac{1}{2}$ special case, which represents the logarithmic negativity entanglement measure [AF09].

Moreover, the important special cases of the Hartley entropy and Shannon entropy are also addressable through the $\alpha \downarrow 0$ and $\alpha \uparrow 1$ limit, respectively.

The Nevanlinna-Herglotz representation allows us to extend Longo and Xu's treatment of entanglement to the more general case of the underlying Rényi entropy and our final analytical result yields the von Neumann entanglement entropy as a special case. Apart from geometrical terms describing the two partitions of the fermionic system, and the multiplicative factor N that indicates the number of fermions in the system, our formula for the Rényi entanglement entropy entails an integral of a function depending on α. The latter integral fully describes the entropy form chosen to characterize the system.

The $(1, +\infty)$ interval of the Rényi index is also of interest for applications in Physics and cryptography, as it contains the important special cases $\alpha = 2$ and $\alpha \to +\infty$, known respectively as collision entropy [BPP12] and min-entropy [VV14]. However, we must note here that the Nevanlinna-Herglotz representation fails whenever $\alpha > 1$, since the power function $t \mapsto t^\alpha$ that enters in Def. 1.3, extended to the complex plane, is not even a self-map in the upper complex half-plane in this case, and therefore we cannot employ our method here. To cope with this issue, we sketch another more general method based on the Cauchy integral that applies to every positive real value of the Rényi index, at the cost of a much more complicated expression for the entanglement entropy, which makes use of a complex line integral.

The latter method may be also applied to other generalized entropy forms, and we demonstrate its flexibility shortly discussing exemplarily an application to the non-extensive entropy [GMT04].

Finally, we conclude the Thesis with a brief discussion on the entanglement entropy of a system of free fermions distributed on a discrete lattice $\mathbb{Z}$. Our approach is to work with a suitable discretized version of the Hilbert operator, which may be readily employed to calculate its resolvent numerically.

Chapter 2

Integral Representation of the Rényi Entropy

In this Chapter we introduce the Rényi entropy function, that was postulated in an information-theoretical context as a generalization of the Shannon entropy, and we seek a suitable integral representation for it employing the Nevanlinna-Herglotz theory of analytic self-maps in the upper complex half-plane.

The advantage of this integral representation is that the independent variable of the function only appears in the denominator of a simple rational integrand. As we shall see in Chapter 3, this form is suitable to express the fermionic Rényi entanglement entropy in the general framework of the von Neumann algebraic formalism.

To fix some basic convention, in this Thesis we shall denote by $\Pi_\pm := \{z \in \mathbb{C} | \pm \mathrm{Im} z > 0\}$ the open upper and lower complex half-planes respectively with the real line removed, and by $\overline{\Pi}_\pm$ their closure.

Furthermore, for any complex number $z \in \mathbb{C} \setminus \{0\}$, we adhere to the following representation in polar coordinates:

$$\mathbb{C} \setminus \{0\} \to \mathbb{R}^+ \times (-\pi, \pi], \qquad z \mapsto (|z|, \arg(z)) \tag{2.1}$$

where $\mathbb{R}^+ := (0, +\infty)$ and

$$|z| := \sqrt{(\mathrm{Re} z)^2 + (\mathrm{Im} z)^2}, \qquad \arg(z) := \begin{cases} \arccos \frac{\mathrm{Re} z}{|z|} & \text{if } \mathrm{Im} z \geq 0 \\ -\arccos \frac{\mathrm{Re} z}{|z|} & \text{if } \mathrm{Im} z < 0. \end{cases} \tag{2.2}$$

2.1 The Nevanlinna-Herglotz Integral Representation

We start with the following (cf. e.g. Ref. [Hia10]):

Definition 2.1.1 (Nevanlinna-Herglotz function[1]). A function $m : \Pi_+ \to \mathbb{C}$ is called Nevanlinna-Herglotz function (NH function in short), if m is analytic on Π_+ and is a self-map, i.e. its range satisfies the property

$$m(\Pi_+) \subseteq \overline{\Pi}_+. \tag{2.3}$$

Moreover, we denote the set of all NH functions as $\mathcal{N}$.

[1] Also known as Pick function in the mathematical literature.

By the Open-Mapping Theorem, if $m \in \mathcal{N}$ and m is not constant, then Eq. 2.3 reduces to $m(\Pi_+) \subset \Pi_+$ automatically.

As customary in the mathematical literature, we always assume that any Nevanlinna-Herglotz function m defined on Π_+ is implicitly extended to the lower complex half-plane Π_- by reflection about the real axis, namely:

$$m(z) := \overline{m(\overline{z})}$$

whenever $z \in \Pi_-$. A further extension of m to either the whole real line $\mathbb{R}$ or a subset of $\mathbb{R}$ will be addressed separately for each Nevanlinna-Herglotz function of interest in Sections 2.2 and 2.3.

From Def. 2.1.1 we derive a few elementary properties that we shall repeatedly employ in our treatment of the Rényi entropy.

Proposition 2.1.1 (Properties of $\mathcal{N}$)**.** *Let $m_1, m_2, m \in \mathcal{N}$ be NH-functions. Then they satisfy:*

1. *$r_1 m_1 + r_2 m_2 \in \mathcal{N}$, for $r_1, r_2 \in \mathbb{R}^+$, i.e. the set $\mathcal{N}$ is a convex cone;*
2. *if m_1 is non-constant, then $m_2 \circ m_1 \in \mathcal{N}$, i.e. the set $\mathcal{N}$ is closed under function composition;*
3. *$(\Pi_+ \to \mathbb{C}, z \mapsto -1/z) \in \mathcal{N}$, and this implies $-1/m \in \mathcal{N}$ by property 2.*

The central result of the Nevanlinna-Herglotz theory is that any NH function may be uniquely represented in integral form [Don74, Hia10, Ges17].

Theorem 2.1.2 (Nevanlinna-Herglotz integral representation)**.** *Any NH function m admits a unique canonical representation of the form:*

$$m(z) = Az + B + \int_{\mathbb{R}} \mathrm{d}\mu(\lambda) \left(\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right), \qquad \forall z \in \Pi_+ \tag{2.4}$$

where $A, B \in \mathbb{R}$, $A \geq 0$ and μ is a positive finite Borel measure on $\mathbb{R}$, i.e. a measure defined on the Borel σ-algebra $\mathcal{B}$ on the real axis and satisfying the relation $\mu(U) < +\infty$ on any bounded set $U \in \mathcal{B}$. Additionally, the measure μ satisfies the condition $\int_{\mathbb{R}} \mathrm{d}\mu(\lambda)\, (\lambda^2 + 1)^{-1} < +\infty$. Conversely, any function that may be cast in form 2.4 is a NH function.

For our purposes, the most significant property of the Nevanlinna-Herglotz representation is that the independent variable z only appears as an argument of a rational function of first order in the integral equation 2.4. We shall see in Chapter 3 that this fact is linked to the concept of the resolvent of a density operator in a quantum-mechanical framework.

The parameters A and B in Theorem 2.1.2 may be derived explicitly [Don74, Hia10].

Lemma 2.1.3. *For the canonical integral representation 2.4 of a NH function $m \in \mathcal{N}$, the following equalities hold:*

$$A = \lim_{\varepsilon \uparrow \infty} \frac{m(i\varepsilon)}{i\varepsilon} \geq 0, \tag{2.5}$$

$$B = \operatorname{Re} m(i). \tag{2.6}$$

Like any Borel measure on the real line $\mathbb{R}$, the measure μ in the Nevanlinna-Herglotz canonical integral representation 2.4 may be generated by a monotone increasing, left-continuous function $F_\mu : \mathbb{R} \to \mathbb{R}$, such that $\mu([a, b[) = F_\mu(b) - F_\mu(a)$ for any $a, b \in \mathbb{R}$, $a < b$ (cf. e.g. Ref. [Bau92], Theorem 6.5), where F_μ is uniquely defined up to an additive constant.

We fix the arbitrary additive constant with the convention:

$$F_\mu(0) = 0, \tag{2.7}$$

and we define the value of F_μ in any real point $\lambda \in \mathbb{R}$ as:

$$F_\mu(\lambda) = \frac{1}{2}(F_\mu(\lambda + 0) + F_\mu(\lambda - 0)), \tag{2.8}$$

to cope with possible discontinuities[2].

Following again Ref. [Don74], we obtain an explicit expression for F_μ.

Lemma 2.1.4. *The generating function F_μ of the measure μ in the Nevanlinna-Herglotz integral representation 2.4, under our conventions 2.7 and 2.8, satisfies:*

$$F_\mu(b) - F_\mu(a) = \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_a^b \mathrm{d}\lambda \, \mathrm{Im}\, m(\lambda + i\varepsilon)$$

for any finite open interval $(a, b) \subset \mathbb{R}$.

In view of Lemma 2.1.4, we may interpret the integral in Eq. 2.4 as a Stieltjes integral (cf. Ref. [Bau92]).

2.2 Nevanlinna-Herglotz Integral Representation of Elementary Functions

2.2.1 The Logarithm Function

We consider the principal branch of the logarithm function upon $\mathbb{C}$ with cut along the negative real semiaxis,

$$\ln : \mathbb{C} \setminus \{z \in \mathbb{C} | \, \mathrm{Re}z \leq 0, \mathrm{Im}z = 0\} \to \mathbb{C}, \qquad z = re^{i\phi} \mapsto \ln z := \ln r + i\phi, \tag{2.9}$$

where $r = |z|$ and $\phi = \arg(z)$.

Theorem 2.2.1. *The principal branch of the complex logarithm is a NH function and admits the unique Nevanlinna-Herglotz canonical integral representation:*

$$\ln z = \int_{-\infty}^{0} \mathrm{d}\lambda \left(\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right). \tag{2.10}$$

Proof. Although the claim is known from the literature (cf. e.g. Ref. [Don74]), we provide here a short explicit proof.

Any complex number in the upper complex half-plane Π_+ may be written in polar coordinates (cf. Eqs. 2.1 and 2.2) as $z = re^{i\phi}$, where $r > 0$ and $0 < \phi < \pi$. In such case, by definition 2.9, the image of z under the logarithm lies in Π_+ as well. In fact

$$\ln(re^{i\phi}) = \ln r + i\phi \in \Pi_+,$$

which yields $\ln \Pi_+ \subseteq \Pi_+$. Moreover, ln is analytic on Π_+. Therefore, it is a NH-function and admits a unique canonical integral representation of the form 2.4.

From Lemma 2.1.3, it follows:

$$A = \lim_{\varepsilon \uparrow \infty} \frac{\ln i\varepsilon}{i\varepsilon} = \lim_{\varepsilon \uparrow \infty} \frac{\ln \varepsilon + i\frac{\pi}{2}}{i\varepsilon} = 0 \tag{2.11}$$

[2] We use here as customary the shorthand notation $F_\mu(\lambda \pm 0) := \lim_{\varepsilon \downarrow 0} F(\lambda \pm \varepsilon)$.

and

$$B = \mathrm{Re} \ln i = \mathrm{Re}\, i\frac{\pi}{2} = 0. \tag{2.12}$$

We now observe that:

$$\ln(\lambda \pm i\varepsilon) = \ln\sqrt{\lambda^2 + \varepsilon^2} \pm i \arccos\frac{\lambda}{\sqrt{\lambda^2 + \varepsilon^2}},$$

as well as:

$$\lim_{\varepsilon \downarrow 0} \ln(\lambda \pm i\varepsilon) = \begin{cases} \ln\lambda & \text{if } \lambda > 0 \\ \ln|\lambda| \pm i\pi & \text{if } \lambda < 0, \end{cases} \tag{2.13}$$

whence, by Eq. 2.7, Theorem 2.1.4, Lebesgue's Dominated Convergence Theorem and Eq. 2.13 we get:

$$\begin{aligned} F_\mu(\lambda + 0) &= F_\mu(\lambda + 0) - F_\mu(0) \\ &= \frac{1}{\pi} \lim_{\eta \downarrow 0} \lim_{\varepsilon \downarrow 0} \int_0^{\lambda+\eta} \mathrm{d}x \, \mathrm{Im} \ln(x + i\varepsilon) \\ &= \frac{1}{\pi} \lim_{\eta \downarrow 0} \int_0^{\lambda+\eta} \mathrm{d}x \, \mathrm{Im} \lim_{\varepsilon \downarrow 0} \ln(x + i\varepsilon) \\ &= \begin{cases} 0 & \text{if } \lambda > 0 \\ \lambda & \text{if } \lambda < 0. \end{cases} \end{aligned} \tag{2.14}$$

Analogously to Eq. 2.14, we also conclude that $F_\mu(\lambda - 0) = F_\mu(\lambda + 0)$. At the discontinuity point $\lambda = 0$ this yields, according to the convention established in Eq. 2.8:

$$F_\mu(\lambda) = \begin{cases} 0 & \text{if } \lambda > 0 \\ \frac{\lambda}{2} & \text{if } \lambda = 0 \\ \lambda & \text{if } \lambda < 0. \end{cases} \tag{2.15}$$

The function $F_\mu(\lambda)$ above generates the measure in the Nevanlinna-Herglotz integral representation of the logarithm function.

Claim 2.10 follows from Eqs. 2.11, 2.12, 2.15 and Theorem 2.1.2 since the function $F_\mu(\lambda)$ in Eq. 2.15 is differentiable for $\lambda < 0$. □

2.2.2 The Power Function

Analogously to our treatment in the previous Section, we define the principal branch of the complex power function with exponent $\alpha \in (0, 1)$:

$$\mathbb{C} \setminus \{z \in \mathbb{C} | \, \mathrm{Re} z \leq 0, \mathrm{Im} z = 0\} \to \mathbb{C}, \qquad z \mapsto z^\alpha := \exp(\alpha \ln z)$$

where ln represents the principal branch of the logarithm function from 2.9 and, as usual, $r = |z|$ and $\phi = \arg(z)$.

Theorem 2.2.2. *The principal branch of the complex power function with exponent $\alpha \in (0, 1)$ is a NH function and admits the unique Nevanlinna-Herglotz canonical integral representation:*

$$z^\alpha = \cos\alpha\frac{\pi}{2} + \frac{\sin\alpha\pi}{\pi} \int_{-\infty}^{0} \mathrm{d}\lambda \, |\lambda|^\alpha \left(\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right). \tag{2.16}$$

Proof. As in the case of the logarithm function, the present claim is known from the literature (cf. e.g. Ref. [Don74]). Nevertheless, we provide here an explicit proof.

For any number $z = re^{i\phi} \in \Pi_+$ (i.e. $r > 0$ and $0 < \phi < \pi$), we get $z^\alpha = \exp(\alpha \ln z) = \exp(\alpha(\ln r + i\phi)) = r^\alpha(\cos\alpha\phi + i\sin\alpha\phi)$. Since $\phi \in (0,\pi)$ and $\alpha \in (0,1)$, it follows $\alpha\phi \in (0,\pi)$ and this implies that $\sin\alpha\phi \in (0,1]$, i.e. $r^\alpha \sin\alpha\phi$ is always a strictly positive number. As a consequence, the image of Π_+ under the power function of exponent α lies in Π_+. Moreover, the function z^α is analytic on Π_+, and therefore we conclude that the power function is a NH-function. As such, it admits a unique canonical integral representation of the form 2.4.

From Lemma 2.1.3, it follows:

$$A_\alpha = \lim_{\varepsilon\uparrow\infty} \frac{(i\varepsilon)^\alpha}{i\varepsilon} = \lim_{\varepsilon\uparrow\infty} \frac{\varepsilon^\alpha\big(\cos\alpha\frac{\pi}{2} + i\sin\alpha\frac{\pi}{2}\big)}{i\varepsilon} = 0, \tag{2.17}$$

since $\cos\alpha\frac{\pi}{2} + i\sin\alpha\frac{\pi}{2}$ is bounded and $\alpha \in (0,1)$.

Moreover,

$$B_\alpha = \operatorname{Re} i^\alpha = \operatorname{Re} e^{i\alpha\frac{\pi}{2}} = \cos\alpha\frac{\pi}{2}. \tag{2.18}$$

We consider now the function $(\lambda \pm i\varepsilon)^\alpha$, with $\varepsilon > 0$. Explicitly, it reads:

$$(\lambda \pm i\varepsilon)^\alpha = \exp\left(\alpha\left(\ln\sqrt{\lambda^2+\varepsilon^2} \pm i \arccos\frac{\lambda}{\sqrt{\lambda^2+\varepsilon^2}}\right)\right).$$

Therefore,

$$\lim_{\varepsilon\downarrow 0}(\lambda + i\varepsilon)^\alpha = \begin{cases} \lambda^\alpha & \text{if } \lambda \geq 0 \\ |\lambda|^\alpha(\cos\alpha\pi \pm i\sin\alpha\pi) & \text{if } \lambda < 0, \end{cases}$$

whence, repeating the same treatment as in Eq. 2.14, we get:

$$\begin{aligned} F_\alpha(\lambda+0) &= \frac{1}{\pi}\lim_{\eta\downarrow 0}\int_0^{\lambda+\eta} \mathrm{d}x \lim_{\varepsilon\downarrow 0}\operatorname{Im}(x+i\varepsilon)^\alpha \\ &= \begin{cases} 0 & \text{if } \lambda \geq 0 \\ \frac{|\lambda|^{\alpha+1}}{\pi(\alpha+1)}\sin\alpha\pi & \text{if } \lambda < 0, \end{cases} \end{aligned} \tag{2.19}$$

and we conclude that $F_\alpha(\lambda - 0) = F_\alpha(\lambda + 0)$. This yields, according to Eq. 2.8:

$$F_\alpha(\lambda) = \begin{cases} 0 & \text{if } \lambda \geq 0 \\ \frac{|\lambda|^{\alpha+1}}{\pi(\alpha+1)}\sin\alpha\pi & \text{if } \lambda < 0. \end{cases} \tag{2.20}$$

From Eqs. 2.17, 2.18 and 2.20 it follows the NH integral representation 2.16 of the power function with exponent $\alpha \in (0,1)$ according to Theorem 2.1.2, since the function $F_\alpha(\lambda)$ from Eq. 2.20 is differentiable for $\lambda < 0$. □

2.3 The Function $z \mapsto \ln\Big(1+\big(\frac{1+z}{-z}\big)^{\alpha}\Big)$

In Section 2.4 we shall see that the Rényi entropy function may be rewritten in a more convenient way as a linear combination of the logarithm and of a second function that we conventionally name L_α. Here we prove that L_α is a NH function and we study it in detail.

Definition 2.3.1. We define the function:

$$L_\alpha : D_L \to \mathbb{C}, \qquad z \mapsto \ln\left(1 + \left(\frac{1+z}{-z}\right)^\alpha\right)$$

for $\alpha \in (0,1)$, on the domain

$$\begin{aligned} D_L : &= \mathbb{C} \setminus (\{z \in \mathbb{C} | \mathrm{Re} z \leq -1, \mathrm{Im} z = 0\} \cup \{z \in \mathbb{C} | \mathrm{Re} z \geq 0, \mathrm{Im} z = 0\}) \\ &= \Pi_+ \cup \Pi_- \cup (-1, 0). \end{aligned} \tag{2.21}$$

Lemma 2.3.1. *The function L_α from Def. 2.3.1 for $\alpha \in (0,1)$ is a Nevanlinna-Herglotz function and admits the unique canonical integral representation:*

$$L_\alpha(z) = B(\alpha) + \int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda \left(\frac{f_\alpha(-\lambda)}{-z - \frac{1}{2} + \lambda} + \frac{f_\alpha(\lambda)}{-z - \frac{1}{2} - \lambda} + \frac{f_\alpha(-\lambda)(\frac{1}{2} - \lambda)}{\left(\frac{1}{2} - \lambda\right)^2 + 1} + \frac{f_\alpha(\lambda)(\frac{1}{2} + \lambda)}{\left(\frac{1}{2} + \lambda\right)^2 + 1} \right) \tag{2.22}$$

where

$$B(\alpha) = \frac{1}{2} \ln\left(1 + 2^\alpha + 2^{\frac{\alpha}{2}+1} \cos\frac{3}{4}\alpha\pi\right), \tag{2.23}$$

and

$$f_\alpha(\lambda) := \frac{1}{\pi} \arctan\left(\frac{\left(\frac{2\lambda-1}{2\lambda+1}\right)^\alpha \sin\alpha\pi}{1 + \left(\frac{2\lambda-1}{2\lambda+1}\right)^\alpha \cos\alpha\pi} \right). \tag{2.24}$$

Proof. By Proposition 2.1.1, the function $z \mapsto \frac{1+z}{-z}$ is NH as linear combination with positive coefficients of the NH function $z \mapsto -\frac{1}{z}$ and of the real constant function -1. Therefore, the function L_α is NH as well, as composition of NH functions.

We now define the functions $A : (0,1) \to \mathbb{R}$ and $B : (0,1) \to \mathbb{R}$ that map each α into the value of the linear coefficient (cf. Eq. 2.5) and of the constant term (cf. Eq. 2.6) of the NH canonical integral representation of L_α, respectively. It turns out that A identically vanishes,

$$\begin{aligned} A(\alpha) &= \lim_{\varepsilon\uparrow\infty} \frac{\ln\left(1 + \left(\frac{1+i\varepsilon}{-i\varepsilon}\right)^\alpha\right)}{i\varepsilon} \\ &= \lim_{\varepsilon\uparrow\infty} \frac{\ln(1 + \varepsilon^{-\alpha}(-\varepsilon + i)^\alpha)}{i\varepsilon} \\ &= \lim_{\varepsilon\uparrow\infty} \frac{\ln\left(1 + \varepsilon^{-\alpha}|-\varepsilon + i|^\alpha e^{i\alpha \arg(-\varepsilon+i)}\right)}{i\varepsilon} \\ &= 0, \end{aligned} \tag{2.25}$$

since the exponential function of a purely imaginary number is bounded and $|-\varepsilon + i|^\alpha \to |\varepsilon|^\alpha$ in the $\varepsilon \uparrow \infty$ limit. Therefore, no linear term in z arises in the integral representation of L_α.

Moreover, we get for $\alpha \in (0,1)$ the constant term:

$$\begin{aligned} B(\alpha) &= \mathrm{Re} \ln\left(1 + \left(\frac{1+i}{-i}\right)^\alpha\right) \\ &= \mathrm{Re} \ln(1 + (-1+i)^\alpha) \end{aligned}$$

$$= \operatorname{Re}\ln\left(1+2^{\frac{\alpha}{2}}e^{i\frac{3}{4}\alpha\pi}\right)$$
$$= \ln\left|1+2^{\frac{\alpha}{2}}e^{i\frac{3}{4}\alpha\pi}\right|, \tag{2.26}$$

from which assertion 2.23 immediately follows.

We consider now for $\lambda \in \mathbb{R} \setminus \{-1, 0\}$ the limit

$$\begin{aligned}
\lim_{\varepsilon\downarrow 0}\left(\frac{1+\lambda\pm i\varepsilon}{-\lambda\mp i\varepsilon}\right)^{\alpha} &= \lim_{\varepsilon\downarrow 0}\left(\frac{-\lambda-\lambda^2-\varepsilon^2\pm i\varepsilon}{\lambda^2+\varepsilon^2}\right)^{\alpha} \\
&= \lim_{\varepsilon\downarrow 0}\exp\left(\alpha\left(\ln\left(\frac{|-\lambda-\lambda^2-\varepsilon^2\pm i\varepsilon|}{\lambda^2+\varepsilon^2}\right)+i\arg\left(-\lambda-\lambda^2-\varepsilon^2\pm i\varepsilon\right)\right)\right) \\
&= \exp\left(\alpha\ln\left(\frac{|\lambda+\lambda^2|}{\lambda^2}\right)\pm i\alpha\arccos\operatorname{sgn}\left(-\lambda-\lambda^2\right)\right) \\
&= \begin{cases}\left(\frac{\lambda+1}{\lambda}\right)^{\alpha}e^{\pm i\alpha\pi} & \text{if } \lambda<-1 \text{ or } \lambda>0 \\ \left(\frac{-\lambda-1}{\lambda}\right)^{\alpha} & \text{if } -1<\lambda<0.\end{cases}
\end{aligned} \tag{2.27}$$

Starting from Eq. 2.27, we further define

$$\begin{aligned}
l_{\pm}(\alpha,\lambda) :&= \lim_{\varepsilon\downarrow 0}\operatorname{Im}\ln\left(1+\left(\frac{1+\lambda\pm i\varepsilon}{-\lambda\mp i\varepsilon}\right)^{\alpha}\right) \\
&= \begin{cases}\operatorname{Im}\ln\left(1+\left(\frac{\lambda+1}{\lambda}\right)^{\alpha}e^{\pm i\alpha\pi}\right) & \text{if } \lambda<-1 \text{ or } \lambda>0 \\ 0 & \text{if } -1<\lambda<0\end{cases} \\
&= \begin{cases}\pm\arccos\left(\frac{1+\left(\frac{\lambda+1}{\lambda}\right)^{\alpha}\cos\alpha\pi}{\sqrt{1+2\left(\frac{\lambda+1}{\lambda}\right)^{\alpha}\cos\alpha\pi+\left(\frac{\lambda+1}{\lambda}\right)^{2\alpha}}}\right) & \text{if } \lambda<-1 \text{ or } \lambda>0 \\ 0 & \text{if } -1<\lambda<0\end{cases} \\
&= \begin{cases}\pm\arctan\left(\frac{\left(\frac{\lambda+1}{\lambda}\right)^{\alpha}\sin\alpha\pi}{1+\left(\frac{\lambda+1}{\lambda}\right)^{\alpha}\cos\alpha\pi}\right) & \text{if } \lambda<-1 \text{ or } \lambda>0 \\ 0 & \text{if } -1<\lambda<0,\end{cases}
\end{aligned} \tag{2.28}$$

where in the last equality we employed the trigonometric identity $\arccos x = \arctan\left(\frac{\sqrt{1-x^2}}{x}\right)$. We notice that $l_{\pm}(\alpha,\lambda)$ vanishes on the $-1<\lambda<0$ interval since the term $\left(\frac{-\lambda-1}{\lambda}\right)^{\alpha}$ in 2.27 is purely real. Moreover, from Eq. 2.28 we also conclude $l_{\pm}(\alpha,-1)=0$, while we set $l_{\pm}(\alpha,0)=\pm\frac{1}{2}\alpha\pi$ at the $\lambda=0$ discontinuity point, according to our convention 2.8.

By Theorem 2.1.2, Lemma 2.1.4 and Eqs. 2.25, 2.26 and 2.28, the NH integral representation of the function $L_{\alpha}(z)$ follows:

$$L_{\alpha}(z) = B(\alpha)+\frac{1}{\pi}\int_{\mathbb{R}\setminus[-1,0]} d\lambda\ \arctan\left(\frac{\left(\frac{\lambda+1}{\lambda}\right)^{\alpha}\sin\alpha\pi}{1+\left(\frac{\lambda+1}{\lambda}\right)^{\alpha}\cos\alpha\pi}\right)\left(\frac{1}{\lambda-z}-\frac{\lambda}{\lambda^2+1}\right).$$

Making suitable linear changes of variable in the improper integral above and recalling Eq. 2.24, this leads to our assertion 2.22. □

Figure 2.1 shows the function f_{α} for α values close to 1.

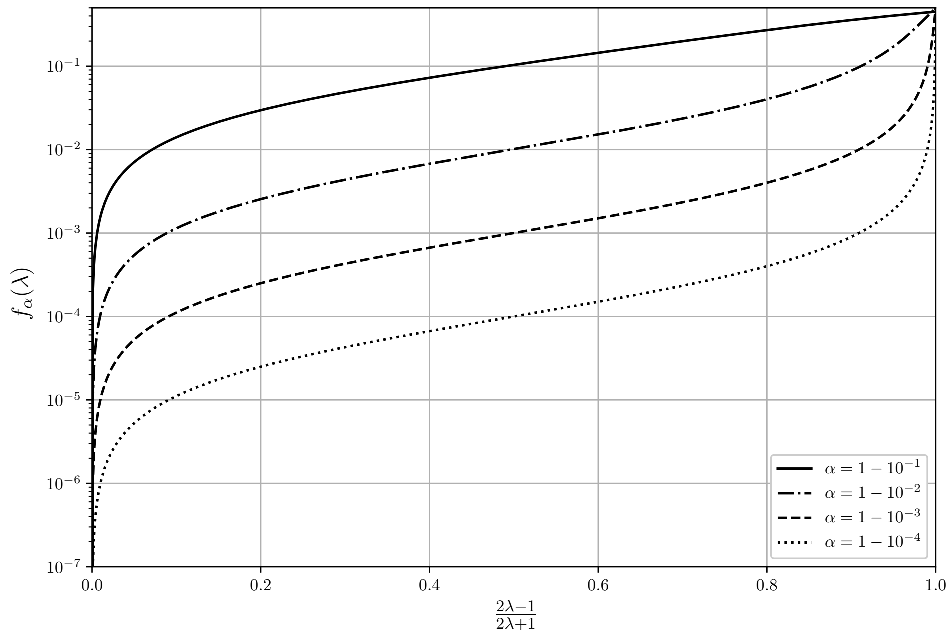

Figure 2.1: Plot of the function f_α of the NH measure for the L_α function (cf. Eq. 2.24) with respect to the ratio $\frac{2\lambda-1}{2\lambda+1}$ for a few values of α close to 1.

2.4 The Rényi Entropy Function

The first concept of information entropy was proposed by Shannon [Sha48] and this led, for a distribution of 2 discrete probabilities $(t, 1-t)$, $t \in [0,1]$, to the following definition of a suitable information measure:

Definition 2.4.1 (Shannon entropy function)**.** The Shannon entropy function H_1 reads

$$H_1 : [0,1] \to \mathbb{R}^+ \cup \{0\}, \qquad t \mapsto \begin{cases} -t\ln t - (1-t)\ln(1-t) & \text{if } t \in (0,1) \\ 0 & \text{if } t \in \{0,1\}. \end{cases}$$

The entropy measure H_1 for a finite discrete probability distribution $(p_1, \dots, p_n)$, i.e. with $0 \le p_1, \dots, p_n \le 1$ and $\sum_{i=1}^n p_i = 1$ is uniquely characterized, up to a normalization constant $k > 0$, by the Axioms [Fad57]:

1. $H_1(p_1, \dots, p_n)$ is a symmetric function of its variables;
2. $H(p, 1-p)$ is a continuous function of p for $0 \le p \le 1$;
3. $H_1\left(\frac{1}{2}, \frac{1}{2}\right) = k$;
4. $H_1(tp_1, (1-t)p_1, p_2, \dots, p_n) = H_1(p_1, p_2, \dots, p_n) + p_1 H_1(t, (1-t))$ for $0 \le t \le 1$.

Axiom 4 implies the additivity property: $H_1(\{p_i q_j | 1 \le i \le n, 1 \le j \le m\}) = H_1(p_1, \dots, p_n) + H_1(q_1, \dots, q_m)$ for any two discrete probability distributions $(p_1, \dots, p_n)$ and $(q_1, \dots, q_m)$, with $0 \le p_1, \dots, p_n, q_1, \dots, q_m \le 1$, $\sum_{i=1}^n p_i = \sum_{j=1}^n q_j = 1$ and $n, m \in \mathbb{N}$.

From Axioms 1 through 3, and relaxing Axiom 4 to the weaker requirement of additivity only, Rényi derived a new parametric entropy function H_α which generalizes Shannon's concept in a natural way [Rén61].

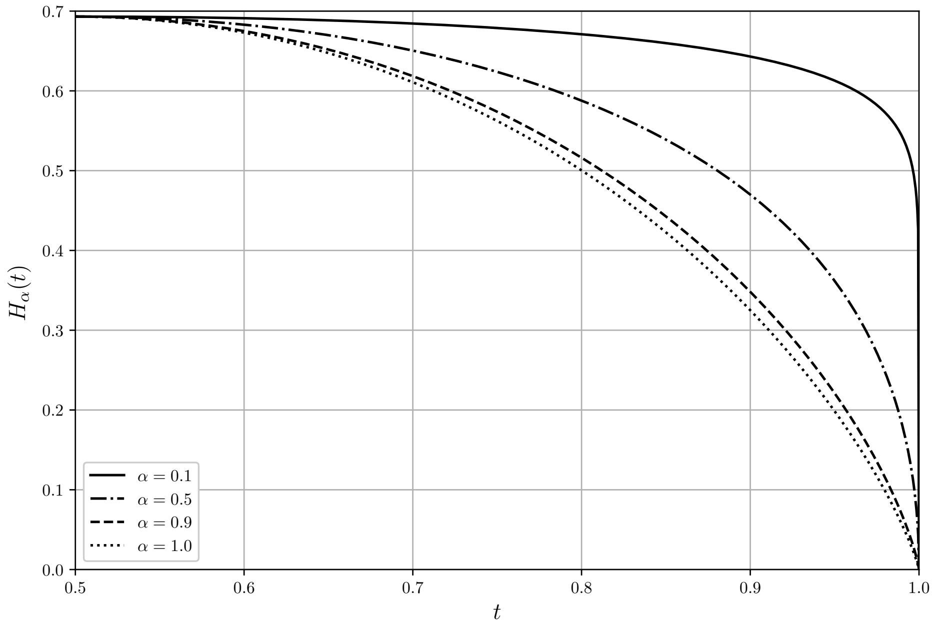

Figure 2.2: Plot of the Rényi entropy function H_α (cf. Def. 2.4.2) for a few values of the Rényi index $\alpha \in (0,1)$ on the interval $t \in \left[\frac{1}{2}, 1\right]$. The Shannon entropy function (cf. Def. 2.4.1) obtained by means of the $\alpha \uparrow 1$ limit is also shown for comparison (dotted line). The $\alpha \downarrow 0$ limit yields the Hartley entropy function with constant value $\ln 2$. The common maximum of all entropy curves at $t = \frac{1}{2}$ reads $\ln 2$.

Definition 2.4.2 (Rényi entropy function)**.** Let $\alpha \in (0,1)$. The Rényi entropy function H_α of order α reads

$$H_\alpha : [0,1] \to \mathbb{R}^+ \cup \{0\}, \qquad t \mapsto \frac{1}{1-\alpha} \ln(t^\alpha + (1-t)^\alpha)$$

where the number α is named Rényi index.

Our Def. 2.4.2 involves the natural logarithm and implies that the normalization constant in Axiom 3 reads $k = \ln 2$ in this case. This corresponds to the choice of a measurement unit for information.

We notice that H_α is symmetric about $t = \frac{1}{2}$, and we show in Figure 2.2 the function H_α for different α values on the right half of its definition domain.

Motivated by Def. 2.4.2, we extend the function H_α to a suitable subset of the complex plane $\mathbb{C}$. Recalling Section 2.2.1 and Eq. 2.21, this leads us to:

Definition 2.4.3 (Complex Rényi entropy function)**.** Let $\alpha \in (0,1)$ be the Rényi index and let $D_{\tilde{H}}$ be the domain

$$\begin{aligned} D_{\tilde{H}} &:= \mathbb{C} \setminus (\{z \in \mathbb{C} | \mathrm{Re} z \leq 0, \mathrm{Im} z = 0\} \cup \{z \in \mathbb{C} | \mathrm{Re} z \geq 1, \mathrm{Im} z = 0\}) \\ &= \Pi_+ \cup \Pi_- \cup (0,1). \end{aligned}$$

Then the complex Rényi entropy function reads

$$\tilde{H}_\alpha : D_{\tilde{H}} \cup \{0,1\} \to \mathbb{C}, \qquad z \mapsto \begin{cases} \frac{1}{1-\alpha} \ln(z^\alpha + (1-z)^\alpha) & \text{if } z \in D_{\tilde{H}} \\ 0 & \text{if } z \in \{0,1\}, \end{cases}$$

and we retrieve H_α as the restriction $H_\alpha = \tilde{H}_\alpha|\mathbb{R}$.

We notice that the complex Rényi entropy function is differentiable with respect to the Rényi index α in the real interval $(0, 1)$.

Employing the Nevanlinna-Herglotz integral representations of the logarithm (cf. Section 2.2.1) and of L_α (cf. Section 2.3) in the complex plane, we seek now a suitable integral representation of the complex Rényi entropy function.

We anticipate here that the complex Rényi entropy function is not a Nevanlinna-Herglotz function, and therefore we cannot exploit Lemmas 2.1.3 and 2.1.4 directly. The lack of the NH property stems from the term $1-z$ in Def. 2.4.3, which is not a self-map on Π_+.

Theorem 2.4.1. *Let $\alpha \in (0,1)$, $z \in D_{\tilde{H}}$ and let R_z be the function*

$$R_z : \mathbb{R} \setminus \left(-\frac{1}{2}, \frac{1}{2}\right) \to \mathbb{C} \qquad \lambda \mapsto R_z(\lambda) := \frac{1}{z - \frac{1}{2} + \lambda}. \tag{2.29}$$

Then, the complex Rényi function $\tilde{H}_\alpha$ on $D_{\tilde{H}}$ admits the integral representation

$$\tilde{H}_\alpha(z) = \frac{B(\alpha)}{1-\alpha} - \frac{1}{1-\alpha} \int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda\, f_\alpha(\lambda) \left(R_z(\lambda) - R_z(-\lambda) + \frac{\frac{1}{2} - \lambda}{\left(\frac{1}{2} - \lambda\right)^2 + 1} - \frac{\frac{1}{2} + \lambda}{\left(\frac{1}{2} + \lambda\right)^2 + 1} \right), \tag{2.30}$$

recalling Defs. 2.23 and 2.24 of B and f_α respectively.

Proof. Rearranging the argument of the logarithm function in Def. 2.4.3, we get

$$\begin{aligned}
\tilde{H}_\alpha(z) &= \frac{1}{1-\alpha} \ln\left(z^\alpha \left(1 + \left(\frac{1-z}{z} \right)^\alpha \right) \right) \\
&= \frac{\alpha}{1-\alpha} \ln z + \frac{1}{1-\alpha} \ln\left(1 + \left(\frac{1-z}{z} \right)^\alpha \right) \\
&= \frac{\alpha}{1-\alpha} \ln z + \frac{1}{1-\alpha} L_\alpha(-z),
\end{aligned} \tag{2.31}$$

where we exploited the definition of the complex function L_α from Section 2.3.

We stress here that, although $L_\alpha(z)$ is a NH function, $L_\alpha(-z)$ is not since $z \mapsto -z$ is not a self-map in Π_+. Consequently, also $\tilde{H}_\alpha(z)$ is not NH. However, we can still use the unique canonical Nevanlinna-Herglotz integral representations of the logarithm and L_α to derive the integral representation of $\tilde{H}_\alpha$.

From Theorem 2.2.1 and Lemma 2.3.1 we get

$$\begin{aligned}
\tilde{H}_\alpha(z) &= \frac{B(\alpha)}{1-\alpha} + \frac{1}{1-\alpha} \int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda \left(\frac{f_\alpha(\lambda)}{z - \frac{1}{2} - \lambda} + \frac{f_\alpha(-\lambda) - \alpha}{z - \frac{1}{2} + \lambda} \right. \\
&\qquad \left. + \frac{f_\alpha(\lambda)(\frac{1}{2} + \lambda)}{\left(\frac{1}{2} + \lambda\right)^2 + 1} + \frac{(f_\alpha(-\lambda) - \alpha)(\frac{1}{2} - \lambda)}{\left(\frac{1}{2} - \lambda\right)^2 + 1} \right) \\
&= \frac{B(\alpha)}{1-\alpha} + \frac{1}{1-\alpha} \int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda\, f_\alpha(\lambda) \left(\frac{1}{z - \frac{1}{2} - \lambda} - \frac{1}{z - \frac{1}{2} + \lambda} + \frac{\frac{1}{2} + \lambda}{\left(\frac{1}{2} + \lambda\right)^2 + 1} - \frac{\frac{1}{2} - \lambda}{\left(\frac{1}{2} - \lambda\right)^2 + 1} \right).
\end{aligned} \tag{2.32}$$

In the last line of Eq. 2.32 we used relation

$$\begin{aligned} f_\alpha(-\lambda) - \alpha &= \frac{1}{\pi} \arctan\left(\frac{\left(\frac{-2\lambda-1}{-2\lambda+1}\right)^\alpha \sin \alpha\pi}{1 + \left(\frac{-2\lambda-1}{-2\lambda+1}\right)^\alpha \cos \alpha\pi} \right) - \alpha \\ &= -\frac{1}{\pi} \arctan\left(\frac{\sin \alpha\pi}{\cos \alpha\pi + \left(\frac{2\lambda+1}{2\lambda-1}\right)^\alpha} \right) \\ &= -f_\alpha(\lambda) \end{aligned}$$

recalling definition 2.24 of f_α and the trigonometric identity $\arctan x - \arctan y = \arctan\left(\frac{x-y}{1+xy}\right)$.
□

In the following Chapter 3, we shall focus on the Rényi entanglement entropy of a relativistic quantum system of quasi-free fermions distributed on the real line. The treatment requires inserting suitable positive operators with upper bound smaller than 1 in representation 2.30, on the ground of the Spectral Theorem. In this context, the function R_z will be interpreted as the resolvent of the operator.

2.5 The Shannon Entropy Function

In this Section, we derive the integral representation of the Shannon entropy function as a special case of our method developed in Sections 2.3 and 2.4. The Shannon entropy function is uniquely determined by the information-theoretical Axioms 1 through 4 (cf. Section 2.4). However, the significance of the function H_1 is much wider. Indeed, in Physics, H_1 is closely linked to the entropy concept of Boltzmann and Gibbs, that was developed in the context of classical statistical mechanics, and in agreement with the definition of entropy in phenomenological thermodynamics. In a quantum-mechanical context, all these equivalent formulations of entropy lead to the concept of von Neumann entropy, where the random variables are replaced by suitable density operators [Neu28].

We now consider a limit in the index α of the complex Rényi entropy function that we introduced previously. This yields a well-known classical result.

Proposition 2.5.1. *The $\alpha \uparrow 1$ limit of the complex Rényi entropy function $\tilde{H}_\alpha$ (cf. Def. 2.4.3) yields*

$$\lim_{\alpha\uparrow 1} \tilde{H}_\alpha(z) = \begin{cases} -z \ln z - (1-z)\ln(1-z) & \text{if } z \in D_{\tilde{H}} \\ 0 & \text{if } z \in \{0,1\}. \end{cases} \tag{2.33}$$

Proof. We note that the function $\tilde{H}_\alpha$ is differentiable with respect to α in $(0,1)$ for any $z \in D_{\tilde{H}}$. Since 1 is an accumulation point of the interval $(0,1)$, we apply the l'Hôpital's rule and we obtain

$$\lim_{\alpha\uparrow 1} \frac{\ln(z^\alpha + (1-z)^\alpha)}{1-\alpha} = -\lim_{\alpha\uparrow 1} \frac{z^\alpha \ln z + (1-z)^\alpha \ln(1-z)}{z^\alpha + (1-z)^\alpha}.$$

The limit above exists and leads to 2.33. □

Motivated by Prop. 2.5.1 and in analogy with Def. 2.4.3, we extend the Shannon entropy function H_1 by analytic continuation to the function $\tilde{H}_1$ defined on a suitable domain in the complex plane.

Definition 2.5.1 (Complex Shannon entropy function)**.** Let $D_{\tilde{H}} \subset \mathbb{C}$ be like in Section 2.2.1. We define the complex Shannon entropy function by

$$\tilde{H}_1 : D_{\tilde{H}} \cup \{0,1\} \to \mathbb{C}, \qquad z \mapsto \begin{cases} -z \ln z - (1-z)\ln(1-z) & \text{if } z \in D_{\tilde{H}} \\ 0 & \text{if } z \in \{0,1\}. \end{cases}$$

It is well known that the Rényi entropy generalizes the Shannon entropy and reduces to it in the $\alpha \uparrow 1$ limit of the Rényi index [Rén61]. We immediately retrieve this result:

Corollary 2.5.1.1 (of Proposition 2.5.1)**.** *The Rényi and Shannon entropy functions from Defs. 2.4.2 and 2.4.1 are linked by the relation*

$$H_1(t) = \lim_{\alpha \uparrow 1} H_\alpha(t).$$

Motivated by Proposition 2.5.1, we seek an integral representation of the complex Shannon entropy function $\tilde{H}_1$.

As a preliminary step we analyse the derivative of the function f_α in the Nevanlinna-Herglotz integral representation of $\tilde{H}_\alpha$.

Lemma 2.5.2. *The first derivative of the function f_α (cf. Eq. 2.24) with respect to the Rényi index α is continuous on the domain $(\alpha, \lambda) \in (0,1) \times \left(\frac{1}{2}, +\infty\right)$ and reads*

$$\frac{\partial f_\alpha}{\partial \alpha}(\lambda) = \frac{1}{\pi} \frac{\left(\frac{2\lambda-1}{2\lambda+1}\right)^\alpha \ln\left(\frac{2\lambda-1}{2\lambda+1}\right) \sin \alpha\pi + \pi \left(\frac{2\lambda-1}{2\lambda+1}\right)^\alpha \cos \alpha\pi + \pi \left(\frac{2\lambda-1}{2\lambda+1}\right)^{2\alpha}}{1 + 2\left(\frac{2\lambda-1}{2\lambda+1}\right)^\alpha \cos \alpha\pi + \left(\frac{2\lambda-1}{2\lambda+1}\right)^{2\alpha}}. \tag{2.34}$$

Moreover, it holds pointwise

$$\lim_{\alpha \uparrow 1} \frac{\partial f_\alpha}{\partial \alpha}(\lambda) = \frac{1}{2} - \lambda. \tag{2.35}$$

Proof. Eqs. 2.34 and 2.35 follow by direct calculation. The first derivative is continuous in α in $(0,1)$ as composition of continuous functions. □

By means of Eq. 2.35, we define the function $f_1^1 : \left(\frac{1}{2}, +\infty\right) \to \mathbb{R}$ by

$$f_1^1(\lambda) := \lim_{\alpha \uparrow 1} \frac{\partial f_\alpha}{\partial \alpha}(\lambda) = \frac{1}{2} - \lambda. \tag{2.36}$$

Additionally, as a shorthand notation, we define the integral kernel

$$K(z, \lambda) := R_z(\lambda) - R_z(-\lambda) + \frac{\frac{1}{2} - \lambda}{\left(\frac{1}{2} - \lambda\right)^2 + 1} - \frac{\frac{1}{2} + \lambda}{\left(\frac{1}{2} + \lambda\right)^2 + 1}, \tag{2.37}$$

on the complex domain $D_{\tilde{H}} \times \left(\frac{1}{2}, +\infty\right)$.

Lemma 2.5.3. *With Defs. 2.36 and 2.37, the following improper integral formula for $z \in D_{\tilde{H}}$ holds:*

$$\int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda \, f_1^1(\lambda) K(z, \lambda) = -\frac{3}{4}\pi + \frac{1}{2}\ln 2 - z \ln z - (1-z)\ln(1-z). \tag{2.38}$$

Proof. Up to an arbitrary additive complex constant, the primitive of the integrand in Eq. 2.38 reads

$$\int \mathrm{d}\lambda \left(\frac{1}{2}-\lambda\right)K(z,\lambda) = \ln\left(\frac{\left(z-\frac{1}{2}+\lambda\right)^{z}\left(-z+\frac{1}{2}+\lambda\right)^{1-z}}{\sqrt{1+\left(\frac{1}{2}+\lambda\right)^2}}\right) - \arctan\left(\lambda-\frac{1}{2}\right) - \arctan\left(\lambda+\frac{1}{2}\right),$$

and the claim follows immediately. □

Lemma 2.5.4. *From Eq. 2.23, it follows*

$$\lim_{\alpha\uparrow 1}\frac{B(\alpha)}{1-\alpha} = \int_{\frac{1}{2}}^{+\infty}\mathrm{d}\lambda\left(\frac{1}{\left(\frac{1}{2}-\lambda\right)^2+1}+\frac{1}{\left(\frac{1}{2}+\lambda\right)^2+1}-\frac{1}{\left(\frac{1}{2}+\lambda\right)\left(\left(\frac{1}{2}+\lambda\right)^2+1\right)}\right) = \frac{3}{4}\pi-\frac{1}{2}\ln 2. \tag{2.39}$$

Proof. Using the l'Hôpital's rule, we get

$$\lim_{\alpha\uparrow 1}\frac{B(\alpha)}{1-\alpha} = -\frac{1}{2}\lim_{\alpha\uparrow 1}\frac{2^{\alpha}\ln 2+2^{\frac{\alpha}{2}}\ln 2\cos\frac{3}{4}\alpha\pi-3\pi\cdot 2^{\frac{\alpha}{2}-1}\sin\frac{3}{4}\alpha\pi}{1+2^{\alpha}+2^{\frac{\alpha}{2}+1}\cos\frac{3}{4}\alpha\pi} = \frac{3}{4}\pi-\frac{1}{2}\ln 2. \tag{2.40}$$

Moreover, we consider the following three improper integral identities:

$$\int_{\frac{1}{2}}^{+\infty}\mathrm{d}\lambda\,\frac{1}{\left(\frac{1}{2}-\lambda\right)^2+1}=\frac{\pi}{2},\quad \int_{\frac{1}{2}}^{+\infty}\mathrm{d}\lambda\,\frac{1}{\left(\frac{1}{2}+\lambda\right)^2+1}=\frac{\pi}{4},\quad \int_{\frac{1}{2}}^{+\infty}\mathrm{d}\lambda\,\frac{1}{\left(\frac{1}{2}+\lambda\right)\left(\left(\frac{1}{2}+\lambda\right)^2+1\right)}=\frac{1}{2}\ln 2,$$

which allow us to equivalently rewrite Eq. 2.40 in integral form. This immediately yields the claim. □

Theorem 2.5.5. *Recalling the definition of function R_z in Eq. 2.29, the integral representation of the complex Shannon entropy $\tilde{H}_1$ (cf. Def. 2.5.1) reads:*

$$\tilde{H}_1(z) = \int_{\frac{1}{2}}^{+\infty}\mathrm{d}\lambda\left(\left(\frac{1}{2}-\lambda\right)\left(R_z(\lambda)-R_z(-\lambda)\right)+\frac{2\lambda}{\lambda+\frac{1}{2}}\right). \tag{2.41}$$

for $z \in D_{\tilde{H}}$.

Proof. Combining the results of Lemmas 2.5.3 and 2.5.4, we may write the complex Shannon entropy function as

$$\tilde{H}_1(z) = \lim_{\alpha\uparrow 1}\frac{B(\alpha)}{1-\alpha} + \int_{\frac{1}{2}}^{+\infty}\mathrm{d}\lambda\, f_1^1(\lambda)K(z,\lambda)$$

$$= \int_{\frac{1}{2}}^{+\infty}\mathrm{d}\lambda\left(\frac{1}{\left(\frac{1}{2}-\lambda\right)^2+1}+\frac{1}{\left(\frac{1}{2}+\lambda\right)^2+1}-\frac{1}{\left(\frac{1}{2}+\lambda\right)\left(\left(\frac{1}{2}+\lambda\right)^2+1\right)}\right)$$

$$+\int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda \left(\frac{1}{2}-\lambda\right)\left(R_z(\lambda)-R_z(-\lambda)+\frac{\frac{1}{2}-\lambda}{\left(\frac{1}{2}-\lambda\right)^2+1}-\frac{\frac{1}{2}+\lambda}{\left(\frac{1}{2}+\lambda\right)^2+1}\right). \quad (2.42)$$

Claim 2.41 follows from Eq. 2.42, rearranging the terms in the integrals. □

We note that, by Theorem 2.5.5, and restricting the definition domain of the function $\tilde{H}_1$ to the real axis, we obtain in the framework of the Nevanlinna-Herglotz theory the same integral representation of the Shannon entropy function given in Ref. [CH09a].

Corollary 2.5.5.1. *Recalling the definition of function R_t in Eq. 2.29, it holds*

$$t\ln t+(1-t)\ln(1-z)=-(\tilde{H}_1|\mathbb{R})(t)=\int_{\frac{1}{2}}^{+\infty}\mathrm{d}\lambda\left(\left(\lambda-\frac{1}{2}\right)(R_t(\lambda)-R_t(-\lambda))-\frac{2\lambda}{\lambda+\frac{1}{2}}\right),$$

for $t\in(0,1)$.

Proof. The claim follows straightforwardly from Theorem 2.5.5, noting that the function on the left-hand side is equal to $-\tilde{H}_1(t)$ on the real axis by Def. 2.5.1. □

Chapter 3

Rényi Entanglement of Free Fermions

In the previous Chapter we introduced the information-theoretical concept of Shannon entropy and its generalization due to Rényi.

In this Chapter we elaborate on the central topic of this Thesis. We consider a statistical relativistic quantum-mechanical system of N quasi-free fermions, we split it into two generic disjoint subsystems and we study the amount of correlations between them, introducing a suitable entanglement measure.

In a quantum-mechanical treatment, the Shannon entropy is linked to the concept of the von Neumann entropy [Neu28]. This leads to the concept of bipartite entanglement entropy, that was recently addressed in a mathematically rigorous way in Ref. [LX17].

Motivated by Ref. [LX17], we generalize the treatment of the entanglement entropy to the case of the Rényi entropy, with Rényi index α restricted to the interval $(0, 1)$.

We make extensive use of our integral representation of the Rényi entropy, that we obtained in Theorem 2.4.1 employing the general results of the Nevanlinna-Herglotz theory of analytic self-maps in the upper complex half-plane.

3.1 The Mathematical Framework of Quantum Spin Systems

3.1.1 C^*-Algebras

A quantum system of $N \in \mathbb{N}$ fermions in a separable one-particle Hilbert space with scalar product $\langle \cdot, \cdot \rangle$ and anticommutation parentheses $[\cdot, \cdot]_+$ is described by a suitable algebra of bounded creation and annihilation operators. This is quantitatively formalized in:

Theorem 3.1.1. *Let $\mathcal{H}$ be a pre-Hilbert space. Up to a *-isomorphism there exists a unique unital C^*-algebra $\mathcal{A}_{\mathcal{H}}$ generated by the identity operator I and further operators $a(f)$ such that $f \mapsto a(f)$ is antilinear for any $f \in \mathcal{H}$, and satisfying the canonical anticommutation relations (CARs),*

$$[a(f), a(g)]_+ = 0, \qquad [a(f), a^*(g)]_+ = \langle f, g \rangle I,$$

for all $f, g \in \mathcal{H}$.

Proof. The claim is a special case of the more general statement of Theorem 5.2.5 in Ref. [BR02]. □

The construction of the Fock space outlined in Ref. [BR02] establishes the existence of bounded operators satisfying the correct anticommutation relations according to the Theorem above.

We now list a few fundamental concepts inherited from the theory of operator algebras that we shall need later. Recalling that a linear operator A on a pre-Hilbert space $\mathcal{H}$ is symmetric if $\langle Af, g\rangle = \langle f, Ag\rangle$ for any f, g lying in the operator definition domain, we start with the concept of a positive operator and that of the operator trace, which is closely associated to it, and is of central importance in mathematical physics.

Definition 3.1.1 (Positive operator)**.** Let A be a linear operator defined on a domain $\mathcal{D}(A) \subseteq \mathcal{H}$. Then A is said to be positive ($A \geq 0$) if it is symmetric and, in addition, $\langle Af, f\rangle \geq 0$ for any $f \in \mathcal{D}(A)$. A is called strictly positive ($A > 0$), if it is positive and $\langle Af, f\rangle = 0$ if and only if $f = 0$. We denote by $\mathcal{A}^+_{\mathcal{H}}$ the subset of all positive operators in the C^*-algebra $\mathcal{A}_{\mathcal{H}}$.

Definition 3.1.2. Let A, B be linear operators defined on domains $\mathcal{D}(A), \mathcal{D}(B) \subseteq \mathcal{H}$. We say that $A \leq B$ if $\mathcal{D}(B) \subseteq \mathcal{D}(A)$ and $B - A \geq 0$.

We now introduce the concept of trace of a finite-rank operator.

Definition 3.1.3 (Trace of a finite-rank operator)**.** Let $L(\mathcal{B})$ be the algebra of all linear bounded operators acting on a complex Banach space $\mathcal{B}$, and let $\mathcal{F}(\mathcal{B})$ be the subalgebra of the finite-rank operators. Then we define the trace of an operator $F \in \mathcal{F}(\mathcal{B})$ of rank $n \in \mathbb{N}$ by

$$\operatorname{tr} F := \sum_{i=1}^{n} \lambda_i(F),$$

where $\lambda_i(F)$, $1 \leq i \leq n$, are the eigenvalues of F, taken with their multiplicity.

Definition 3.1.4 (Adjoint and self-adjoint operator)**.** Let A be a linear operator defined on a domain $\mathcal{D}(A) \subseteq \mathcal{H}_1$ and with range in $\mathcal{H}_2$, where $\mathcal{H}_1, \mathcal{H}_2$ are Hilbert spaces. A linear operator A^* defined on $\mathcal{D}(A^*) \subseteq \mathcal{H}_2$ and with range in $\mathcal{H}_1$ is said to be adjoint to A if

$$\langle Af, g\rangle = \langle f, A^* g\rangle \tag{3.1}$$

holds for any $f \in \mathcal{D}(A)$ and $g \in \mathcal{D}(A^*)$. If A is such that $\overline{\mathcal{D}(A)} = \mathcal{H}$ with range in $\mathcal{H}$, where $\mathcal{H}$ is a Hilbert space and moreover, if $A = A^*$ holds, then A is called self-adjoint.

We now introduce the concepts of compact operators and of trace-class operators, extending Def. 3.1.3 accordingly. We recall that a linear operator A defined on $\mathcal{D}(A) \subseteq \mathcal{H}_1$ with range in $\mathcal{H}_2$, where $\mathcal{H}_1, \mathcal{H}_2$ are normed spaces, is compact if any bounded sequence $(f_k)_{k\in\mathbb{N}} \subseteq \mathcal{D}(A)$ contains a subsequence $(f_{k_m})_{m\in\mathbb{N}}$ such that the sequence $(Af_{k_m})_{m\in\mathbb{N}}$ converges in $\mathcal{H}_2$. It is well-known that the set of the non-zero eigenvalues of a compact operator is finite or at most countable, each eigenvalue has a finite algebraic multiplicity, and 0 is the only possible accumulation point of the spectrum.

When a bounded operator A is defined on a Hilbert space, the compactness of A is equivalent to the compactness of A^*A, where A^* is the adjoint of A. The operator A^*A is by definition self-adjoint and thus its spectrum is purely real and moreover, all its eigenvalues are non-zero in this case. This makes possible the following:

Definition 3.1.5 (Singular values)**.** Let A be a bounded compact operator acting in a Hilbert space and let A^* be its adjoint operator. Let

$$\lambda_1(A^*A) \geq \lambda_2(A^*A) \geq \cdots \geq 0$$

be the sequence of all non-zero eigenvalues of the operator A^*A, with their multiplicity taken into account. Let the eigenvalues of A^*A be labelled by an index from a set $I \subseteq \mathbb{N}$. Then, the

i-th singular value of A is the number

$$s_i(A) := \sqrt{\lambda_i(A^*A)}$$

for $i \in I$.

Definition 3.1.6 (Trace-class operator)**.** Let A be a bounded compact operator acting in a Hilbert space with singular values $s_i(A)$, for $i \in I \subseteq \mathbb{N}$. Then A is called a trace-class operator whenever

$$\sum_{i \in I} s_i(A) < \infty.$$

For a separable Hilbert space $\mathcal{H}$, we denote by $\mathcal{S}_1$ the set of all trace-class operators. The latter may be endowed with the trace-norm

$$\|A\|_1 := \sum_{i \in I} s_i(A),$$

for all $A \in \mathcal{S}_1$.

The functional tr introduced in Def. 3.1.3 on the set of the finite-rank operators $\mathcal{F}(\mathcal{H})$ defined on $\mathcal{H}$ may be extended by continuity to $\mathcal{S}_1$, with respect to the trace-norm above.

For trace-class operators, the trace can be explicitly expressed in a particularly straightforward form.

Theorem 3.1.2 (Lidskii Theorem)**.** *Let A be a trace-class operator, $A \in \mathcal{S}_1$, and let $\lambda_i(A)$, $i \in I \subseteq \mathbb{N}$, be the non-zero eigenvalues of A, with their multiplicities considered. Then:*

$$\operatorname{tr} A = \sum_{i \in I} \lambda_i(A).$$

Proof. Cf. e.g. Theorem 6.1 in Ref. [GGK00]. □

Before concluding, we also recall the cyclic invariance property of trace.

Theorem 3.1.3. *Let A, B be linear operators acting in a Hilbert space such that both AB and BA are trace-class. Then the trace is invariant under cyclic permutations:*

$$\operatorname{tr}(AB) = \operatorname{tr}(BA).$$

Proof. Cf. e.g. Theorem 5.8 in Ref. [GGK00]. □

3.1.2 States in CAR Algebras and Entanglement

After the short review of the relevant fundamental theoretical topics in the previous Section, we now move forward and define the mathematical properties of a state describing a quantum-mechanical system of relativistic fermions in the formalism of C^*-algebras.

Definition 3.1.7. A state ω over a CAR algebra $\mathcal{A}_{\mathcal{H}}$ on the Hilbert space $\mathcal{H}$ is a linear functional $\omega : \mathcal{A}_{\mathcal{H}} \to \mathbb{C}$ with $\omega(I) = 1$ and $\omega(X^*X) \geq 0$ for all $X \in \mathcal{A}_{\mathcal{H}}$.

According to Example 5.2.20 in Ref. [BR02] and Chapter 3 in Ref. [Ara70] (cf. especially Lemma 3.3 therein for the proof of uniqueness), we introduce the concept of quasi-free state.

Definition 3.1.8 (Quasi-free state)**.** A state ω over a CAR algebra $\mathcal{A}_{\mathcal{H}}$ is called quasi-free if there exists a bounded linear self-adjoint operator $D \in \mathcal{A}_{\mathcal{H}}$ with $0 \leq D \leq I$, such that

$$\omega(a^*(f_1)\cdots a^*(f_m)a(g_1)\cdots a(g_n)) = \begin{cases} 0 & \text{if } m \neq n \\ \det\langle g_i, Df_j\rangle & \text{if } m = n, 1 \leq i \leq n, 1 \leq j \leq m \end{cases}$$

for any finite set $\{f_1, \ldots, f_m, g_1, \ldots, g_n\} \subset \mathcal{H}$ and $n, m \in \mathbb{N}$. The operator D is called the one-particle density operator of the state ω. The relation between quasi-free states and operators with the properties mentioned above is bijective.

Let $H_\alpha(t)$ be the Rényi entropy function for $t \in [0,1]$ and Rényi index $\alpha \in (0,1)$ as in Def. 2.4.2. Since the one-particle density operator D associated with a quasi-free state satisfies the operator inequality $0 \leq D \leq I$, the Spectral Theorem for self-adjoint operators ensures that the operator $H_\alpha(D)$ is well-defined (cf. e.g. Ref. [Car09]). The following definition, stemming from that of the von Neumann entropy, is therefore adequate.

Definition 3.1.9 (Rényi entropy of a quasi-free state)**.** Let D be the one-particle density operator that identifies the quasi-free state ω and let $\alpha \in (0,1)$ be the Rényi index. In case that the operator $H_\alpha(D)$ is trace-class, we define the Rényi entropy of ω as

$$S_\alpha(\omega) := \operatorname{tr} H_\alpha(D).$$

We now proceed towards the definition of a suitable measure for the entanglement of a system, when it is split into two subsystems. Given a state ω and a bipartite orthogonal decomposition $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ of the underlying Hilbert space into two closed subspaces $\mathcal{H}_1$ and $\mathcal{H}_2$, we use the isomorphism between the C^*-algebras $\mathcal{A}_{\mathcal{H}}$ and $\mathcal{A}_{\mathcal{H}_1} \otimes \mathcal{A}_{\mathcal{H}_1}$ to define partial states ω_1, ω_2 on the subalgebras $\mathcal{A}_{\mathcal{H}_1}$ and $\mathcal{A}_{\mathcal{H}_2}$ by

$$\begin{aligned} \omega_1(X) &:= \omega(X \otimes I), \quad X \in \mathcal{A}_{\mathcal{H}_1} \\ \omega_2(X) &:= \omega(I \otimes X), \quad X \in \mathcal{A}_{\mathcal{H}_2}, \end{aligned} \tag{3.2}$$

respectively.

If ω is a quasi-free state, then the partial states ω_1, ω_2 identified through Eq. 3.2 are quasi-free as well. If ω is characterized by the one-particle density operator D on the Hilbert space $\mathcal{H}$, then the partial states are characterized by the pinched operators $D_i := P_i D P_i$ (cf. Ref. [Dav59]), where $P_i : \mathcal{H} \to \mathcal{H}_i$ is the orthogonal projection from $\mathcal{H}$ onto $\mathcal{H}_i$, for $i = 1, 2$.

In the literature, several proposals for suitable measures of entanglement have been suggested and investigated based on the von Neumann entropy, including the relative and the mutual entropy of the bipartite system, cf. e.g. Ref. [Nis18]. The latter was also employed by Longo and Xu in their treatment [LX17]. It seems therefore reasonable and immediate to extend the concept of the von Neumann mutual entropy of a bipartite system to the Rényi case as an estimate of the amount of quantum correlations between the subsystems described by ω_1, ω_2 with respect to the original state ω.

Definition 3.1.10 (Bipartite Rényi entanglement entropy)**.** Let ω be a quasi-free state of a relativistic fermionic quantum system and let us consider a bipartition into two subsystems characterized by quasi-free states ω_1, ω_2, according to Eq. 3.2. Let $\alpha \in (0,1)$ be the Rényi index. Then the bipartite Rényi entanglement entropy between the quasi-free states ω and $\omega_1 \otimes \omega_2$ reads (cf. Def. 3.1.9)

$$\Delta S_\alpha(\omega, \omega_1 \otimes \omega_2) := S_\alpha(\omega_1 \otimes \omega_2) - S_\alpha(\omega).$$

Proposition 3.1.4. *For the bipartite Rényi entanglement entropy from Def. 3.1.10 between states ω and $\omega_1 \otimes \omega_2$ and Rényi index $\alpha \in (0,1)$, it holds:*

$$\Delta S_\alpha(\omega, \omega_1 \otimes \omega_2) = S_\alpha(\omega_1) + S_\alpha(\omega_2) - S_\alpha(\omega),$$

whenever the Rényi entropies of the states $\omega, \omega_1, \omega_2$ are well-defined.

Proof. According to e.g. Chapter II, Section 2 in Ref. [Thi02], the Rényi entropy of states ω_i, $i \in \{1,2\}$ may be written as $S_\alpha(\omega_i) = \frac{1}{1-\alpha} \ln \operatorname{tr} W_i^\alpha$ where W_i is a density operator in the fermionic Fock space $\mathcal{F}(\mathcal{H})$ upon the Hilbert space $\mathcal{H}$.

Therefore:

$$\begin{aligned}
S_\alpha(\omega_1 \otimes \omega_2) &= \frac{1}{1-\alpha} \ln(\operatorname{tr}(W_1 \otimes W_2)^\alpha) \\
&= \frac{1}{1-\alpha} \ln(\operatorname{tr} W_1^\alpha \cdot \operatorname{tr} W_2^\alpha) \\
&= \frac{1}{1-\alpha} (\ln(\operatorname{tr} W_1^\alpha) + \ln(\operatorname{tr} W_2^\alpha)) \\
&= S_\alpha(\omega_1) + S_\alpha(\omega_2)
\end{aligned}$$

where, in the second line, we used the property $\operatorname{tr}(A \otimes B) = \operatorname{tr} A \cdot \operatorname{tr} B$ for trace-class operators A, B. □

Motivated by Def. 3.1.9 and Proposition 3.1.4, we consider the following:

Definition 3.1.11 (Bipartite Rényi entanglement entropy operator)**.** Let $\alpha \in (0,1)$ be the Rényi index. Let P_i be the orthogonal projection operators from the Hilbert space $\mathcal{H}$ onto the subspaces $\mathcal{H}_i$, $i = 1, 2$. Let D be a one-particle density operator in $\mathcal{A}_\mathcal{H}$ and let $D_i := P_i D P_i$ be the corresponding pinched operators with $i = 1, 2$. We define the bipartite Rényi entanglement entropy operator as

$$\begin{aligned}
\sigma(\alpha, D, D_1, D_2) := \frac{1}{1-\alpha}(&-P_1 \ln(D^\alpha + (I-D)^\alpha)P_1 + P_1 \ln(D_1^\alpha + (P_1 - D_1)^\alpha)P_1 \\
&- P_2 \ln(D^\alpha + (I-D)^\alpha)P_2 + P_2 \ln(D_2^\alpha + (P_2 - D_2)^\alpha)P_2), \quad (3.3)
\end{aligned}$$

under the necessary condition that the operator $\sigma(\alpha, D, D_1, D_2)$ is trace-class.

By Defs. 3.1.10 and 3.1.11, the bipartite Rényi entanglement entropy between the composite state ω, characterized by the one-particle density operator D and the state $\omega_1 \otimes \omega_2$, where ω_i are characterized by the one-particle density operators D_i, $i = 1, 2$, simplifies to the trace of operator $\sigma(\alpha, D, D_1, D_2)$:

$$\Delta S_\alpha(\omega, \omega_1 \otimes \omega_2) = \operatorname{tr} \sigma(\alpha, D, D_1, D_2). \quad (3.4)$$

Eq. 3.4 is at this point just a formal one. To award a physical significance to it, two important questions must be clarified.

On one hand, the question concerning the traceability of the Rényi entanglement entropy operator σ, such that Eq. 3.4 is well-defined at all. This point will be analyzed in detail in Section 3.6, at least for the operator σ of a system of quasi-free fermions distributed on a finite subset of the real line.

On the other hand, the question concerning the positivity of the trace in Eq. 3.4 in the Rényi context. The von Neumann mutual entropy is known to be positive-definite, owing to the subadditivity property of the von Neumann entropy. The positivity of the Rényi operator will be addressed in the next Section starting from general considerations on its concavity.

3.2 Concavity of the Rényi Entanglement Entropy Operator

In this Section, we investigate the concavity property of the bipartite Rényi entanglement entropy operator that we introduced in Def. 3.1.11, which leads to the positivity of the quantity in Eq. 3.4.

As a high-level motivation for the present topic, we note along with Lieb [Lie14] that concavity is an essential property for the theory of thermodynamics as it was developed by Maxwell and Gibbs. Moreover, the positivity of the bipartite Rényi entanglement entropy operator σ also stems from the concavity property and, additionally, this has further important implications on its traceability, as we shall prove in Section 3.6. Therefore, concavity ensures that the bipartite Rényi entanglement entropy 3.4 is meaningful at all.

Definition 3.2.1. A function $f : I \to \mathbb{R}$, $I \subseteq \mathbb{R}^+$, is said to be operator-monotone whenever

$$A \leq B \implies f(A) \leq f(B)$$

for all positive operators $A, B \geq 0$ defined on a Hilbert space with spectra $\sigma(A), \sigma(B) \subseteq I$.

Definition 3.2.2. A function $f : I \to \mathbb{R}$, $I \subseteq \mathbb{R}^+$, is said to be operator-convex whenever

$$f((1-t)A + tB) \leq (1-t)f(A) + tf(B)$$

for all positive operators $A, B \geq 0$ defined on a Hilbert space with spectra $\sigma(A), \sigma(B) \subseteq I$ and $0 \leq t \leq 1$. A function f is said to be operator-concave if $-f$ is operator-convex.

Lemma 3.2.1. *The function $t \mapsto 1-t$, defined on $\mathbb{R}^+$, is operator-convex and operator-concave.*

Proof. The claim follows from the operator equality $I-((1-t)A+tB) = (1-t)(I-A)+t(I-B)$ that holds for all positive operators A, B. □

Lemma 3.2.2. *The set of operator-concave functions and the set of operator-monotone functions are closed under conical combinations.*

Proof. We consider two operator-concave functions $f_1 : I_1 \to \mathbb{R}$, $f_2 : I_2 \to \mathbb{R}$, $I_1, I_2 \subseteq \mathbb{R}^+$, and two non-negative weights $a_1, a_2 \geq 0$. Due to concavity, the relations

$$f_i((1-t)A + tB) \geq (1-t)f_i(A) + tf_i(B), \quad i = 1, 2$$

hold for all positive operators A, B defined on a Hilbert space with spectra $\sigma(A), \sigma(B) \in I_1 \cap I_2$.

Therefore:

$$\begin{aligned}(a_1 f_1 + a_2 f_2)((1-t)A + tB) &= a_1 f_1((1-t)A + tB) + a_2 f_2((1-t)A + tB)) \\ &\geq a_1((1-t)f_1(A) + tf_1(B)) + a_2((1-t)f_2(A) + tf_2(B)) \\ &= (1-t)(a_1 f_1 + a_2 f_2)(A) + t(a_1 f_1 + a_2 f_2)(B),\end{aligned}$$

since a_1, a_2 are non-negative. Hence the function $a_1 f_1 + a_2 f_2$, defined on $I_1 \cap I_2$ is operator-concave.

We now consider two operator-monotone functions $g_1 : I_1 \to \mathbb{R}$, $g_2 : I_2 \to \mathbb{R}$, with I_1, I_2 as above. Then, for positive operators $A \leq B$ defined on a Hilbert space with spectra $\sigma(A), \sigma(B) \in I_1 \cap I_2$, we get

$$\begin{aligned}(a_1 g_1 + a_2 g_2)(A) &= a_1 g_1(A) + a_2 g_2(A) \\ &\leq a_1 g_1(B) + a_2 g_2(B) \\ &= (a_1 g_1 + a_2 g_2)(B)\end{aligned}$$

since a_1, a_2 are non-negative, and hence the function $a_1 g_1 + a_2 g_2$ is operator-monotone. □

Theorem 3.2.3 (Löwner-Heinz). *Let $t \in [0,1]$. For $-1 \leq p \leq 0$, the function $f(t) = -t^p$ is operator-monotone and operator-concave. For $0 \leq p \leq 1$, the function $f(t) = t^p$ is operator-monotone and operator-concave. For $1 \leq p \leq 2$, the function $f(t) = t^p$ is operator-convex. Furthermore, let now $t \in (0,1)$. Then, $f(t) = \ln t$ is operator-concave and operator-monotone, while $f(t) = t \ln t$ is operator-convex.*

Proof. Cf. Refs. [Car09, Fur08]. □

Theorem 3.2.4. *Let S, T be bounded self-adjoint operators on a Hilbert space. Then:*

$$0 \leq S \leq T \implies S^\alpha \leq T^\alpha$$

for each α in the interval $[0,1]$.

Proof. Cf. Ref. [Löw34], Theorem 3 in Ref. [Hei51], as well as Ref. [Ped72]. □

Lemma 3.2.5. *Let $g : I \to \mathbb{R}$, $I \subseteq \mathbb{R}^+$, be operator-concave and operator-monotone and let $f : J \to \mathbb{R}$, $J \subseteq \mathbb{R}^+$, such that $f(J) \subseteq I$, be operator-concave. Then $g \circ f$ is operator-concave. If the function f is additionally operator-monotone, then $g \circ f$ is operator-monotone as well.*

Proof. Because function f is operator-concave, the relation

$$f((1-t)A + tB) \geq (1-t)f(A) + tf(B),$$

holds for all operators A, B on a Hilbert space with spectra $\sigma(A), \sigma(B) \subseteq J$ and every $0 \leq t \leq 1$.

Therefore, it follows

$$(g \circ f)((1-t)A + tB) \geq g((1-t)f(A) + tf(B)) \geq (1-t)(g \circ f)(A) + t(g \circ f)(B),$$

where we used, in the first inequality, the operator-monotonicity of g as well as the operator-concavity of f and, in the second inequality, the operator-concavity of g. This proves that $g \circ f$ is operator-concave.

In case f is additionally operator-monotone, we get for positive operators $A \leq B$ that

$$(g \circ f)(A) = g(f(A)) \leq g(f(B)) = (g \circ f)(B).$$

□

Theorem 3.2.6. *Let $\alpha \in (0,1)$. Then the Rényi entropy function $H_\alpha : [0,1] \to \mathbb{R}$, $H_\alpha(t) := \ln(t^\alpha + (1-t)^\alpha)$ is operator-concave.*

Proof. By Theorems 3.2.3 and 3.2.4 the function $g : [0,1] \to \mathbb{R}$, $g(t) := t^\alpha$, with $\alpha \in (0,1)$ is operator-monotone and operator-concave. By Lemma 3.2.1, the function $f : [0,1] \to \mathbb{R}$, $f(t) = 1 - t$ is operator-concave. Using Lemma 3.2.5 we may conclude that $(g \circ f) = (1-t)^\alpha$ is operator-concave. Lemma 3.2.2 guarantees the operator-concavity of the function $t^\alpha + (1-t)^\alpha$. Again, by Theorems 3.2.3 and 3.2.4 and Lemma 3.2.5 the claim follows. □

Theorem 3.2.7 (Davis-Sherman inequality). *For all operator-convex functions f on $\mathbb{R}^+$ and all orthogonal projections P, the inequality*

$$Pf(PAP)P \leq Pf(A)P$$

holds for every bounded self-adjoint positive operator A defined on a Hilbert space.

Proof. Cf. Refs. [Dav57] and [Dav59]. □

Theorem 3.2.8. *Let $f : \mathbb{R}^+ \to \mathbb{R}, t \mapsto f(t)$ be a continuous function. If f is operator-monotone increasing/convex/strictly convex, so is the mapping $A \mapsto \mathrm{tr} f(A)$, for every bounded self-adjoint positive operator A defined on a Hilbert space.*

Proof. Cf. Theorem 2.10 in Ref. [Car09]. □

It was pointed out in the literature [AIDS03], that plugging the Rényi entropy function directly into the definition of a mutual entropy is critical, since the trace of the Rényi bipartite entanglement entropy operator may become negative for some values of the Rényi index α. In the following result, we rule out this issue, in the $\alpha \in (0, 1)$ interval that we study in this Thesis.

Theorem 3.2.9. *Let $\alpha \in (0, 1)$. Then the Rényi bipartite entanglement entropy operator $\sigma(\alpha, D, D_1, D_2)$ originating from the one-particle density operator D and the pinched one-particle density operators $D_i := P_i D P_i$, $i = 1, 2$ (cf. Eq. 3.3) is positive. Moreover, the bipartite Rényi entanglement entropy satisfies the inequality*

$$\mathrm{tr}\, \sigma(\alpha, D, D_1, D_2) \geq 0.$$

Proof. By Theorems 3.2.6 and 3.2.7, by Def. 3.1.11, and recalling that the one-particle density operator D is by definition self-adjoint (cf. Def. 3.1.8), we get

$$-P_i \ln(D^\alpha + (I - D)^\alpha) P_i \geq -P_i \ln(D_i^\alpha + (P_i - D_i)^\alpha) P_i$$

for both $i = 1, 2$, whence $\sigma(\alpha, D, D_1, D_2) \geq 0$.

By Theorem 3.2.8, the trace preserves operator inequalities. Therefore, we get

$$\mathrm{tr}(P_i \ln(D^\alpha + (I - D)^\alpha) P_i) \leq \mathrm{tr}(P_i \ln(D_i^\alpha + (P_i - D_i)^\alpha) P_i)$$

and the second claim follows immediately. □

The Theorem above completely answers the second of the questions listed at the end of Section 3.1.2. Therefore, our definition 3.4 as a mutual entropy is adequate as a measure of entanglement.

The issue of the traceability of the bipartite Rényi entanglement entropy operator remains still open and will be discussed later in Section 3.6. We shall see that even in the proof of traceability the positivity enters as a central necessary requirement.

3.3 Fermionic Quasi-Free States on the Real Line

Here we intend to make the formal discussion from the previous Sections more concrete. Since we are going to study in detail a 1D system, we introduce the definition of the Hilbert transform and the related concept of projection operator onto the Hardy space on the real line.

We start with the well-known definition of the Hilbert space L^2.

Definition 3.3.1 (Hilbert space L^2 on the real line)**.** Let $D \subseteq \mathbb{R}$ be a Lebesgue-measurable set and let

$$L^2(D) := \{f : D \to \mathbb{C} : f \text{ Lebesgue-measurable}, |f|^2 \text{ Lebesgue-integrable}\}$$

be a vector space over $\mathbb{C}$ with scalar product and seminorm defined by, respectively,

$$\langle f, g\rangle_{L^2(D)} := \int_D \mathrm{d}x\, f(x)\overline{g(x)}, \qquad \|f\|_{L^2(D)} := \sqrt{\langle f, f\rangle_{L^2}}$$

for $f, g \in L^2(D)$. We define the Hilbert space $\mathcal{L}^2(D)$ as the quotient space $L^2(D)/\{f \in L^2(D) : \|f\|_{L^2(D)} = 0\}$ with scalar product $\langle [f], [g]\rangle_{\mathcal{L}^2(D)} := \langle f, g\rangle_{L^2(D)}$ and norm $\|[f]\|_{\mathcal{L}^2(D)} := \|f\|_{L^2(D)}$ for $[f], [g] \in \mathcal{L}^2(D)$. As customary in the mathematical literature, and to avoid cumbersome notation, we identify the space $\mathcal{L}^2(D)$ with the space $L^2(D)$, i.e. we do not distinguish between equivalence classes in $\mathcal{L}^2(D)$ and their representants in $L^2(D)$.

Following Ref. [RR94], we now define the Hardy space $H^2(\Pi_+)$ on the upper half-plane and from this we subsequently introduce the Hardy space on the real line as the vector space of the boundary functions of functions in $H^2(\Pi_+)$ in the limit of vanishing imaginary part.

Definition 3.3.2 (Hardy space on the upper complex half-plane Π_+)**.** Let

$$H^2(\Pi_+) := \left\{ F : \Pi_+ \to \mathbb{C} : F \text{ holomorph on } \Pi_+ \text{ and } \sup_{y>0} \left(\int_{-\infty}^{+\infty} \mathrm{d}x\, |F(x+iy)|^2 \right) < \infty \right\}$$

be a vector space over $\mathbb{C}$ with scalar product and seminorm defined by

$$\langle F, G\rangle_{H^2(\Pi_+)} := \sup_{y>0} \left(\int_{-\infty}^{+\infty} \mathrm{d}x\, F(x+iy)\overline{G(x+iy)} \right), \qquad \|F\|_{H^2(\Pi_+)} := \sqrt{\langle F, F\rangle_{H^2(\Pi_+)}}$$

for $F, G \in H^2(\Pi_+)$. We define the Hilbert space $\mathcal{H}^2(\Pi_+)$ as the quotient space $H^2(\Pi_+)/\{F \in H^2(\Pi_+) : \|F\|_{H^2(\Pi_+)} = 0\}$ with scalar product $\langle [F], [G]\rangle_{\mathcal{H}^2(\Pi_+)} := \langle F, G\rangle_{H^2(\Pi_+)}$ and norm $\|[F]\|_{\mathcal{H}^2(\Pi_+)} := \|F\|_{H^2(\Pi_+)}$ for $[F], [G] \in \mathcal{H}^2(\Pi_+)$. In analogy with our convention in Def. 3.3.1, we identify the space $\mathcal{H}^2(\Pi_+)$ with the space $H^2(\Pi_+)$.

Referring to Refs. [RR85, RR94], we specialize Def. 3.3.2 to the limit case of the real line.

Definition 3.3.3 (Hardy space on the real line)**.** The Hardy space over $\mathbb{C}$ on the real line is defined as the Hilbert space

$$H^2(\mathbb{R}) := \left\{ f : \mathbb{R} \to \mathbb{C} : \exists F \in H^2(\Pi_+) \text{ such that } f(x) = \lim_{y \downarrow 0} F(x+iy) \right\},$$

with the same scalar product as $L^2(\mathbb{R})$, i.e. $\langle f, g\rangle_{H^2(\mathbb{R})} := \langle f, g\rangle_{L^2(\mathbb{R})}$, for $f, g \in H^2(\mathbb{R})$.

With the help of a Theorem due to Riesz (cf. e.g. Ref. [RR94]), the following operator is well-defined and bounded.

Definition 3.3.4 (Hilbert transform)**.** The Hilbert transform is the operator on $L^2(\mathbb{R})$ onto itself that maps any $\phi \in L^2(\mathbb{R})$ into the function

$$\tilde{\phi}(x) := \frac{1}{\pi} \int_{-\infty}^{+\infty} \mathrm{d}y\, \frac{\phi(y)}{y-x},$$

which exists almost everywhere on the real line with respect to the Lebesgue measure. The integral above is intended as the Cauchy's principal integral.

We come now to a fundamental result from the theory of Hardy Spaces:

Theorem 3.3.1. *Let H be the Hilbert transform operator on $L^2(\mathbb{R})$ (cf. Def. 3.3.4) and let $P^0_{\mathbb{R}}$ be the projection operator of the Hilbert space $L^2(\mathbb{R})$ on the Hilbert space $H^2(\mathbb{R})$. Then:*

$$P^0_{\mathbb{R}} = \frac{1}{2}(I - iH), \tag{3.5}$$

i.e., equivalently,

$$(P^0_{\mathbb{R}}\phi)(x) = \frac{1}{2}\phi(x) + \frac{1}{2\pi i}\int_{-\infty}^{+\infty} \mathrm{d}y \, \frac{\phi(y)}{y-x}$$

for any $\phi \in L^2(\mathbb{R})$. The integral above is intended as the Cauchy's principal integral. Moreover, the projection operator $P^0_{\mathbb{R}}$ is orthogonal.

Proof. Result 3.5 follows from Ref. [RR94], Section 5.

The orthogonality of the projection operator $P^0_{\mathbb{R}}$ follows from the fact that the Hardy space $H^2(\mathbb{R})$ is a closed subspace of the Hilbert space $L^2(\mathbb{R})$, cf. Ref. [Bel92]. □

The orthogonal projection operator $P^0_{\mathbb{R}}$ from Theorem 3.3.1 above is of central significance. Since it is orthogonal, it is additionally self-adjoint and symmetric and it satisfies the relation $0 \leq P^0_{\mathbb{R}} \leq I$. Therefore, it describes a quasi-free state of a system of scalar particles.

For relativistic massless spin-$\frac{1}{2}$ particles, the system may be decomposed into states of definite chirality. Considering a spin-$\frac{1}{2}$ fermionic field in 1+1 time- and space-dimension, we choose the gamma matrices

$$\gamma^0 := \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma^1 := -i\sigma_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

as a basis of the 2-dimensional Clifford algebra [Pai62,Ken80], where we denote by $\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ the first two Pauli matrices.

We define the chirality operator as $\gamma^3 := \gamma^0\gamma^1$ (cf. e.g. Appendix A.2.1 in Ref. [Frè12]), and from this it follows immediately that it is Hermitian and fulfils the property $\gamma^3\gamma^3 = I$.

Operator $P^0_{\mathbb{R}}$ may be generalized in the case of fermions as follows[1] (cf. Refs. [CH09b, CH09a]):

$$P_{\mathbb{R}} := \frac{1}{2}(I - iH\gamma^3). \tag{3.6}$$

In the scientific physical literature (cf. e.g. Refs. [GR96], [Ker98]), the Dirac correlation operator describing a fermionic field for a pure quasi-free state in the massless limit is defined as the integral kernel $C(x,y)$ of operator $P_{\mathbb{R}}$ in Eq. 3.6. We implicitly define C by $(P_{\mathbb{R}}\phi)(x) = \int_{-\infty}^{+\infty} \mathrm{d}y \, C(x,y)\phi(y)$ for any 2-vector $\phi \in L^2(\mathbb{R}, \mathbb{C}^2)$.

According to Ref. [CH09b], the operator $P_{\mathbb{R}}$ is positive with eigenvalues in $[0,1]$. Therefore, it represents a valid one-particle density operator which generates exactly one fermionic quasi-free

[1] Note that, to avoid cumbersome notation, we employ throughout this Thesis the same symbol I for several identity operators defined on different spaces, e.g. on $L^2(\mathbb{R})$ in Eq. 3.5, on $\mathbb{C}^2$ in the discussion of the chirality operator and on $L^2(\mathbb{R}, \mathbb{C}^2)$ in Eq. 3.6.

state ω in the C^*-algebra on the Hilbert space $L^2(\mathbb{R}, \mathbb{C}^2)$ (cf. Def. 3.1.8). The quasi-free state ω is characterized by

$$\omega(a^*(f_1)\cdots a^*(f_m)a(g_1)\cdots a(g_n)) = \begin{cases} 0 & \text{if } m \neq n \\ \det\langle g_i, P_{\mathbb{R}} f_j\rangle & \text{if } m = n, 1 \leq i \leq n, 1 \leq j \leq m \end{cases}$$

for any finite set $\{f_1, \ldots, f_m, g_1, \ldots, g_n\} \subset L^2(\mathbb{R}, \mathbb{C}^2)$ and $m, n \in \mathbb{N}$.

3.4 The Regularized Rényi Entropy Operator

In this Section, our aim is to calculate the bipartite Rényi entanglement entropy $\operatorname{tr}\sigma(\alpha, D, D_1, D_2)$ for $\alpha \in (0, 1)$ (cf. Def. 3.1.11 and Eq. 3.4), where D is the one-particle density operator describing the fermionic quasi-free state of a multiparticle system and D_1, D_2 are the one-particle density operators of a partition of the system.

According to our discussion in Section 3.3, we take as one-particle density operator the self-adjoint orthogonal projection operator from Eq. 3.6. Therefore, we make the identification $D := P_{\mathbb{R}}$.

Relying on the Spectral Theorem, we plan to plug the one-particle density operator D into the bipartite Rényi entanglement entropy operator σ (cf. Def. 3.1.11), and we intend to employ our Nevanlinna-Herglotz integral representation of the Rényi entropy function that we derived in Theorem 2.4.1. However, the restriction of the Nevanlinna-Herglotz integral representation to the real line is defined on the open interval $(0, 1)$ only, while the one-particle density operator satisfies the weaker inequality $0 \leq D \leq I$. Therefore, care is required when plugging D into operator σ.

To circumvent this issue, we introduce the regularized operator $E_\epsilon := \frac{1}{1+2\epsilon}(D + \epsilon I)$, which may be plugged into σ without concern because

$$0 < \frac{\epsilon}{1+2\epsilon} I \leq E_\epsilon \leq \frac{1+\epsilon}{1+2\epsilon} I < I \tag{3.7}$$

for $\epsilon > 0$. On the other hand, in the $\epsilon \to 0$ limit, the regularized operator E_ϵ tends to D strongly, since the limit

$$\left\| D - \frac{1}{1+2\epsilon}(D + \epsilon I) \right\| = \frac{\epsilon}{1+2\epsilon} \|2D - I\| \to 0$$

holds in the $L^2(\mathbb{R}, \mathbb{C}^2)$ operator norm.

In our Nevanlinna-Herglotz integral representation of the complex Rényi entropy function (cf. Theorem 2.4.1) a central role is played by the function $R_z(\lambda) := \frac{1}{z - \frac{1}{2} + \lambda}$ in Eq. 2.29. By virtue of the Spectral Theorem for self-adjoint operators, inserting the regularized operator E_ϵ into R_z we get the expression

$$\begin{aligned} R_{E_\epsilon}(\lambda) &:= \left(E_\epsilon - \left(\frac{1}{2} - \lambda \right) I \right)^{-1} \\ &= \left(\frac{1}{1+2\epsilon}(D + \epsilon I) - \left(\frac{1}{2} - \lambda \right) I \right)^{-1} \\ &= (1+2\epsilon) \left(D - \left(\frac{1}{2} - (1+2\epsilon)\lambda \right) I \right)^{-1} \\ &= (1+2\epsilon) R_D((1+2\epsilon)\lambda), \end{aligned} \tag{3.8}$$

which represents the resolvent of operator E_ϵ on $L^2(\mathbb{R})$, defined for values of λ for which the operator $E_\epsilon - \left(\frac{1}{2} - \lambda\right) I$ is invertible.

In Theorem 3.5.1 we shall address the question for which real λ values the inversion of the latter operator is possible and the resolvent is well-defined, at least for the special case of a system of fermions distributed on the real line. We anticipate here that this is possible on the set $\mathbb{R} \setminus \left[-\frac{1}{2}, \frac{1}{2}\right]$. Therefore, by Theorem 2.4.1 and Eq. 3.8, we are allowed to plug without concern the regularized operator E_ϵ into our Nevanlinna-Herglotz integral representation of the Rényi entropy function.

Therefore, the Rényi entropy operator reads

$$\begin{aligned}
&\frac{1}{1-\alpha}\ln(E_\epsilon^\alpha + (I - E_\epsilon)^\alpha) = \\
&= \frac{B(\alpha)}{1-\alpha} - \frac{1}{1-\alpha}\int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda\, f_\alpha(\lambda)\left(R_{E_\epsilon}(\lambda) - R_{E_\epsilon}(-\lambda) + \frac{\frac{1}{2}-\lambda}{\left(\frac{1}{2}-\lambda\right)^2+1} - \frac{\frac{1}{2}+\lambda}{\left(\frac{1}{2}+\lambda\right)^2+1}\right) \\
&= \frac{B(\alpha)}{1-\alpha} - \frac{1}{1-\alpha}\int_{\frac{1}{2}(1+2\epsilon)}^{+\infty} \mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right)\left(R_D(\lambda) - R_D(-\lambda)\right. \\
&\qquad \left. + \frac{\frac{1}{2}-\frac{\lambda}{1+2\epsilon}}{\left(\frac{1}{2}-\frac{\lambda}{1+2\epsilon}\right)^2+1} - \frac{\frac{1}{2}+\frac{\lambda}{1+2\epsilon}}{\left(\frac{1}{2}+\frac{\lambda}{1+2\epsilon}\right)^2+1}\right),
\end{aligned} \tag{3.9}$$

where the functions B and f_α were defined in Defs. 2.23 and 2.24 and as usual $\alpha \in (0, 1)$.

3.5 Integral Representation of the Bipartite Rényi Entanglement Entropy Operator

3.5.1 Quasi-Free Fermionic States

We want now to apply Def. 3.1.11 of the bipartite Rényi entanglement entropy operator to a concrete quantum system that may be treated analytically.

To this aim, we define in detail the spatial domain of the system. Let us pick $n \in \mathbb{N}$, choose $2n$ real numbers in ascending order, $a_1 < b_1 < a_2 < b_2 < \cdots < a_n < b_n$, and denote the index set $\mathbb{N}_n := \{1, \ldots, n\}$. Let $\mathcal{I} := \bigcup_{i\in\mathbb{N}_n} \mathcal{I}_i$ be the finite set where the intervals $\mathcal{I}_i := (a_i, b_i)$ are pairwise disjoint, i.e. $\overline{\mathcal{I}}_i \cap \overline{\mathcal{I}}_j = \emptyset$, $i, j \in \mathbb{N}_n$, $i \neq j$. We consider the case of a fermionic quasi-free system stretched across the open set $\mathcal{I} \subset \mathbb{R}$ on the real axis.

Since we aim at calculating the bipartite Rényi entanglement entropy of the system, we partition it into two disjoint subsystems, distributed on the sets $\mathcal{I}^1, \mathcal{I}^2$ of the real axis respectively. To this purpose, we choose two integers $n_1, n_2 > 0$ such that $n_1 + n_2 = n$ and we take two index partitions $I_1, I_2 \subset \mathbb{N}_n$ of n_1, n_2 elements each, such that $I_1 \cup I_2 = \mathbb{N}_n$ and $I_1 \cap I_2 = \emptyset$. We then set $\mathcal{I}^i := \bigcup_{j\in I_i} \mathcal{I}_j$, $i = 1, 2$, in the notation discussed above.

3.5.2 Resolvent of the One-Particle Density Operator

We denote by $D_\mathcal{I}$ the one-particle density operator derived by $D := P_\mathbb{R}$ (cf. Section 3.4), restricting the Cauchy's principal value integral to the real set $\mathcal{I}$ defined in Section 3.5.1. The corresponding pinched one-particle density operators of the two system partitions are then given by $D_{\mathcal{I}^1}, D_{\mathcal{I}^2}$, through restrictions of the Cauchy's principal value integral to the subsets $\mathcal{I}^1, \mathcal{I}^2$.

Eq. 3.9 expresses the Rényi entropy operator in an integral form that is suitable to evaluate $\sigma(\alpha, D_\mathcal{I}, D_{\mathcal{I}^1}, D_{\mathcal{I}^2})$, since the system's one-particle density operator $D_\mathcal{I}$ appears in the

Nevanlinna-Herglotz integral representation only through its resolvent

$$R_{D_{\mathcal{I}}}(\lambda) := \left(D_{\mathcal{I}} - \left(\frac{1}{2} - \lambda\right)I\right)^{-1} \tag{3.10}$$

calculated in the point $\frac{1}{2} - \lambda$, for real $\lambda > \frac{1}{2}(1 + 2\epsilon)$. In the following Theorem, we prove that Eq. 3.10 is well-defined, and we seek an explicit form of the resolvent.

Theorem 3.5.1. *Let $D_{\mathcal{I}}$ be the one-particle density operator such that*

$$(D_{\mathcal{I}}\phi)(x) = \frac{1}{2}\phi(x) + \frac{1}{2\pi i}\int_{\mathcal{I}} \mathrm{d}y\, \frac{1}{y-x}\gamma^3\phi(y) \tag{3.11}$$

for any $\phi \in L^2(\mathcal{I}, \mathbb{C}^2)$, $x \in \mathcal{I}$, where the integral above is intended as the Cauchy's principal integral value. Let $R_{D_{\mathcal{I}}}(\lambda)$ be the inverse of the operator $D_{\mathcal{I}} - \left(\frac{1}{2} - \lambda\right)I$ (cf. Eq. 3.10).

Then the operator $R_{D_{\mathcal{I}}}(\lambda)$ is well-defined for $\lambda \in \mathbb{C}\setminus\left\{z \in \mathbb{C} | -\frac{1}{2} \leq \mathrm{Re}z \leq \frac{1}{2}, \mathrm{Im}z = 0\right\}$ and reads explicitly

$$(R_{D_{\mathcal{I}}}(\lambda)\chi)(x) = \frac{1}{\lambda^2 - \frac{1}{4}}\left(\lambda\chi(x) - \frac{1}{2\pi i}\int_{\mathcal{I}} \mathrm{d}y\, K_{\mathcal{I}}(\lambda, x, y)\chi(y)\right) \tag{3.12}$$

for $\chi \in H^2(\mathcal{I}, \mathbb{C}^2)$, where the integral is again intended as the Cauchy's principal integral value. The integration kernel in 3.12 reads

$$K_{\mathcal{I}}(\lambda, x, y) := \frac{1}{y-x}\gamma^3 \exp\left(\frac{1}{2\pi i}\ln\left(\frac{2\lambda - 1}{2\lambda + 1}\right)(Z_{\mathcal{I}}(y) - Z_{\mathcal{I}}(x))\gamma^3\right), \tag{3.13}$$

with the definition

$$Z_{\mathcal{I}}(w) := \ln\left(\frac{\prod_{i\in\mathbb{N}_n}(w - a_i)}{\prod_{i\in\mathbb{N}_n}(w - b_i)}\right). \tag{3.14}$$

Proof. We search for complex numbers μ, such that the equation:

$$((D_{\mathcal{I}} - \mu I)\phi)(x) = \chi(x), \tag{3.15}$$

has a solution for any function $\chi \in H^2(\mathcal{I}, \mathbb{C}^2)$.

Eq. 3.15 is equivalent to the singular integral equation

$$\left(\frac{1}{2} - \mu\right)\phi(x) + \frac{1}{2\pi i}\int_{\mathcal{I}} \mathrm{d}y\, \frac{1}{y-x}\gamma^3\phi(y) = \chi(x), \tag{3.16}$$

where as usual the integral above is intended as the Cauchy's principal integral.

The general solution of a singular integral equation of the type above for an integration contour of n disjoint arcs of continuously changing curvature was derived in §27 of Ref. [Mik64] and Chapter 14 of Ref. [Mus53]. Recalling that, in our definition, $\mathcal{I}$ is a subset of the real line and therefore, it may be interpreted as the image of n curves of constant curvature, the results from Refs. [Mus53, Mik64] may be employed. However, special caution is required since Eq. 3.16, owing to γ^3, represents a linear system of equations with matrix coefficients instead of a single scalar equation.

The general solution of Eq. 3.16 reads

$$\phi(x) = \frac{1}{\left(\frac{1}{2} - \mu\right)^2 - \frac{1}{4}}\left(\left(\frac{1}{2} - \mu\right)\chi(x)\right.$$

$$- \frac{1}{2\pi i} \prod_{k \in N_n} \left(\frac{x - a_k}{x - b_k} \right)^m \sum_{i \in N_n} \int_{a_i}^{b_i} \mathrm{d}y \prod_{k \in N_n} \left(\frac{y - b_k}{y - a_k} \right)^m \frac{1}{y - x} \gamma^3 \chi(y) \Bigg) \tag{3.17}$$

where $a := \left(\frac{1}{2} - \mu\right) I$, $b := \frac{1}{2}\gamma^3$ and m is a function of a, b. The exponent m may be explicitly expressed by

$$\begin{aligned}
m :&= \frac{1}{2\pi i}(\ln(a+b) - \ln(a-b)) \\
&= \frac{1}{2\pi i}\left(\ln\left(\left(\frac{1}{2} - \mu \right) I + \frac{1}{2}\gamma^3 \right) - \ln\left(\left(\frac{1}{2} - \mu \right) I - \frac{1}{2}\gamma^3 \right) \right) \\
&= \frac{1}{2\pi i} \sum_{n=1}^{\infty} \frac{1}{n} \left(\frac{1}{1 - 2\mu} \right)^n ((-1)^{n+1} + 1)(\gamma^3)^n \\
&= \frac{1}{\pi i} \sum_{k=0}^{\infty} \frac{1}{2k+1} \left(\frac{1}{1 - 2\mu} \right)^{2k+1} (\gamma^3)^{2k+1} \\
&= \frac{1}{\pi i} \operatorname{arctanh}\left(\frac{1}{1 - 2\mu} \right) \gamma^3 \\
&= \frac{1}{2\pi i} \ln\left(\frac{\mu - 1}{\mu} \right) \gamma^3,
\end{aligned} \tag{3.18}$$

where we used the identities $\operatorname{arctanh} x = \frac{1}{2}\log\left(\frac{1+x}{1-x}\right)$, $(\gamma^3)^{2k+1} = (\gamma^3\gamma^3)^k\gamma^3 = \gamma^3$ and the fact that the factor $(-1)^{n+1} + 1 = 2$ for odd values of n while it vanishes for even values of n.

Solution 3.17 is only well-defined for $\mu \in \mathbb{C} \setminus \{z \in \mathbb{C} | 0 \leq \mathrm{Re} z \leq 1, \mathrm{Im} z = 0\}$, since the argument $\frac{\mu-1}{\mu}$ of the logarithm in Eq. 3.18 must be strictly positive when restricted to the real axis and moreover, the denominator $\left(\frac{1}{2} - \mu\right)^2 - \frac{1}{4}$ in 3.17 must not vanish. Therefore, the invertibility of operator $D_{\mathcal{I}} - \mu I$ is guaranteed on the complex domain $\mathbb{C} \setminus \{z \in \mathbb{C} | 0 \leq \mathrm{Re} z \leq 1, \mathrm{Im} z = 0\}$ only.

Rearranging the terms in 3.17 and setting $\mu = \frac{1}{2} - \lambda$, Eq. 3.17 leads to the claim. □

Proceeding towards a suitable representation of operator $\frac{1}{1-\alpha}\ln(D_{\mathcal{I}}^\alpha + (I - D_{\mathcal{I}})^\alpha)$ in integral form, we recall that the difference of the resolvent operators $R_{D_{\mathcal{I}}}(\lambda) - R_{D_{\mathcal{I}}}(-\lambda)$ appears in the Nevanlinna-Herglotz integral representation (cf. Eq. 3.9). Therefore, we investigate this difference more thoroughly.

Lemma 3.5.2. *The difference of the resolvent operators of $D_{\mathcal{I}}$ calculated in $\pm\lambda$ for values $\lambda \in \mathbb{R} \setminus \left[-\frac{1}{2}, +\frac{1}{2}\right]$ is expressed by the operator*

$$((R_{D_{\mathcal{I}}}(\lambda) - R_{D_{\mathcal{I}}}(-\lambda))\chi)(x) = \frac{2\lambda}{\lambda^2 - \frac{1}{4}}\chi(x) + \int_{\mathcal{I}} \mathrm{d}y\, \Delta K_{\mathcal{I}}(\lambda, x, y)\chi(y)$$

for $\chi \in H^2(\mathcal{I}, \mathbb{C}^2)$. The integration kernel reads

$$\begin{aligned}
\Delta K_{\mathcal{I}}(\lambda, x, y) :&= -\frac{1}{2\pi i\left(\lambda^2 - \frac{1}{4}\right)}(K_{\mathcal{I}}(\lambda, x, y) - K_{\mathcal{I}}(-\lambda, x, y)) \\
&= \frac{\sin\left(\frac{1}{2\pi}\ln\left(\frac{2\lambda-1}{2\lambda+1}\right)(Z_{\mathcal{I}}(y) - Z_{\mathcal{I}}(x))\right)}{\pi\left(\lambda^2 - \frac{1}{4}\right)(y - x)} I,
\end{aligned} \tag{3.19}$$

and is defined for $\lambda \in \mathbb{R} \setminus \left[-\frac{1}{2}, \frac{1}{2}\right]$ and $x, y \in \mathcal{I}$.

Proof. The statement follows from Theorem 3.5.1 by direct calculation. Indeed:

$$((R_{D_{\mathcal{I}}}(\lambda) - R_{D_{\mathcal{I}}}(-\lambda))\chi)(x) = \frac{2\lambda}{\lambda^2 - \frac{1}{4}}\chi(x) - \frac{1}{2\pi i(\lambda^2 - \frac{1}{4})}\int_{\mathcal{I}} \mathrm{d}y\,(K_{\mathcal{I}}(\lambda, x, y) - K_{\mathcal{I}}(-\lambda, x, y))\chi(y)$$

where (cf. Eq. 3.13)

$$\begin{aligned}
K_{\mathcal{I}}(\lambda, x, y) - K_{\mathcal{I}}(-\lambda, x, y) &= \frac{1}{y-x}\gamma^3\left(e^{\frac{1}{2\pi i}\ln\left(\frac{2\lambda-1}{2\lambda+1}\right)(Z_{\mathcal{I}}(y)-Z_{\mathcal{I}}(x))\gamma^3} - e^{\frac{1}{2\pi i}\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)(Z_{\mathcal{I}}(y)-Z_{\mathcal{I}}(x))\gamma^3}\right)\\
&= \frac{1}{y-x}\gamma^3\left(e^{\frac{1}{2\pi i}\ln\left(\frac{2\lambda-1}{2\lambda+1}\right)(Z_{\mathcal{I}}(y)-Z_{\mathcal{I}}(x))\gamma^3} - e^{-\frac{1}{2\pi i}\ln\left(\frac{2\lambda-1}{2\lambda+1}\right)(Z_{\mathcal{I}}(y)-Z_{\mathcal{I}}(x))\gamma^3}\right)\\
&= \frac{1}{y-x}\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{1}{2\pi i}\ln\left(\frac{2\lambda-1}{2\lambda+1}\right)(Z_{\mathcal{I}}(y)-Z_{\mathcal{I}}(x))\right)^n(1-(-1)^n)(\gamma^3)^{n+1}\\
&= \frac{2}{y-x}\sum_{k=0}^{\infty}\frac{1}{(2k+1)!}\left(\frac{1}{2\pi}\ln\left(\frac{2\lambda-1}{2\lambda+1}\right)(Z_{\mathcal{I}}(y)-Z_{\mathcal{I}}(x))\right)^{2k+1}(-i)^{2k+1}(\gamma^3)^{2(k+1)}\\
&= -\frac{2i}{y-x}\sum_{k=0}^{\infty}\frac{(-1)^k}{(2k+1)!}\left(\frac{1}{2\pi}\ln\left(\frac{2\lambda-1}{2\lambda+1}\right)(Z_{\mathcal{I}}(y)-Z_{\mathcal{I}}(x))\right)^{2k+1}I^{k+1}\\
&= -\frac{2i}{y-x}\sin\left(\frac{1}{2\pi}\ln\left(\frac{2\lambda-1}{2\lambda+1}\right)(Z_{\mathcal{I}}(y)-Z_{\mathcal{I}}(x))\right)I
\end{aligned}$$

where we exploited the property of the chirality operator that $\gamma^3\gamma^3 = I$ and the fact that $1-(-1)^n = 2$ for odd values of n whereas it vanishes for even values. The last equality immediately yields the claim. □

To simplify the notation, from now on we shall suppress the identity operator I appearing in the definition of operator $\Delta K_{\mathcal{I}}$ or any other operator derived from it. We tacitly assume that I is always present whenever operators are applied to χ.

3.5.3 Integral Kernel of the Bipartite Rényi Entanglement Entropy Operator

The operator $\sigma(\alpha, D_{\mathcal{I}}, D_{\mathcal{I}^1}, D_{\mathcal{I}^2})$ with $\alpha \in (0,1)$ from Def. 3.1.10 contains two terms of the form

$$\frac{1}{1-\alpha}(-P_i\ln(D_{\mathcal{I}}^\alpha + (I - D_{\mathcal{I}})^\alpha)P_i + P_i\ln(D_{\mathcal{I}^i}^\alpha + (P_i - D_{\mathcal{I}^i})^\alpha)P_i) \tag{3.20}$$

arising from each of the disjoint subsystems $i = 1, 2$ in which we split the fermionic quasi-free state under investigation (cf. Section 3.5.1). By Eq. 3.9, operator 3.20 in its regularized form (cf. Section 3.4) admits an integral representation involving the resolvents of $D_{\mathcal{I}}$ and $D_{\mathcal{I}^i}$ only, each of which evaluated in the points λ and $-\lambda$. For any $\chi \in H^2(\mathcal{I}, \mathbb{C}^2)$ and $i = 1, 2$, we get the following form of the i-th part of the regularized bipartite Rényi entanglement entropy operator

$$\begin{aligned}
&\frac{1}{1-\alpha}\int_{\frac{1}{2}(1+2\epsilon)}^{+\infty}\mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right)((P_iR_{D_{\mathcal{I}}}(\lambda)P_i - P_iR_{D_{\mathcal{I}}}(-\lambda)P_i - P_iR_{D_{\mathcal{I}^i}}(\lambda)P_i + P_iR_{D_{\mathcal{I}^i}}(-\lambda)P_i)\chi)(x)\\
&= \frac{1}{1-\alpha}\int_{\frac{1}{2}(1+2\epsilon)}^{+\infty}\mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right)\int_{\mathcal{I}^i}\mathrm{d}y\,(\Delta K_{\mathcal{I}}(\lambda, x, y) - \Delta K_{\mathcal{I}^i}(\lambda, x, y))\chi(y).
\end{aligned} \tag{3.21}$$

Note that the integration domain in the inner integral of Eq. 3.21 is restricted to the interval $\mathcal{I}^i$ only where subsystem i is localized as a result of pinching the resolvents $R_{D_{\mathcal{I}}}(\pm\lambda)$ with the orthogonal projection operator P_i onto the spatial domain of subsystem i.

The integral kernel $\Delta K_{\mathcal{I}}(\lambda,x,y)-\Delta K_{\mathcal{I}^i}(\lambda,x,y)$ in Eq. 3.21 does not contain any information about the functional form of the underlying entropy which describes the fermionic system, i.e. the same kernel applies equally well to either the von Neumann or the Rényi entropy. It only depends on the spatial domains $\mathcal{I}$ and $\mathcal{I}^1,\mathcal{I}^2$ of the whole system and of the two subsystems, according to Eq. 3.19. Its analytic properties are summarized in Lemma 3.5.3 below. Instead, the detailed information on the functional form of the entropy is localized in the function $\frac{1}{1-\alpha}f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right)$, where as usual f_α comes from Eq. 2.24. We recall that the latter function may be interpreted as the derivative of the generating function of the measure in the Nevanlinna-Herglotz integral representation (cf. Lemma 2.1.4).

Lemma 3.5.3. *For $i=1,2$ and on the domain $\mathcal{D}_{G_i}:=\left(\frac{1}{2},+\infty\right)\times\mathcal{I}^i\times\mathcal{I}^i$, it holds:*

$$
\begin{aligned}
G_{\mathcal{I},\mathcal{I}^i}(\lambda,x,y) &:= \pi\left(\lambda^2-\frac{1}{4}\right)(\Delta K_{\mathcal{I}}(\lambda,x,y)-\Delta K_{\mathcal{I}^i}(\lambda,x,y))\\
&= \begin{cases} \frac{\sin\left(\frac{1}{2\pi}\ln\left(\frac{2\lambda-1}{2\lambda+1}\right)(Z_{\mathcal{I}}(y)-Z_{\mathcal{I}}(x))\right)-\sin\left(\frac{1}{2\pi}\ln\left(\frac{2\lambda-1}{2\lambda+1}\right)(Z_{\mathcal{I}^i}(y)-Z_{\mathcal{I}^i}(x))\right)}{y-x} & \text{if } x\neq y\\ \frac{1}{2\pi}\ln\left(\frac{2\lambda-1}{2\lambda+1}\right)(Z'_{\mathcal{I}}(x)-Z'_{\mathcal{I}^i}(x)) & \text{if } x=y. \end{cases}
\end{aligned}
$$

The functions $Z_{\mathcal{I}},Z_{\mathcal{I}^i}$ are defined in 3.14 and their derivatives read

$$
Z'_{\mathcal{I}}(x)=\sum_{j\in\mathbb{N}_n}\left(\frac{1}{x-a_j}-\frac{1}{x-b_j}\right),\qquad Z'_{\mathcal{I}^i}(x)=\sum_{j\in I_i}\left(\frac{1}{x-a_j}-\frac{1}{x-b_j}\right). \tag{3.22}
$$

Moreover, the kernel $G_{\mathcal{I},\mathcal{I}^i}(\lambda,x,y)$ as a function of λ,x,y is continuous in each of the variables on the definition domain $\mathcal{D}_{G_i}$ and is bounded according to inequality

$$
|G_{\mathcal{I},\mathcal{I}^i}(\lambda,x,y)|\leq\frac{M}{2\pi}\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)
$$

for a positive constant M.

Proof. As discussed before the claim of the present Lemma, operator $G_{\mathcal{I},\mathcal{I}^i}$ does not depend on the explicit functional form of the entropy. Therefore, we inherit here the results from Lemmas 3.13 and 3.14 in Ref. [LX17], that were derived in the case of the von Neumann-entropy.

Formulas 3.22 follow from 3.14 by direct calculation of the first derivative. □

Combining Eqs. 3.20 and 3.21 with the help of Lemmas 3.5.2 and 3.5.3, the contribution of the regularized operator E_ϵ from subsystem i to the bipartite Rényi entanglement operator reads

$$
\begin{aligned}
&\frac{1}{1-\alpha}((-P_i\ln(E_\epsilon^\alpha+(I-E_\epsilon)^\alpha)P_i+P_i\ln((P_iE_\epsilon P_i)^\alpha+(P_i-P_iE_\epsilon P_i)^\alpha)P_i)\chi)(x)\\
&=\frac{1}{1-\alpha}\int_{\frac{1}{2}(1+2\epsilon)}^{+\infty}\mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right)\int_{\mathcal{I}^i}\mathrm{d}y\,(\Delta K_{\mathcal{I}}(\lambda,x,y)-\Delta K_{\mathcal{I}^i}(\lambda,x,y))\chi(y)\\
&=\frac{1}{\pi(1-\alpha)}\int_{\frac{1}{2}(1+2\epsilon)}^{+\infty}\mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right)\frac{1}{\lambda^2-\frac{1}{4}}\int_{\mathcal{I}^i}\mathrm{d}y\,G_{\mathcal{I},\mathcal{I}^i}(\lambda,x,y)\chi(y)
\end{aligned} \tag{3.23}
$$

for any $\chi\in H^2(\mathcal{I},\mathbb{C}^2)$.

3.5.4 Analytic Properties of the Integral Kernel

To study the behaviour of operator 3.23 in the $\epsilon \to 0$ limit, we introduce yet another integral kernel,

$$\tilde{K}_i(\epsilon, \alpha, x, y) := \frac{1}{\pi(1-\alpha)} \int_{\frac{1}{2}(1+2\epsilon)}^{+\infty} \mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right) \frac{G_{\mathcal{I},\mathcal{I}^i}(\lambda, x, y)}{\lambda^2 - \frac{1}{4}}, \tag{3.24}$$

with definition domain $(0, +\infty) \times (0, 1) \times \mathcal{I}^i \times \mathcal{I}^i$, $i = 1, 2$, and image in $\mathbb{R}$.

To start with the analysis of $\tilde{K}_i$, we first prove two straightforward properties of the function f_α that, as we recall, represents the derivative of the generating function of the Nevanlinna-Herglotz measure and summarizes the whole information on the exact form of the entropy.

Lemma 3.5.4. *The function*

$$f_\alpha(\lambda) := \frac{1}{\pi} \arctan\left(\frac{\left(\frac{2\lambda-1}{2\lambda+1}\right)^\alpha \sin\alpha\pi}{1 + \left(\frac{2\lambda-1}{2\lambda+1}\right)^\alpha \cos\alpha\pi}\right)$$

from 2.24 is continuous and strictly monotone increasing on the interval $\lambda \in \left[\frac{1}{2}, +\infty\right)$ for any fixed $\alpha \in (0, 1)$.

Proof. The function f_α is continuous as composition of continuous functions.

Regarding monotonicity, we first observe that $\frac{2\lambda-1}{2\lambda+1}$ is strictly monotone increasing in the considered interval since its first derivative with respect to λ reads $\frac{4}{(2\lambda+1)^2} > 0$.

Moreover, for $\lambda \geq \frac{1}{2}$, and setting $y := \frac{2\lambda-1}{2\lambda+1}$, $C := \cos\alpha\pi$ and $S := \sin\alpha\pi$, with $0 < y < 1$, $-1 < C < 1$ and $0 < S \leq 1$, the function $\frac{y^\alpha S}{1+y^\alpha C}$ is strictly monotone increasing as well, since its first derivative with respect to variable y reads $\frac{\alpha S}{y^{1-\alpha}(1+y^\alpha C)^2} > 0$.

The statement follows because f_α is the composition of strictly monotone increasing functions. □

Lemma 3.5.5. *Let $\alpha \in (0, 1)$. Then, it exists a positive constant N_α such that*

$$0 \leq f_\alpha(\lambda) = |f_\alpha(\lambda)| \leq N_\alpha \left(\lambda - \frac{1}{2}\right)^\alpha$$

for $\lambda \in \left[\frac{1}{2}, +\infty\right)$.

Additionally, the following upper bound holds as well:

$$N_\alpha \leq \frac{1}{1-\alpha}, \tag{3.25}$$

dependent on the value of the Rényi parameter α.

Proof. The function $\frac{2\lambda-1}{2\lambda+1}$ is continuous and strictly monotone increasing for $\lambda \geq \frac{1}{2}$, with bounds $0 \leq \frac{2\lambda-1}{2\lambda+1} < 1$ (cf. proof of Lemma 3.5.4). Therefore, f_α is by definition always non-negative in the λ interval.

Combining the inequality $\arctan x \leq x$ for non-negative x values with the inequality

$$1 + \left(\frac{2\lambda-1}{2\lambda+1}\right)^\alpha \cos\alpha\pi \geq 1 - \left(\frac{2\lambda-1}{2\lambda+1}\right)^\alpha |\cos\alpha\pi| \geq 1 - |\cos\alpha\pi|,$$

we get

$$f_\alpha(\lambda) \leq \frac{1}{\pi}\frac{\left(\frac{2\lambda-1}{2\lambda+1}\right)^\alpha \sin\alpha\pi}{1+\left(\frac{2\lambda-1}{2\lambda+1}\right)^\alpha \cos\alpha\pi} \leq \frac{\sin\alpha\pi}{\pi(1-|\cos\alpha\pi|)}\left(\frac{2\lambda-1}{2\lambda+1}\right)^\alpha \leq \frac{\sin\alpha\pi}{\pi(1-|\cos\alpha\pi|)}\left(\lambda-\frac{1}{2}\right)^\alpha$$

whence the assertion follows, since $0 \leq |\cos\alpha\pi| < 1$ for $\alpha \in (0,1)$.

We consider now $N_\alpha := \frac{\sin\alpha\pi}{\pi(1-|\cos\alpha\pi|)}$. As a function of α, N_α is symmetric with respect to $\alpha = \frac{1}{2}$, since $\sin\left(\frac{1}{2}+x\right)\pi = \sin\left(\frac{1}{2}-x\right)\pi$ and $\left|\cos\left(\frac{1}{2}+x\right)\pi\right| = \left|-\cos\left(\frac{1}{2}-x\right)\pi\right| = \left|\cos\left(\frac{1}{2}-x\right)\pi\right|$ for $0 \leq x < \frac{1}{2}$. Therefore, we restrict our analysis to the smaller interval $\alpha \in \left[\frac{1}{2},1\right)$, where we may write $N_\alpha = \frac{\sin\alpha\pi}{\pi(1+\cos\alpha\pi)}$. We find that N_α is strictly monotone increasing, since its first derivative reads $\frac{1+\cos\alpha\pi}{(1+\cos\alpha\pi)^2} = \frac{1}{1+\cos\alpha\pi} > 0$. Moreover, $\frac{\sin\alpha\pi}{1-|\cos\alpha\pi|} = O((1-\alpha)^{-1})$ in the $\alpha \uparrow 1$ limit. This implies inequality 3.25. □

We now turn to the analysis of the improper integral in the definition of the integral kernel $\tilde{K}_i$ in Eq. 3.24. Using Lemmas 3.5.3 and 3.5.5, the integral in the variable λ may be majorated as follows:

$$\left|\int\limits_{\frac{1}{2}(1+2\epsilon)}^{+\infty} \mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right)\frac{G_{\mathcal{I},\mathcal{I}^i}(\lambda,x,y)}{\lambda^2-\frac{1}{4}}\right| \leq \frac{MN_\alpha}{2\pi}\int\limits_{\frac{1}{2}}^{+\infty}\mathrm{d}\lambda\left(\lambda-\frac{1}{2}\right)^\alpha \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2-\frac{1}{4}}, \tag{3.26}$$

with constants $M, N_\alpha > 0$.

In the Lemma below, we address the convergence behaviour of the latter integral.

Lemma 3.5.6. *For any fixed $\alpha \in (0,1)$, the improper integral 3.26 exists and is equal to a non-negative constant P_α. In the von Neumann limit $\alpha \uparrow 1$, it follows $P_1 = \frac{\pi^2}{6}$.*

Proof. By variable substitution we get

$$\int\limits_{\frac{1}{2}}^{+\infty}\mathrm{d}\lambda\left(\lambda-\frac{1}{2}\right)^\alpha \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2-\frac{1}{4}} = \int\limits_0^{+\infty}\mathrm{d}t\,\frac{t}{(e^t-1)^\alpha}. \tag{3.27}$$

Because the integrand satisfies $\frac{t}{(e^t-1)^\alpha} = O(t^{1-\alpha})$ in the $t \to 0$ limit and $\frac{t}{(e^t-1)^\alpha} = O(te^{-\alpha t})$ in the $t \to \infty$ limit, the integral in 3.27 converges to a number P_α.

Moreover, the integrand in 3.27 is non-negative in the interval $t \in (0,+\infty)$, whence the non-negativity of the integral follows.

The claim for P_1 follows from Lemma 3.15 (2) in Ref. [LX17]. □

With the results of Lemmas 3.5.4, 3.5.5 and 3.5.6, we may now start the investigation of the analytic properties of the integral kernel $\tilde{K}_i$.

Lemma 3.5.7. *The integral kernel $\tilde{K}_i$, $i = 1,2$ defined in Eq. 3.24 is continuous in the variables ϵ, α, x, y on the domain $\left(0,\frac{1}{2}\right) \times (0,1) \times \mathcal{I}^i \times \mathcal{I}^i$.*

For a fixed α value, $\tilde{K}_i$ converges uniformly according to

$$\tilde{K}_i(\epsilon,\alpha,x,y) \to K_i(\alpha,x,y) := \frac{1}{\pi(1-\alpha)}\int\limits_{\frac{1}{2}}^{+\infty}\mathrm{d}\lambda\, f_\alpha(\lambda)\frac{G_{\mathcal{I},\mathcal{I}^i}(\lambda,x,y)}{\lambda^2-\frac{1}{4}}$$

for $\epsilon \to 0$ and $(\alpha, x, y) \in (0,1) \times \mathcal{I}^i \times \mathcal{I}^i$.

Moreover, the family $\{\tilde{K}_i, \epsilon > 0\}$ for a fixed α value is uniformly bounded.

Proof. We define the sequence $(s_k(\epsilon, \alpha, x, y))_{k\in\mathbb{N}}$ for any $(\epsilon, \alpha, x, y) \in \left(0, \frac{1}{2}\right) \times (0,1) \times \mathcal{I}^i \times \mathcal{I}^i$ and a fixed i by

$$s_k(\epsilon, \alpha, x, y) := \frac{1}{\pi} \int_{\frac{1}{2}(1+2\epsilon)}^{k} \mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right) \frac{G_{\mathcal{I},\mathcal{I}^i}(\lambda, x, y)}{\lambda^2 - \frac{1}{4}}.$$

For any $\epsilon \in \left(0, \frac{1}{2}\right)$ and $\forall k \in \mathbb{N}$ it holds $\frac{1}{2}(1+2\epsilon) \le k$. Then, by Lemma 3.5.3 and since by definition f_α is bounded as $|f_\alpha| \le \frac{1}{2}$ (cf. Lemma 2.3.1), we get

$$\begin{aligned}
|(1-\alpha)\tilde{K}_i(\epsilon, \alpha, x, y) - s_k(\epsilon, \alpha, x, y)| &= \frac{1}{\pi}\left| \int_{k}^{+\infty} \mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right) \frac{G_{\mathcal{I},\mathcal{I}^i}(\lambda, x, y)}{\lambda^2 - \frac{1}{4}} \right| \\
&\le \frac{1}{\pi} \int_{k}^{+\infty} \mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right) \frac{|G_{\mathcal{I},\mathcal{I}^i}(\lambda, x, y)|}{\lambda^2 - \frac{1}{4}} \\
&\le \frac{1}{2\pi} \int_{k}^{+\infty} \mathrm{d}\lambda\, \frac{|G_{\mathcal{I},\mathcal{I}^i}(\lambda, x, y)|}{\lambda^2 - \frac{1}{4}} \\
&\le \frac{M}{4\pi^2} \int_{k}^{+\infty} \mathrm{d}\lambda\, \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2 - \frac{1}{4}} \\
&\le -\frac{M}{8\pi^2} \left(\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)\right)^2 \Bigg|_{k}^{+\infty} \\
&\le \frac{M}{8\pi^2} \left(\ln\left(\frac{2k+1}{2k-1}\right)\right)^2
\end{aligned}$$

that converges to 0 in the $k \to \infty$ limit. Since none of the variables ϵ, α, x and y appears in the last expression on the r.h.s. of the inequality chain above, the convergence of the sequence $(s_k(\epsilon, \alpha, x, y))_{k\in\mathbb{N}}$ is uniform, and this implies that the improper parameter integral in the definition of $\tilde{K}_i(\epsilon, \alpha, x, y)$ in Eq. 3.24 is continuous on $\left(0, \frac{1}{2}\right) \times (0,1) \times \mathcal{I}^i \times \mathcal{I}^i$ and therefore, $\tilde{K}_i(\epsilon, \alpha, x, y)$ is continuous as well on the same domain.

The uniform boundedness of the function family $\{\tilde{K}_i(\epsilon, \alpha, x, y), \epsilon > 0\}$, for a fixed value $\alpha \in (0,1)$ and for any $\epsilon > 0$, follows from Lemmas 3.5.3, 3.5.5 and 3.5.6:

$$\begin{aligned}
|\tilde{K}_i(\epsilon, \alpha, x, y)| &= \frac{1}{\pi(1-\alpha)} \left| \int_{\frac{1}{2}(1+2\epsilon)}^{+\infty} \mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right) \frac{G_{\mathcal{I},\mathcal{I}^i}(\lambda, x, y)}{\lambda^2 - \frac{1}{4}} \right| \\
&\le \frac{1}{\pi(1-\alpha)} \int_{\frac{1}{2}(1+2\epsilon)}^{+\infty} \mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right) \frac{|G_{\mathcal{I},\mathcal{I}^i}(\lambda, x, y)|}{\lambda^2 - \frac{1}{4}} \\
&\le \frac{M}{2\pi^2(1-\alpha)} \int_{\frac{1}{2}(1+2\epsilon)}^{+\infty} \mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right) \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2 - \frac{1}{4}}
\end{aligned}$$

$$
\begin{aligned}
&\le \frac{MN_\alpha}{2\pi^2(1-\alpha)} \int_{\frac{1}{2}(1+2\epsilon)}^{+\infty} \mathrm{d}\lambda \left(\frac{\lambda}{1+2\epsilon}-\frac{1}{2}\right)^\alpha \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2-\frac{1}{4}} \\
&\le \frac{M}{2\pi^2(1-\alpha)^2} \int_{\frac{1}{2}(1+2\epsilon)}^{+\infty} \mathrm{d}\lambda \left(\frac{\lambda}{1+2\epsilon}-\frac{1}{2}\right)^\alpha \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2-\frac{1}{4}} \\
&\le \frac{M}{2\pi^2(1-\alpha)^2} \int_{\frac{1}{2}(1+2\epsilon)}^{+\infty} \mathrm{d}\lambda \left(\lambda-\frac{1}{2}\right)^\alpha \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2-\frac{1}{4}} \\
&\le \frac{M}{2\pi^2(1-\alpha)^2} \int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda \left(\lambda-\frac{1}{2}\right)^\alpha \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2-\frac{1}{4}} \\
&= \frac{MP_\alpha}{2\pi^2(1-\alpha)^2},
\end{aligned}
$$

since the last expression does not depend on ϵ, x, y.

We now focus on the convergence property of the integral kernel $\tilde{K}_i(\epsilon,\alpha,x,y)$ in the $\epsilon \to 0$ limit, for a fixed value $\alpha \in (0,1)$. To this aim we consider the function

$$
k_n^\alpha(\lambda,x,y) := \frac{1}{\pi(1-\alpha)} f_\alpha\left(\frac{\lambda}{1+\frac{2}{n}}\right) \frac{G_{\mathcal{I},\mathcal{I}^i}(\lambda,x,y)}{\lambda^2-\frac{1}{4}} \chi_{\left(\frac{1}{2}\left(1+\frac{2}{n}\right),+\infty\right)}(\lambda),
$$

for an integer $n \in \mathbb{N}$, where we denote the indicator function on a real interval $A \subseteq \mathbb{R}$ by χ_A.

We have that $k_n^\alpha(\lambda,x,y) \to k^\alpha(\lambda,x,y) := \frac{1}{\pi(1-\alpha)} f_\alpha(\lambda) \frac{G_{\mathcal{I},\mathcal{I}^i}(\lambda,x,y)}{\lambda^2-\frac{1}{4}}$ pointwise. We also observe that $f_\alpha(\lambda) > f_\alpha\left(\frac{\lambda}{1+\frac{2}{n}}\right)$ for $n \in \mathbb{N}$ by Lemma 3.5.4, and therefore we may find an integrable function that dominates $|k_n^\alpha(\lambda,x,y)|$, for any $(x,y) \in \mathcal{I}^i \times \mathcal{I}^i$:

$$
\begin{aligned}
|k_n^\alpha(\lambda,x,y)| &= \frac{1}{\pi(1-\alpha)} f_\alpha\left(\frac{\lambda}{1+\frac{2}{n}}\right) \frac{|G_{\mathcal{I},\mathcal{I}^i}(\lambda,x,y)|}{\lambda^2-\frac{1}{4}} \chi_{\left(\frac{1}{2}\left(1+\frac{2}{n}\right),+\infty\right)}(\lambda) \\
&\le \frac{1}{\pi(1-\alpha)} f_\alpha\left(\frac{\lambda}{1+\frac{2}{n}}\right) \frac{|G_{\mathcal{I},\mathcal{I}^i}(\lambda,x,y)|}{\lambda^2-\frac{1}{4}} \\
&\le \frac{1}{\pi(1-\alpha)} f_\alpha(\lambda) \frac{|G_{\mathcal{I},\mathcal{I}^i}(\lambda,x,y)|}{\lambda^2-\frac{1}{4}} \\
&\le \frac{M}{2\pi^2(1-\alpha)} f_\alpha(\lambda) \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2-\frac{1}{4}} \\
&\le \frac{M}{2\pi^2(1-\alpha)^2} \left(\lambda-\frac{1}{2}\right)^\alpha \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2-\frac{1}{4}} \\
&\le \frac{M}{2\pi^2(1-\alpha)^2} \left(\lambda-\frac{1}{2}\right) \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2-\frac{1}{4}}.
\end{aligned}
$$

The integrability on $\left(\frac{1}{2},+\infty\right)$ of the function

$$
k^\alpha(\lambda,x,y) := \frac{M}{2\pi^2(1-\alpha)^2} \left(\lambda-\frac{1}{2}\right) \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2-\frac{1}{4}} \tag{3.28}
$$

on the last line of the inequality chain is ensured by Lemma 3.5.6.

By Lebesgue's Dominated Convergence Theorem, the uniform convergence follows:

$$0 \leq \lim_{n\to\infty} \left| \tilde{K}_i\left(\frac{1}{n}, \alpha, x, y\right) - K_i(\alpha, x, y) \right| \leq \lim_{n\to\infty} \int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda \, |k_n^\alpha(\lambda, x, y) - k^\alpha(\lambda, x, y)| = 0,$$

for a fixed $\alpha \in (0, 1)$. □

3.6 Traceability of the Bipartite Rényi Entanglement Entropy Operator

In this Section we want to answer the last of the open questions from Section 3.1.2, that is concerned with the traceability of the operator $\sigma(\alpha, D_{\mathcal{I}}, D_{\mathcal{I}^1}, D_{\mathcal{I}^2})$ that we expressed in integral form in Section 3.5.3.

The positivity of σ, that we already proved in Theorem 3.2.9 starting from general considerations about operator-concavity, plays an essential role.

The finiteness of the spatial definition domain $\mathcal{I}$ of the fermionic system and, consequently of the two partitions $\mathcal{I}^1, \mathcal{I}^2$ as well, is also a necessary requirement.

Theorem 3.6.1. *Let $X \subseteq \mathbb{R}$ and let $A \geq 0$ be a positive Hilbert-Schmidt integral operator on the Hilbert space $L^2(X)$ with integral kernel $a(x, y)$ defined on X^2. Let $\tilde{a}(x, x)$ be the diagonal component of the kernel averaged upon symmetric intervals of the real line centered in the origin, $[-r, r]$, $r > 0$, defined by*

$$\tilde{a}(x, x) := \lim_{r\to 0} \frac{1}{2r} \int_{-r}^{r} \mathrm{d}t \, a(x + t, x + t). \tag{3.29}$$

If $\tilde{a}(x, x)$ exists almost everywhere on X with respect to the Lebesgue measure, then the integral operator A is trace-class if and only if the integral $T := \int_X \mathrm{d}x \, \tilde{a}(x, x)$ is finite. In this case $\operatorname{tr} A = T$.

Proof. This is a simplified version of Corollary 4.4 in Ref. [Bri88] restricted to the real line.

The averaging procedure 3.29 was derived from Section 3 in Ref. [Bri88]. □

Theorem 3.6.2. *The bipartite Rényi entanglement entropy operator σ from Def. 3.1.11 of the system discussed in Section 3.5.3 is trace-class.*

Proof. We focus here on the subsystem $i = 1$ of the operator σ, that may be written in integral form as shown in Eq. 3.23. The analogous operator of the remaining subsystem, for $i = 2$, may be treated in exactly the same way.

As shown in the proof of Theorem 3.2.9, each of the two subsystems of the bipartite Rényi entanglement operator $\sigma(\alpha, D, D_1, D_2)$ is positive. This ensures in turn (cf. Eq. 3.23 and recall that $f_\alpha \geq 0$ by Lemma 3.5.5) that the integral operator A_λ^1 defined by

$$(A_\lambda^1 \chi)(x) := \int_{\mathcal{I}^1} \mathrm{d}y \, G_{\mathcal{I},\mathcal{I}^1}(\lambda, x, y) \chi(y) \tag{3.30}$$

for any $\chi \in H^2(\mathcal{I}, \mathbb{C}^2)$ is positive as well whenever $\lambda \in \left(\frac{1}{2}, +\infty\right)$. We also note that $H^2(\mathcal{I}, \mathbb{C}^2) \subset L^2(\mathcal{I}, \mathbb{C}^2)$, and $\mathcal{I} \subset \mathbb{R}$.

Moreover, A^1_λ is a Hilbert-Schmidt operator. Indeed, by Lemma 3.5.3, there exists a positive constant M such that

$$\int_{\mathcal{I}^1} \mathrm{d}x \int_{\mathcal{I}^1} \mathrm{d}y\, |G_{\mathcal{I},\mathcal{I}^1}(\lambda, x, y)|^2 \leq \frac{M^2}{4\pi^2}\left(\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)\sum_{j\in I_1}(b_j - a_j)\right)^2 < \infty$$

for any $\lambda \in \left(\frac{1}{2}, +\infty\right)$.

Following Def. 3.29 and Section 2 in Ref. [Bri88], we focus now on the averaged diagonal component $\tilde{G}^\lambda_{\mathcal{I},\mathcal{I}^1}$ of the integral kernel $G_{\mathcal{I},\mathcal{I}^1}$ on the interval $[-r, r] \subset \mathbb{R}$ centered in the origin of the real line and of length $2r$, for arbitrary $r > 0$. We get

$$\tilde{G}^\lambda_{\mathcal{I},\mathcal{I}^1}(x, x) := \lim_{r\to 0} \frac{1}{2r}\int_{-r}^{r} \mathrm{d}t\, G_{\mathcal{I},\mathcal{I}^1}(\lambda, x+t, x+t). \tag{3.31}$$

By Lemma 3.5.3:

$$\begin{aligned}
G_{\mathcal{I},\mathcal{I}^1}(\lambda, x+t, x+t) &= -\frac{1}{2\pi}\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)(Z'_{\mathcal{I}}(x+t) - Z'_{\mathcal{I}^1}(x+t)) \\
&= -\frac{1}{2\pi}\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)\left(\sum_{j\in N_n}\left(\frac{1}{x+t-a_j} - \frac{1}{x+t-b_j}\right)\right. \\
&\qquad \left. - \sum_{j\in I_1}\left(\frac{1}{x+t-a_j} - \frac{1}{x+t-b_j}\right)\right) \\
&= -\frac{1}{2\pi}\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)\sum_{j\in I_2}\left(\frac{1}{x+t-a_j} - \frac{1}{x+t-b_j}\right),
\end{aligned} \tag{3.32}$$

since $\mathbb{N}_n \setminus I_1 = I_2$.

Combining Eqs. 3.31 and 3.32, it follows

$$\begin{aligned}
\tilde{G}^\lambda_{\mathcal{I},\mathcal{I}^1}(x, x) &= -\frac{1}{4\pi}\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)\sum_{j\in I_2}\lim_{r\to 0}\frac{1}{r}\int_{-r}^{r}\mathrm{d}t\left(\frac{1}{x+t-a_j} - \frac{1}{x+t-b_j}\right) \\
&= -\frac{1}{4\pi}\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)\sum_{j\in I_2}\lim_{r\to 0}\frac{1}{r}\ln\left(\left|\frac{(r+x-a_j)(r-x+b_j)}{(r-x+a_j)(r+x-b_j)}\right|\right) \\
&= \frac{1}{2\pi}\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)\sum_{j\in I_2}\frac{b_j - a_j}{(x-a_j)(x-b_j)},
\end{aligned} \tag{3.33}$$

where we used the Taylor expansion

$$\ln\left(\left|\frac{(r+x-a_j)(r-x+b_j)}{(r-x+a_j)(r+x-b_j)}\right|\right) = -\frac{2(b_j-a_j)}{(x-a_j)(x-b_j)}r + O(r^2)$$

in the determination of the $r \to 0$ limit.

The averaged kernel $\tilde{G}^\lambda_{\mathcal{I},\mathcal{I}^1}(x, x)$ is well-defined for values $x \in \mathcal{I}$, since $\mathcal{I}$ is a finite set union of open intervals.

Starting from Eqs. 3.30 and 3.33, we deduce the boundedness of the integral

$$T_\lambda := \int_{\mathcal{I}^1} \mathrm{d}x\, \tilde{G}^\lambda_{\mathcal{I},\mathcal{I}^1}(x,x) = \frac{1}{2\pi} \ln\left(\frac{2\lambda+1}{2\lambda-1}\right) \sum_{j\in I_2} \int_{\mathcal{I}^1} \mathrm{d}x\, \frac{b_j - a_j}{(x-a_j)(x-b_j)} < \infty, \tag{3.34}$$

since the integrand function does not have any singularity in $\mathcal{I}^1$. Indeed, the poles a_j, b_j of the intervals in $\mathcal{I}^2$, with $j \in I_2$, all lie outside the integration domain $\mathcal{I}^1$. Moreover, we note that, whenever $x \in \mathcal{I}^1$, the two terms $x - a_j$ and $x - b_j$ are both either strictly positive or negative, for any $j \in I_2$, since $(a_j, b_j) \subset \mathcal{I}^2$ and $(a_j, b_j) \cap \mathcal{I}^1 = \emptyset$. Therefore, the function $\frac{1}{(x-a_j)(x-b_j)}$ in the integrand in Eq. 3.34 is always positive, and so is the integral T_λ.

Finally, we may now apply Theorem 3.6.2 to the positive Hilbert-Schmidt operator A^1_λ, and we deduce its traceability with trace $T_\lambda > 0$, for any $\lambda \in \left(\frac{1}{2}, +\infty\right)$. The traceability of the bipartite Rényi entanglement operator $\sigma(\alpha, D_\mathcal{I}, D_{\mathcal{I}^1}, D_{\mathcal{I}^2})$ follows from that of operator A^1_λ and from the linearity of the trace, as well as from Lemma 3.5.6. □

3.7 Entanglement Entropy of Quasi-Free Fermionic States

Here we shortly recall and summarize what was proven until now. After defining the regularized one-particle density operator E_ϵ of the system, we expressed the contribution from the subsystem i to the bipartite Rényi entanglement operator through the integral kernel $\tilde{K}_i(\epsilon, \alpha, x, y)$ defined in Eq. 3.24. In Lemma 3.5.7 we analyzed the behaviour of $\tilde{K}_i$ in the $\epsilon \to 0$ limit.

Since the bipartite Rényi entanglement entropy is defined as the trace of the corresponding entanglement entropy operator in 3.3, it is now necessary to focus on the trace of the operator expressed by the integral kernel $\tilde{K}_i$, and especially to study its behaviour in the $\epsilon \to 0$ limit. The following general Theorem clarifies how to calculate the trace of an operator that is defined by means of an integral kernel.

Theorem 3.7.1. *Let K be an integral trace-class operator on $L^2(\mathbb{R})$ with continuous integral kernel $\tilde{K}$, i.e. $(K\phi)(x) = \int \mathrm{d}y\, \tilde{K}(x,y)\phi(y)$, for $\phi \in L^2(\mathbb{R})$. Then:*

$$\mathrm{tr}K = \int \mathrm{d}x\, \tilde{K}(x,x).$$

Proof. Cf. Theorem 3.1 in Ref. [Bri88] and Theorem 8.1 in Ref. [GGK00]. □

Proposition 3.7.2. *Let $i = 1, 2$ and α be a fixed number in $(0,1)$. Then the trace of the operator defined through the integral kernel K_i (cf. Lemma 3.5.7) is given by*

$$\int_{\mathcal{I}^i} \mathrm{d}x\, K_i(\alpha, x, x) = \lim_{\epsilon\to 0} \int_{\mathcal{I}^i} \mathrm{d}x\, \tilde{K}_i(\epsilon, \alpha, x, x).$$

Proof. The existence of the $\epsilon \to 0$ limit of the parametric integral $\int_{\mathcal{I}^i} \mathrm{d}x\, \tilde{K}_i(\epsilon, \alpha, x, x)$ is ensured by the uniform convergence of $\tilde{K}_i$ shown in Lemma 3.5.7 for a fixed α.

By Theorem 3.6.2 we know that the integral operator with kernel K_i is trace-class. It is therefore possible to apply Theorem 3.7.1 to $\tilde{K}_i$, which directly yields the claim. □

The contribution of the regularized operator E_ϵ from the first subsystem to the bipartite Rényi entanglement operator in the $\epsilon \to 0$ limit is now given by

$$\frac{1}{1-\alpha} \lim_{\epsilon\to 0} \mathrm{tr}(-P_1 \ln(E^\alpha_\epsilon + (I - E_\epsilon)^\alpha)P_1 + P_1 \ln((P_1 E_\epsilon P_1)^\alpha + (P_1 - P_1 E_\epsilon P_1)^\alpha)P_1)$$

$$= \lim_{\epsilon\to 0} \int_{\mathcal{I}_1} \mathrm{d}x\, \tilde{K}_1(\epsilon,\alpha,x,x)$$
$$= \int_{\mathcal{I}_1} \mathrm{d}y\, K_1(\alpha,x,x), \tag{3.35}$$

where we employed Eqs. 3.23, 3.24 and Proposition 3.7.2.

We now deduce an explicit expression for this trace.

Lemma 3.7.3. *Let I_1, I_2 be index partitions such that $\mathcal{I}^i := \bigcup_{j\in I_i}(a_j,b_j)$, $i=1,2$, according to our definition in Section 3.5.1.*

The contribution of subsystem 1 to the Rényi-entanglement entropy of a 1-fermion system reads

$$\int_{\mathcal{I}^1} \mathrm{d}y\, K_1(\alpha,x,x) = \sum_{i\in I_1}\sum_{j\in I_2} \ln\left(\frac{|a_i-a_j||b_i-b_j|}{|a_i-b_j||b_i-a_j|}\right) \frac{1}{2\pi^2(1-\alpha)} \int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda\, f_\alpha(\lambda) \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2-\frac{1}{4}}. \tag{3.36}$$

The contribution of subsystem 2 is identical to that of subsystem 1 above.

Proof. We start with subsystem 1. From Eq. 3.35 and Proposition 3.7.2, we have

$$\int_{\mathcal{I}_1} \mathrm{d}y\, K_1(\alpha,x,x) = \lim_{\epsilon\to 0}\int_{\mathcal{I}^1} \mathrm{d}x\, \tilde{K}_1(\epsilon,\alpha,x,x)$$
$$= \frac{1}{\pi(1-\alpha)} \lim_{\epsilon\to 0} \int_{\frac{1}{2}(1+2\epsilon)}^{+\infty} \mathrm{d}\lambda\, f_\alpha\left(\frac{\lambda}{1+2\epsilon}\right) \frac{1}{\lambda^2-\frac{1}{4}} \int_{\mathcal{I}^1} \mathrm{d}x\, G_{\mathcal{I},\mathcal{I}^1}(\lambda,x,x)$$
$$= \frac{1}{\pi(1-\alpha)} \int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda\, f_\alpha(\lambda) \frac{1}{\lambda^2-\frac{1}{4}} \int_{\mathcal{I}^1} \mathrm{d}x\, G_{\mathcal{I},\mathcal{I}^1}(\lambda,x,x), \tag{3.37}$$

where the exchange of limit and integral is allowed by Lemma 3.5.7 (especially the result concerning the uniform boundedness of $\tilde{K}_1$ in the $\epsilon\to 0$ limit).

By Lemma 3.5.3, the function $G_{\mathcal{I},\mathcal{I}^1}$ is expressed by

$$G_{\mathcal{I},\mathcal{I}^1}(\lambda,x,x) = -\frac{1}{2\pi}\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)(Z'_{\mathcal{I}}(x) - Z'_{\mathcal{I}^1}(x)) \tag{3.38}$$

where, recalling that $I_2 = \mathbb{N}_n \setminus I_1$ (cf. Section 3.5.1),

$$Z'_{\mathcal{I}}(x) - Z'_{\mathcal{I}^1}(x) = \sum_{j\in\mathbb{N}_n}\left(\frac{1}{x-a_j} - \frac{1}{x-b_j}\right) - \sum_{j\in I_1}\left(\frac{1}{x-a_j} - \frac{1}{x-b_j}\right)$$
$$= \sum_{j\in I_2}\left(\frac{1}{x-a_j} - \frac{1}{x-b_j}\right). \tag{3.39}$$

Integrating Eq. 3.39 upon the domain $\mathcal{I}^1$, it follows

$$\int_{\mathcal{I}^1} \mathrm{d}x\, (Z'_{\mathcal{I}}(x) - Z'_{\mathcal{I}^1}(x)) = \sum_{j\in I_2}\int_{\mathcal{I}^1} \mathrm{d}x\left(\frac{1}{x-a_j} - \frac{1}{x-b_j}\right)$$

$$= \sum_{i\in I_1}\sum_{j\in I_2}\int_{a_i}^{b_i} \mathrm{d}x \left(\frac{1}{x-a_j} - \frac{1}{x-b_j}\right)$$
$$= \sum_{i\in I_1}\sum_{j\in I_2} \ln\left(\frac{|x-a_j|}{|x-b_j|}\right)\Big|_{a_i}^{b_i}$$
$$= \sum_{i\in I_1}\sum_{j\in I_2} \ln\left(\frac{|b_i-a_j||a_i-b_j|}{|b_i-b_j||a_i-a_j|}\right). \tag{3.40}$$

Therefore, from Eqs. 3.37, 3.38, 3.39 and 3.40 we deduce the first claim.

The contribution of subsystem 2 may be obtained from 3.36 by exchanging the index sets I_1 and I_2 in the summations. However, the argument $\frac{|a_i-a_j||b_i-b_j|}{|a_i-b_j||b_i-a_j|}$ of the logarithm is invariant under the exchange of indices i and j. Therefore, the contributions of subsystems 1 and 2 are identical. □

To simplify the result in Lemma 3.7.3, we introduce the following shorthand notation that characterizes in a compact manner any union of open intervals on the real line.

Definition 3.7.1. Let I be a finite index set and let $\mathcal{J} := \bigcup_{i\in I}(a_i, b_i)$ be the set union of intervals where the numbers a_i, b_i are chosen in increasing order as in Section 3.5.1. Then we define the number

$$g(\mathcal{J}) := \sum_{i\in I}\sum_{j\in I} \ln|b_i-a_j| - \sum_{\substack{i,j\in I\\ i<j}} \ln|a_i-a_j| - \sum_{\substack{i,j\in I\\ i<j}} \ln|b_i-b_j|.$$

Let I_1, I_2 be as usual the index sets that characterize the two partitions of a bipartite system, i.e. $\mathcal{I}^i := \bigcup_{j\in I_i}(a_j, b_j)$, $i = 1, 2$, and $\mathcal{I} = \mathcal{I}^1 \cup \mathcal{I}^2$, according to our definition in Section 3.5.1. The index set of $\mathcal{I}$ is then $\mathbb{N}_n = I_1 \cup I_2$.

Lemma 3.7.4. *The following relation holds:*

$$2\sum_{i\in I_1}\sum_{j\in I_2} \ln\left(\frac{|a_i-a_j||b_i-b_j|}{|a_i-b_j||b_i-a_j|}\right) = g(\mathcal{I}^1) + g(\mathcal{I}^2) - g(\mathcal{I}).$$

Proof. According to Def. 3.7.1, and by direct calculation:

$$\begin{aligned}
g(\mathcal{I}) - g(\mathcal{I}^1) - g(\mathcal{I}^2) &= g(\mathcal{I}^1\cup\mathcal{I}^2) - g(\mathcal{I}^1) - g(\mathcal{I}^2)\\
&= \sum_{i\in I_1\cup I_2}\sum_{j\in I_1\cup I_2} \ln|b_i-a_j| - \sum_{\substack{i,j\in I_1\cup I_2\\ i<j}} \ln|a_i-a_j| - \sum_{\substack{i,j\in I_1\cup I_2\\ i<j}} \ln|b_i-b_j|\\
&\quad - \sum_{i\in I_1}\sum_{j\in I_1} \ln|b_i-a_j| + \sum_{\substack{i,j\in I_1\\ i<j}} \ln|a_i-a_j| + \sum_{\substack{i,j\in I_1\\ i<j}} \ln|b_i-b_j|\\
&\quad - \sum_{i\in I_2}\sum_{j\in I_2} \ln|b_i-a_j| + \sum_{\substack{i,j\in I_2\\ i<j}} \ln|a_i-a_j| + \sum_{\substack{i,j\in I_2\\ i<j}} \ln|b_i-b_j|\\
&= \sum_{i\in I_1}\sum_{j\in I_2} \ln|b_i-a_j| - \sum_{\substack{i\in I_1, j\in I_2\\ i<j}} \ln|a_i-a_j| - \sum_{\substack{i\in I_1, j\in I_2\\ i<j}} \ln|b_i-b_j|\\
&\quad + \sum_{i\in I_2}\sum_{j\in I_1} \ln|b_i-a_j| - \sum_{\substack{i\in I_2, j\in I_1\\ i<j}} \ln|a_i-a_j| - \sum_{\substack{i\in I_2, j\in I_1\\ i<j}} \ln|b_i-b_j|
\end{aligned}$$

$$= \sum_{i\in I_1}\sum_{j\in I_2} \ln\left(\frac{|b_i - a_j||a_i - b_j|}{|b_i - b_j||a_i - a_j|}\right) + \sum_{i\in I_2}\sum_{j\in I_1} \ln\left(\frac{|b_i - a_j||a_i - b_j|}{|b_i - b_j||a_i - a_j|}\right).$$

As noted in the proof of Lemma 3.7.3, the two terms in the equation above are identical, from which the claim follows. □

Now, collecting the results of the previous Lemmas, we establish our central result in this Thesis.

Theorem 3.7.5. *The bipartite Rényi entanglement entropy ΔS_α of the system described by the relativistic quantum state ω of N quasi-free fermions spatially distributed on the real-line set $\mathcal{I} = \mathcal{I}^1 \cup \mathcal{I}^2$ reads*

$$\Delta S_\alpha(\omega, \omega_1 \otimes \omega_2) = N\Xi(\alpha)(g(\mathcal{I}^1) + g(\mathcal{I}^2) - g(\mathcal{I})) \tag{3.41}$$

where

$$\Xi(\alpha) := \frac{1}{2\pi^2(1-\alpha)} \int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda\, f_\alpha(\lambda) \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2 - \frac{1}{4}}, \tag{3.42}$$

is a number depending on the Rényi index $\alpha \in (0,1)$. We name $\Xi(\alpha)$ entanglement coefficient.

Proof. The claim follows from formula 3.4, applying Lemma 3.7.3 to each component of the bipartite system, and employing Lemma 3.7.4.

The number $\Xi(\alpha)$ is well-defined thanks to Lemmas 3.5.5 and 3.5.6.

We now observe that the bipartite Rényi entanglement entropy for a quasi-free state of N fermions is N times the bipartite Rényi entanglement entropy of the 1-fermion state. In fact, the trace operator on the N-particle Hilbert space $\bigoplus_{i=1}^N L^2(\mathbb{R})$ is N times the trace operator defined on the 1-particle Hilbert space $L^2(\mathbb{R})$. This yields the linear proportionality of the bipartite Rényi entanglement entropy on the number N of quasi-free fermions in the system. □

Our Theorem above generalizes the results of Section 3.1.7 in Ref. [CH09a] and Theorem 3.18 in Ref. [LX17], that were obtained assuming that the underlying quantum entropy form is of von Neumann type. We formalize this observation in the following:

Corollary 3.7.5.1 (of Theorem 3.7.5)**.** *The bipartite von Neumann entanglement entropy ΔS_1 of the system described by the relativistic quantum state ω of N quasi-free fermions spatially distributed on the real-line set $\mathcal{I} = \mathcal{I}^1 \cup \mathcal{I}^2$ reads*

$$\Delta S_1(\omega, \omega_1 \otimes \omega_2) = \frac{N}{12}(g(\mathcal{I}^1) + g(\mathcal{I}^2) - g(\mathcal{I})).$$

Proof. The entanglement coefficient $\Xi(\alpha)$, defined in Eq. 3.42 of Theorem 3.7.5 reduces in the von Neumann limit to

$$\Xi(1) := -\frac{1}{2\pi^2} \int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda\, f_1^1(\lambda) \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2 - \frac{1}{4}} = \frac{1}{2\pi^2} \int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda \left(\lambda - \frac{1}{2}\right) \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda^2 - \frac{1}{4}} = \frac{1}{2\pi^2} \int_{\frac{1}{2}}^{+\infty} \mathrm{d}\lambda\, \frac{\ln\left(\frac{2\lambda+1}{2\lambda-1}\right)}{\lambda + \frac{1}{2}}, \tag{3.43}$$

according to the discussion in Section 2.5.

Integral 3.43 was calculated in Lemma 3.15(3) in Ref. [LX17] and its explicit value reads $\frac{1}{12}$. The claim stems from Lemma 3.7.4. □

3.8 The Entanglement Coefficient $\Xi(\alpha)$

In the important case of the logarithmic negativity, i.e. $\alpha = \frac{1}{2}$, the entanglement coefficient may be calculated explicitly.

Lemma 3.8.1. *The logarithmic negativity entanglement coefficient reads*

$$\Xi\left(\frac{1}{2}\right) = \frac{1}{8}.$$

Proof. Employing the definition 2.24 of the function f_α, by the variable substitution $t = \left(\frac{2\lambda-1}{2\lambda+1}\right)^\alpha$ the entanglement coefficient from Eq. 3.42 becomes

$$\Xi(\alpha) = -\frac{1}{2\pi^3\alpha^2(1-\alpha)} \int_0^1 \mathrm{d}t \, \arctan\left(\frac{t\sin\alpha\pi}{1+t\cos\alpha\pi}\right)\frac{\ln t}{t}.$$

Recalling the Taylor series of the arctan function, valid for $|t| \le 1$,

$$\arctan t = \sum_{n=0}^{\infty} (-1)^n \frac{t^{2n+1}}{2n+1},$$

we get, integrating by parts:

$$\begin{aligned}
\Xi\left(\frac{1}{2}\right) &= -\frac{4}{\pi^3}\int_0^1 \mathrm{d}t \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} t^{2n}\ln t \\
&= -\frac{4}{\pi^3}\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)^2}\left(t^{2n+1}\ln t\Big|_0^1 - \int_0^1 \mathrm{d}t\, t^{2n}\right) \\
&= \frac{4}{\pi^3}\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)^3},
\end{aligned} \tag{3.44}$$

which yields the claim since $\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)^3} = \frac{\pi^3}{32}$.

The exchange of integral and infinite sum in Eq. 3.44 is possible by Fubini's and Tonelli's Theorems applied to the special case of the measure defined by the product of the counting measure on $\mathbb{N}\cup\{0\}$ and the Lebesgue measure on $[0,1]$, since $\sum_{n=0}^{\infty}\int_0^1 \mathrm{d}t\,|f_n(t)| = \sum_{n=0}^{\infty}\frac{1}{(2n+1)^3} < \infty$ with $f_n(t) := \frac{(-1)^n}{2n+1}t^{2n}\ln t$. □

The result from Lemma 3.8.1 is a special case of a more general formula that expresses $\Xi(\alpha)$ on the whole $\alpha \in (0,1)$ interval.

Theorem 3.8.2. [2] *Let $\alpha \in (0,1)$. Then the entanglement coefficient may be written as*

$$\Xi(\alpha) = \frac{1}{24}\frac{1+\alpha}{\alpha}.$$

Proof. By the variable substitution $t = \left(\frac{2\lambda+1}{2\lambda-1}\right)^\alpha$ the entanglement coefficient defined in Eq. 3.42 becomes

$$\Xi(\alpha) = \frac{1}{2\pi^3\alpha^2(1-\alpha)}\int_1^{+\infty}\mathrm{d}t\,\arctan\left(\frac{\sin\alpha\pi}{t+\cos\alpha\pi}\right)\frac{\ln t}{t}. \tag{3.45}$$

[2] Proof devised by Prof. Dr. W. Spitzer.

We denote the integral in Eq. 3.45 by $I(\alpha) := \int_1^{+\infty} \mathrm{d}t \, \arctan\Big(\frac{\sin \alpha\pi}{t+\cos\alpha\pi}\Big)\frac{\ln t}{t}$. Processing $I(\alpha)$ further, we obtain

$$\begin{aligned} I(\alpha) &= \frac{1}{2}\arctan\Big(\frac{\sin\alpha\pi}{t+\cos\alpha\pi}\Big)(\ln t)^2\Big|_1^{+\infty} + \frac{1}{2}\sin\alpha\pi\int_1^{+\infty}\mathrm{d}t\,\frac{(\ln t)^2}{t^2+2t\cos\alpha\pi+1} \\ &= \frac{1}{2}\sin\alpha\pi\int_1^{+\infty}\mathrm{d}t\,\frac{(\ln t)^2}{t^2+2t\cos\alpha\pi+1} \\ &= -\frac{1}{4i}\int_1^{+\infty}\mathrm{d}t\,(\ln t)^2\Big(\frac{1}{t+e^{i\alpha\pi}}-\frac{1}{t+e^{-i\alpha\pi}}\Big), \end{aligned} \tag{3.46}$$

where we integrated by parts and we employed $t^2+2t\cos\alpha\pi+1=(t+e^{i\alpha\pi})(t+e^{-i\alpha\pi})$.

Again, by the variable substitution $u=\ln t$, and expressing the fractions in the integrand as geometric series[3], Eq. 3.46 yields

$$\begin{aligned} I(\alpha) &= -\frac{1}{4i}\int_0^{+\infty}\mathrm{d}u\,u^2\Big(\frac{1}{1+e^{-u+i\alpha\pi}}-\frac{1}{1+e^{-u-i\alpha\pi}}\Big), \\ &= -\frac{1}{4i}\int_0^{+\infty}\mathrm{d}u\,u^2\Big(\sum_{n=0}^{\infty}(-1)^n e^{-nu+in\alpha\pi}-\sum_{n=0}^{\infty}(-1)^n e^{-nu-in\alpha\pi}\Big) \\ &= -\frac{1}{4i}\sum_{n=1}^{\infty}(-1)^n(e^{in\alpha\pi}-e^{-in\alpha\pi})\int_0^{+\infty}\mathrm{d}u\,u^2e^{-nu} \\ &= \frac{i}{2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n^3}(e^{in\alpha\pi}-e^{-in\alpha\pi}), \end{aligned} \tag{3.47}$$

where the integral $\int_0^{+\infty}\mathrm{d}u\,u^2e^{-nu}=\frac{2}{n^3}$ was evaluated applying integration by parts twice.

We now define the polylogarithm of order $s\in\mathbb{C}$ for complex $z\in\mathbb{C}$ with $|z|<1$ [Jon89],

$$\mathrm{Li}_s(z) := \sum_{n=1}^{\infty}\frac{z^n}{n^s}. \tag{3.48}$$

The polylogarithm satisfies the addition formula (cf. Eq. 1 in Ref. [Jon89])

$$\mathrm{Li}_s(z)+(-1)^s\mathrm{Li}_s(z^{-1}) = -\frac{(2\pi i)^s}{s!}B_s\Big(\frac{\ln z}{2\pi i}\Big), \qquad s\in\mathbb{N}, \tag{3.49}$$

where (cf. e.g. Section 23.1 in Ref. [AS70])

$$B_s(z) = \sum_{n=0}^{s}\frac{1}{n+1}\sum_{k=0}^{n}(-1)^k\binom{n}{k}(z+k)^s \tag{3.50}$$

represents the Bernoulli polynomial[4] of order s.

[3] Note that $|e^{-u\pm i\alpha\pi}|<1$ in the interval $u\in(0,+\infty)$.

[4] Note that the Bernoulli polynomials are defined in Ref. [Jon89] by means of the generating function $\frac{te^{zt}}{e^t-1}=\sum_{s=0}^{\infty}B_s(z)t^s$, whereas our definition in Eq. 3.50 relies instead on the generating function $\frac{te^{zt}}{e^t-1}=\sum_{s=0}^{\infty}B_s(z)\frac{t^s}{s!}$ for $|t|<2\pi$. This discrepancy in the definition leads to the additional factor $\frac{1}{s!}$ in Eq. 3.49.

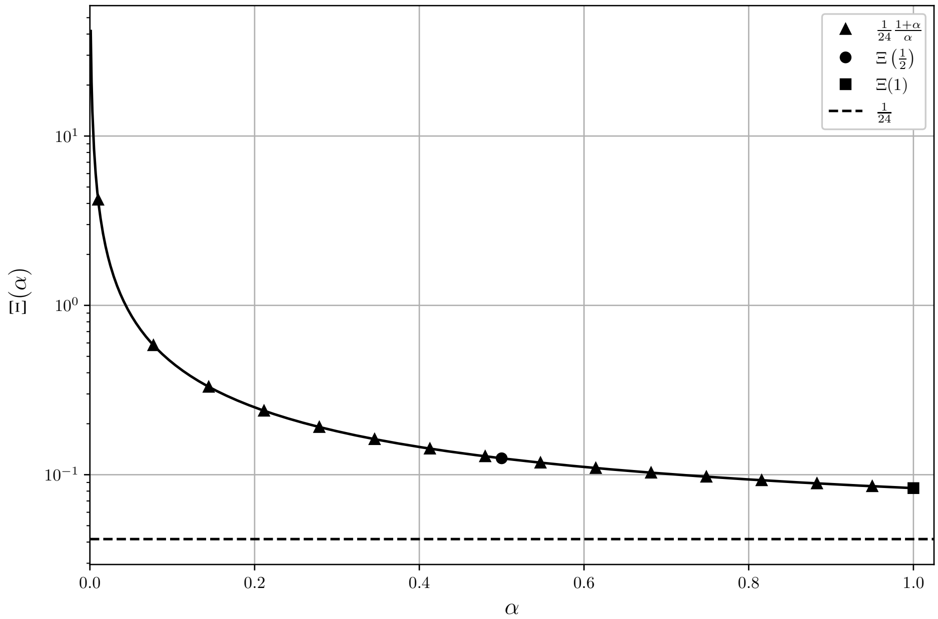

Figure 3.1: Plot of the entanglement coefficient $\Xi(\alpha)$ defined in 3.42 and of our hyperbolic formula from Lemma 3.8.2 on the Rényi-index interval $\alpha \in (0,1)$. The entanglement coefficient values $\Xi\left(\frac{1}{2}\right)$ (logarithmic negativity, cf. Lemma 3.8.1) and $\Xi(1)$ (von Neumann limit, cf. Eq. 3.43) are also marked (cf. points at $\alpha = \frac{1}{2}$ and $\alpha = 1$). The horizontal asymptote is shown as a dashed line.

By Eqs. 3.48, 3.49 and 3.50, and taking $s = 3$ and $z = -e^{i\alpha\pi}$, we may rewrite integral 3.47 as

$$\begin{aligned} I(\alpha) &= \frac{i}{2}(\mathrm{Li}_3(-e^{i\alpha\pi}) - \mathrm{Li}_3(-e^{-i\alpha\pi})) \\ &= \frac{i}{2}(\mathrm{Li}_3(e^{i(1+\alpha)\pi}) - \mathrm{Li}_3(e^{i(1-\alpha)\pi})) \\ &= -\frac{i}{2}\frac{(2\pi i)^3}{3!}B_3\left(\frac{1}{2}(\alpha+1)\right) \\ &= \frac{\pi^3}{12}\alpha(1-\alpha^2). \end{aligned} \tag{3.51}$$

In Eq. 3.51 we employed the explicit representation $B_3(z) = z^3 - \frac{3}{2}z^2 + \frac{1}{2}z$ of the Bernoulli polynomial of order 3 (cf. e.g. Table 23.1 in Ref [AS70] for the polynomial coefficients).

Combining Eqs. 3.45 and 3.51, the claim follows. □

The agreement between the entanglement coefficient $\Xi(\alpha)$ calculated numerically from its definition in Eq. 3.42 and the hyperbolic formula from Theorem 3.8.2 is demonstrated graphically in Fig. 3.1. Remarkably, our formula $\frac{1}{24}\frac{1+\alpha}{\alpha}$ is identical to the scaling law derived in Ref. [LSS14] and it agrees with the von Neumann result in Ref. [LX17].

Chapter 4

Advanced Topics and Outlook

In this Chapter we deal with several generalizations of our bipartite Rényi entanglement entropy results from Chapter 3. Here we only provide a short discussion, we sketch our proposals of method extension and we give best guesses of the expected generalized results. However, we refrain from detailed and formal proofs, which lie outside of the scope of this Thesis.

4.1 Quasi-Free Fermions on a Jordan Curve of Smooth Curvature

The method we employed in Chapter 3 and especially in Section 3.5.2 for the determination of the Rényi entanglement entropy relies on the explicit form of the resolvent of the one-particle density operator.

The resolvent was provided in Theorem 3.5.1 and the proof was based on classical results of the theory of singular equations from Refs. [Mus53, Mik64], applied to the special case of the integration domain $\mathcal{I} \subset \mathbb{R}$. The latter was chosen as the union of finitely many open real intervals.

Our main result in Theorem 3.7.5 may be readily generalized to the case of a finite open subset of a suitable integration contour. To this aim, we define a closed Jordan curve of continuous curvature in the plane $\gamma : [0,1] \to \mathbb{R}^2$, with $\gamma(0) = \gamma(1)$[1] and we assume that the orientation of the curve is chosen in such a way that the region bounded by γ lies to the left. We then use the orientation on γ to orient any subset of $\gamma([0,1])$.

In complete analogy with our definition in Section 3.5.1, we choose $2n$ real numbers $0 < \alpha_1 < \beta_1 < \alpha_2 < \beta_2 < \cdots < \alpha_n < \beta_n < 1$, and we now assume that the fermionic quasi-free state is defined on the domain $\mathcal{K} \subset \gamma([0,1])$, which we define as the set union $\mathcal{K} := \bigcup_{i \in \mathbb{N}_n} \mathcal{K}_i$, where the sets $\mathcal{K}_i := \gamma((\alpha_i, \beta_i))$ are pairwise disjoint for $i \in \mathbb{N}_n$.

Moreover, as customary, we partition the domain $\mathcal{K}$ into two subdomains $\mathcal{K}^i := \bigcup_{j \in K_i} \gamma((\alpha_j, \beta_j))$, $i = 1, 2$, with index sets

$$
\begin{aligned}
&K_1, K_2 \subset \mathbb{N}_n, \\
&|K_1| = n_1, |K_2| = n_2 \\
&K_1 \cup K_2 = \mathbb{N}_n \\
&K_1 \cap K_2 = \emptyset
\end{aligned}
$$

where $n_1, n_2 > 0$ and $n_1 + n_2 = n$.

[1] We identify here the equivalence class of the Jordan curves with one of its elements by choosing a specific parametrization.

Theorem 4.1.1. *Let γ be a Jordan curve as described above, and let L_γ be the arc length between any two points on γ. Moreover, let $\Xi(\alpha)$ be the entanglement coefficient defined in Theorem 3.7.5 for any Rényi-index $\alpha \in (0,1)$. Then the bipartite Rényi entanglement entropy ΔS_α^γ of the system described by the quantum state ω of N quasi-free fermions distributed on the set $\mathcal{K} = \mathcal{K}^1 \cup \mathcal{K}^2$ on the Jordan curve γ as described above reads*

$$\Delta S_\alpha^\gamma(\omega, \omega_1 \otimes \omega_2) = N\Xi(\alpha)(g_\gamma(\mathcal{K}^1) + g_\gamma(\mathcal{K}^2) - g_\gamma(\mathcal{K})) \tag{4.1}$$

where

$$g_\gamma(\mathcal{K}) := \sum_{i\in K}\sum_{j\in K} \ln\left(L_\gamma(\alpha_j, \beta_i)\right) - \sum_{\substack{i,j\in K\\ i<j}} \ln\left(L_\gamma(\alpha_i, \alpha_j)\right) - \sum_{\substack{i,j\in K\\ i<j}} \ln\left(L_\gamma(\beta_i, \beta_j)\right),$$

and analogous definitions hold for $g_\gamma(\mathcal{K}^1)$ and $g_\gamma(\mathcal{K}^2)$.

4.2 The $\alpha > 1$ Case

For a Rényi index $\alpha > 1$, the method we developed in this Thesis cannot be directly extended. This difficulty arises from the fact that our method relies on the canonical integral representation of the Rényi entropy function (cf. Section 2.4.1) that we derived from the Nevanlinna-Herglotz theory. However, the power function $z : \mathbb{C} \setminus \{z \in \mathbb{C}|\mathrm{Re}z \le 0, \mathrm{Im}z = 0\} \to \mathbb{C}$ with $z \mapsto z^\alpha$ is not NH in the present case. This may be shown explicitly considering the power $(re^{i\phi})^\alpha = r^\alpha(\cos\alpha\phi + i\sin\alpha\phi)$ (cf. Section 2.2.2) of a complex number in the open upper complex half-plane, i.e. $re^{i\phi} \in \Pi_+$ with $r > 0, \phi \in (0,\pi)$. Since $\alpha > 1$, it follows that $\alpha\phi$ may become larger than π and therefore $\sin\alpha\phi$ may also possibly take negative values. This means that the power function is not a self-map of the open upper half-plane Π_+ and, as a consequence, it fails to be NH according to Def. 2.1.1.

In this Section we sketch an alternative method that may be applied for arbitrary values of the Rényi index $\alpha \in (0,1) \cup (1,+\infty)$. The method relies on the analytic functional calculus, which is founded on the following fundamental theoretical result that precisely describes the conditions under which an operator may be inserted into an analytic scalar function.

Theorem 4.2.1. *Let T be an operator defined on a Hilbert space with spectrum $\sigma(T)$, and let U be an open set such that $\sigma(T) \subseteq U$. Let f be an analytic function in a domain containing the closure of U, and suppose that the boundary ∂U of U consists of a finite number of closed rectifiable Jordan curves, oriented in the positive sense customary in the theory of complex variables[2]. Then $f(T)$ may be expressed as a contour integral over ∂U by the following formula:*

$$f(T) = \frac{1}{2\pi i}\oint_{\partial U} \mathrm{d}z\, f(z)(zI - T)^{-1},$$

where $(zI - T)^{-1}$ is the resolvent of operator T in z.

Proof. Cf. Theorem 10 in Ref. [DS57]. □

The power function is well-defined on its definition domain even for $\alpha > 1$, and so is the complex Rényi entropy function (cf. Def. 2.4.3) $\tilde{H}_\alpha : D_{\tilde{H}} \cup \{0,1\} \to \mathbb{C}$, with $z \mapsto \frac{1}{1-\alpha}\ln(z^\alpha + (1-z)^\alpha)$ on the domain

$$D_{\tilde{H}} := \mathbb{C} \setminus (\{z \in \mathbb{C}|\mathrm{Re}z \le 0, \mathrm{Im}z = 0\} \cup \{z \in \mathbb{C}|\mathrm{Re}z \ge 1, \mathrm{Im}z = 0\}) = \Pi_+ \cup \Pi_- \cup (0,1),$$

[2] Cf. definition in Section 4.1.

and $\tilde{H}_\alpha(0) = \tilde{H}_\alpha(1) = 0$. The function $\tilde{H}_\alpha$ is additionally analytic on $D_{\tilde{H}}$.

In Section 3.4, we introduced the regularized operator E_ϵ, which converges strongly to the operator D in the $\epsilon \to 0$ limit with respect to the $L^2(\mathbb{R}, \mathbb{C}^2)$ operator norm. We now define the open disk $\Delta\left(\frac{1}{2}, \frac{1}{2(1+\epsilon)}\right) := \left\{z \in \mathbb{C} : \left|z - \frac{1}{2}\right| < \frac{1}{2(1+\epsilon)}\right\}$, and we note that, by the operator inequality 3.7,

$$\sigma(E_\epsilon) \subseteq \left[\frac{\epsilon}{1+2\epsilon}, \frac{1+\epsilon}{1+2\epsilon}\right] \subset \Delta\left(\frac{1}{2}, \frac{1}{2(1+\epsilon)}\right) \subset \overline{\Delta\left(\frac{1}{2}, \frac{1}{2(1+\epsilon)}\right)} \subset D_{\tilde{H}},$$

and therefore $\tilde{H}_\alpha$ is analytic on the closure of $\Delta\left(\frac{1}{2}, \frac{1}{2(1+\epsilon)}\right)$ for any $\epsilon > 0$.

Moreover, we denote by $\partial\Delta\left(\frac{1}{2}, \frac{1}{2(1+\epsilon)}\right)$ the circle centered in the real point $\frac{1}{2}$ and of radius $\frac{1}{2(1+\epsilon)}$ and oriented counterclockwise.

According to our treatment in Section 3.5, we focus here on the contribution of subsystem 1 to the Rényi entanglement entropy operator $\sigma(\alpha, D_{\mathcal{I}}, D_{\mathcal{I}^1}, D_{\mathcal{I}^2})$, cf. Def. 3.1.11. The corresponding contribution to the Rényi entanglement entropy is given by the trace of operator σ.

By Theorems 3.5.1, 3.7.1 and 4.2.1, Proposition 3.7.2 and employing Eq. 3.40:

$$\begin{aligned}
&\frac{1}{1-\alpha}\lim_{\epsilon\to 0} \operatorname{tr}(-P_1 \ln(E_\epsilon^\alpha + (I - E_\epsilon)^\alpha)P_1 + P_1 \ln((P_1 E_\epsilon P_1)^\alpha + (P_1 - P_1 E_\epsilon P_1)^\alpha)P_1) \\
&\quad = \frac{1}{2\pi i(1-\alpha)} \lim_{\epsilon\to 0} \oint_{\partial\Delta\left(\frac{1}{2}, \frac{1}{2(1+\epsilon)}\right)} \mathrm{d}z \, \ln(z^\alpha + (1-z)^\alpha) \cdot \operatorname{tr}\big((zI - D_{\mathcal{I}^1})^{-1} - (zI - D_{\mathcal{I}})^{-1}\big) \\
&\quad = \frac{1}{2\pi i(1-\alpha)} \lim_{\epsilon\to 0} \oint_{\partial\Delta\left(0, \frac{1}{2(1+\epsilon)}\right)} \mathrm{d}z \, \ln\left(\left(\frac{1}{2} - z\right)^\alpha + \left(\frac{1}{2} + z\right)^\alpha\right) \operatorname{tr}\big(R_{D_{\mathcal{I}^1}}(z) - R_{D_{\mathcal{I}}}(z)\big) \\
&\quad = -\frac{1}{4\pi^2(1-\alpha)} \lim_{\epsilon\to 0} \oint_{\partial\Delta\left(0, \frac{1}{2(1+\epsilon)}\right)} \mathrm{d}z \, \frac{\ln\left(\left(\frac{1}{2} - z\right)^\alpha + \left(\frac{1}{2} + z\right)^\alpha\right)}{z^2 - \frac{1}{4}} \\
&\qquad\qquad \cdot \lim_{x\to y} \int_{\mathcal{I}^1} \mathrm{d}y \, (K_{\mathcal{I}}(z,x,y) - K_{\mathcal{I}^1}(z,x,y)) \\
&\quad = \frac{1}{8\pi^3 i(1-\alpha)} \lim_{\epsilon\to 0} \oint_{\partial\Delta\left(0, \frac{1}{2(1+\epsilon)}\right)} \mathrm{d}z \, \frac{\ln\left(\left(\frac{1}{2} - z\right)^\alpha + \left(\frac{1}{2} + z\right)^\alpha\right)}{z^2 - \frac{1}{4}} \ln\left(\frac{2z+1}{2z-1}\right) \\
&\qquad\qquad \cdot \int_{\mathcal{I}^1} \mathrm{d}x \, (Z'_{\mathcal{I}}(x) - Z'_{\mathcal{I}^1}(x)) \\
&\quad = \frac{1}{8\pi^3 i(1-\alpha)} \lim_{\epsilon\to 0} \oint_{\partial\Delta\left(0, \frac{1}{2(1+\epsilon)}\right)} \mathrm{d}z \, \frac{\ln\left(\left(\frac{1}{2} - z\right)^\alpha + \left(\frac{1}{2} + z\right)^\alpha\right)}{z^2 - \frac{1}{4}} \ln\left(\frac{2z+1}{2z-1}\right) \\
&\qquad\qquad \cdot \sum_{i\in I_1} \sum_{j\in I_2} \ln\left(\frac{|b_i - a_j||a_i - b_j|}{|b_i - b_j||a_i - a_j|}\right).
\end{aligned} \tag{4.2}$$

Combining Eq. 4.2 for both subsystems 1 and 2 with Lemma 3.7.4, we may now state a generalized form of Theorem 3.7.5 for Rényi-index $\alpha \in (0,1) \cup (1, +\infty)$. We get

$$\Delta S_\alpha(\omega, \omega_1 \otimes \omega_2) = N\tilde{\Xi}(\alpha)(g(\mathcal{I}^1) + g(\mathcal{I}^2) - g(\mathcal{I})) \tag{4.3}$$

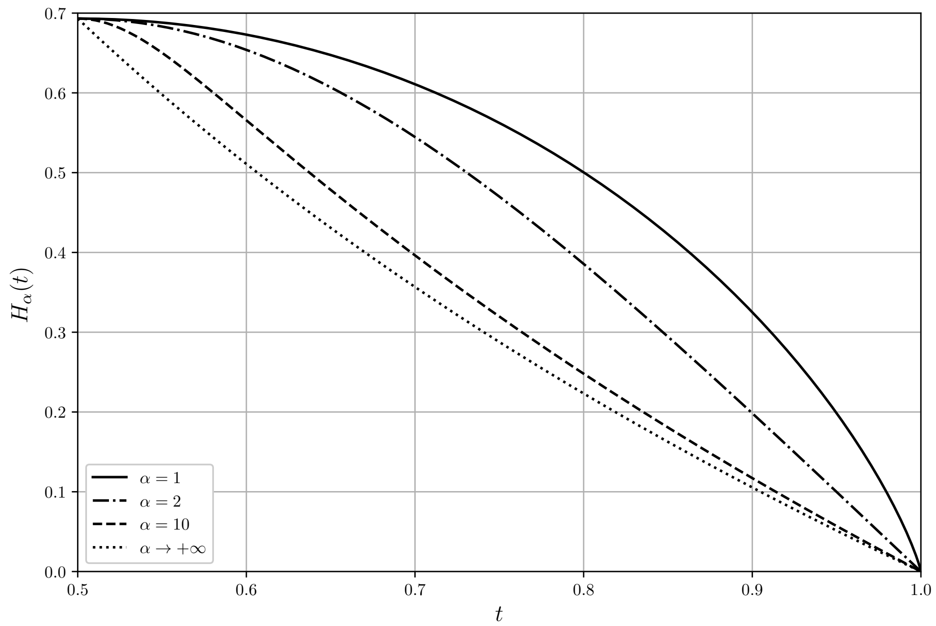

Figure 4.1: Plot of the Rényi entropy function H_α (cf. Def. 2.4.2) for a few values of the Rényi index $\alpha \in (1, +\infty)$ on the interval $t \in \left[\frac{1}{2}, 1\right]$. The Shannon entropy function (cf. Def. 2.4.1) obtained by means of the $\alpha \downarrow 1$ limit is also shown for comparison (solid line). The $\alpha \to +\infty$ limit represents the min-entropy function (dotted line). The common maximum of all entropy curves at $t = \frac{1}{2}$ reads $\ln 2$.

where the entanglement coefficient $\tilde{\Xi}(\alpha)$ now reads

$$\tilde{\Xi}(\alpha) := \frac{1}{8\pi^3 i(1-\alpha)} \lim_{\epsilon \to 0} \oint_{\partial\Delta\left(0, \frac{1}{2(1+\epsilon)}\right)} \mathrm{d}z \, \ln\left(\left(\frac{1}{2} - z\right)^\alpha + \left(\frac{1}{2} + z\right)^\alpha\right) \frac{\ln\left(\frac{2z+1}{2z-1}\right)}{z^2 - \frac{1}{4}}. \tag{4.4}$$

We conclude with two warnings. For $\alpha > 1$ the Rényi entropy function fails to be globally concave, cf. Fig. 4.1. Our argument for the traceability of the bipartite Rényi entanglement entropy (cf. Theorem 3.6.2) fails in this case as well, since it requires the positivity of the entanglement operator that in turn is based on the property of concavity. Therefore, the question of the traceability must be addressed separately.

Moreover, in the literature it was pointed out that, in the $\alpha = 2$ case, the Rényi mutual entropy, upon which our definition of the entanglement entropy is based (cf. Eqs. 3.3 and 3.4), is in general not subadditive and may become negative, e.g. in two-qubit systems [AGS12]. However, in the same paper it was shown that the $\alpha = 2$ mutual information for two-mode Gaussian states is non-negative and it measures the quadrature correlations of the total state.

4.3 Non-Extensive Entropy

The concept of a non-extensive entropy was applied in many physical problems of nonlinear systems out of thermal equilibrium (cf. e.g. Refs. [GMT04, Cho02]). For any $q \in \mathbb{R}$, we define the complex non-extensive entropy function as follows:

$$\tilde{H}_q : D_{\tilde{H}} \to \mathbb{C}, \qquad z \mapsto \frac{1}{1-q}(1 - z^q - (1-z)^q) \tag{4.5}$$

on the same complex domain $D_{\tilde{H}}$ defined in Section 4.2. From the point of view of information theory, even in this case the $q \to 1$ limit yields the usual Shannon entropy, when considering the restriction $\tilde{H}_q|\mathbb{R}$ on the real axis.

Applying the same line of argumentation as in Section 4.2, we may adapt results 4.3 and 4.4 with Eq. 4.5, and obtain

$$\Delta S_q(\omega, \omega_1 \otimes \omega_2) = N\tilde{\Xi}(q)(g(\mathcal{I}^1) + g(\mathcal{I}^2) - g(\mathcal{I}))$$

where the entanglement coefficient $\tilde{\Xi}(q)$ now reads

$$\tilde{\Xi}(q) := \frac{1}{8\pi^3 i(1-q)} \lim_{\epsilon\to 0} \oint_{\partial\Delta\left(0,\frac{1}{2(1+\epsilon)}\right)} \mathrm{d}z \left(1 - \left(\frac{1}{2} - z\right)^q - \left(\frac{1}{2} + z\right)^q\right) \frac{\ln\left(\frac{2z+1}{2z-1}\right)}{z^2 - \frac{1}{4}}.$$

4.4 Fermions on a Discrete Lattice

The one-particle density operator $D := \frac{1}{2}(I - iH\gamma^3)$ we introduced in Theorem 3.3.1 and Eq. 3.6 to describe a system of quasi-free fermions (cf. Section 3.5.2) was defined using the Hilbert transform operator H from Def. 3.3.4 and the matrix $\gamma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

Assuming now that the system is defined on $\mathbb{Z}$, we search for a discrete expression for the resolvent of D, in analogy to its counterpart on $\mathbb{R}$ in Theorem 3.5.1.

Let $f := \{f[i] : i \in \mathbb{Z}\}$ denote a discrete sequence on $\mathbb{Z}$, where $f[i] \in \mathbb{C}$ for $i \in \mathbb{Z}$. We define the discrete Hilbert transform of f on the lattice by

$$(Hf)[j] := \frac{1}{\pi} \sum_{k=-\infty}^{+\infty} H_{jk} f[k] \tag{4.6}$$

where

$$H_{jk} := \begin{cases} \frac{1-(-1)^{j-k}}{j-k} & \text{if } j \neq k \\ 0 & \text{if } j = k \end{cases} \tag{4.7}$$

according to Eqs. 13.175 and 13.176 in Ref. [Kin09]. We note that the matrix H_{jk} is skew-symmetric, i.e. $H_{jk} = -H_{kj}$.

In analogy to our treatment in Section 3.3, we now define the domain $\mathcal{I}$ of the fermionic system as a finite subset of $\mathbb{Z}$, and we take $\mathcal{I}^1, \mathcal{I}^2 \subset \mathbb{Z}$ such that $\mathcal{I} = \mathcal{I}^1 \cup \mathcal{I}^2$ and $\mathcal{I}^1 \cap \mathcal{I}^2 = \emptyset$.

Let $H_{\mathcal{I}}$ mean the discrete Hilbert operator 4.7 with summation restricted to the subset $\mathcal{I}$ of $\mathbb{Z}$. Then recalling Theorem 3.5.1, we search for the formal resolvent $R_{D_{\mathcal{I}}}$, i.e. the inverse of the matrix operator $M^{\pm}_{\mathcal{I}}(\lambda) := D^{\pm}_{\mathcal{I}} - \left(\frac{1}{2} - \lambda\right)I = \lambda I \mp \frac{i}{2} H_{\mathcal{I}}$ on $\mathbb{Z}$, for real λ. By the superscript symbol $\pm$ we denote the eigenvalues ± 1 of the γ^3 matrix.

By Eqs. 4.6 and 4.7, the matrix operator reads

$$(M^{\pm}_{\mathcal{I}}(\lambda) f)[j] = \pm\frac{1}{2\pi i} \sum_{k\in\mathcal{I}} H_{jk} f[k] + \lambda \sum_{k\in\mathcal{I}} \delta_{jk} f[k] \tag{4.8}$$

for any discrete sequence f on $\mathcal{I}$.

In general, considering a finite discrete linear space of dimension $n \in \mathbb{N}$ on which we define a vector $x \neq 0$ and a skew-symmetric $n \times n$ matrix A, we get for any real number $\mu \neq 0$ through matrix multiplication:

$$(\mu I - A) \cdot (\mu I + A) = \mu^2 I - AA = \mu^2 I + A^T A. \tag{4.9}$$

Additionally, we note the scalar product

$$\langle x, (\mu^2 I + A^T A)x \rangle = \mu^2 \langle x, x \rangle + \langle x, A^T A x \rangle = \mu^2 \langle x, x \rangle + \langle Ax, Ax \rangle = \mu^2 \|x\|^2 + \|Ax\|^2 > 0. \tag{4.10}$$

Eqs. 4.9 and 4.10 together yield $\det(\mu I \pm A) \neq 0$ and therefore both matrices $\mu I \pm A$ are invertible.

From this discussion, since H_{jk} is skew-symmetric, we conclude that the matrix $\pm \frac{1}{2\pi i} H_{jk} + \lambda \delta_{jk}$ in Eq. 4.8 is invertible for any real $\lambda \neq 0$, i.e. the resolvent matrix exists and may be computed e.g. numerically. Analogously we may proceed with the matrix operators of subsystems $i = 1, 2$.

The traces of the resolvent matrices may be then inserted directly into Eq. 3.21 to calculate the contributions of each subsystem to the Rényi entanglement entropy for $\alpha \in (0, 1)$ (cf. Def. 3.3 and Eq. 3.4). Then, the treatment follows the same argumentation line already outlined in Section 3.7.

Chapter 5

Conclusions

In this Thesis we studied the entanglement entropy of a 1D system of N relativistic quasi-free fermions distributed on the real line. Our results employ the Rényi entropy and generalize and extend those of Longo and Xu [LX17] who, for the first time, rigorously calculated the entanglement of such system on the basis of the Shannon entropy.

The idea we pursued in Chapter 2 is to employ the Nevanlinna-Herglotz theory of analytic self-maps in the open upper complex half-plane to express the Rényi entropy function in a suitable way for our subsequent treatment. In fact, Nevanlinna-Herglotz functions admit the unique canonical integral representation 2.4, where the independent variable z only appears in the rational terms $R_z(\pm\lambda) := \frac{1}{z-\frac{1}{2}\pm\lambda}$. This is convenient since, in a quantum mechanical treatment, replacing z with a suitable one-particle density operator D, $R_D(\pm\lambda)$ may be interpreted as the resolvent of D in $\frac{1}{2} \mp \lambda$.

Unfortunately, the complex Rényi entropy function partly breaks the Nevanlinna-Herglotz property since the term $(1-t)^\alpha$ for generic real positive α is not a self-map in the upper complex half-plane. Nevertheless, if we restrict the interval of the Rényi index to $\alpha \in (0,1)$, the Rényi entropy function may be cast in the form

$$H_\alpha(t) = \frac{\alpha}{1-\alpha} \ln t + \frac{1}{1-\alpha} L_\alpha(-t), \tag{5.1}$$

as we showed in the proof of Theorem 2.4.1, for values $t \in (0,1)$ and for a suitably defined function L_α, where the only place where the break occurs is the term $-t$ in the argument of L_α. In Eq. 5.1 both the logarithm and L_α are Nevanlinna-Herglotz functions (cf. Theorem 2.2.1 and Lemma 2.3.1), and this yields our representation 2.30 of the Rényi entropy in Theorem 2.4.1. Despite its apparent complexity, a simple structure emerges in Eq. 2.30: The whole information concerning the underlying entropy form is summarized in the function $\frac{f_\alpha(\lambda)}{1-\alpha}$ which may be interpreted as the derivative of the generating function of the measure in the Nevanlinna-Herglotz integral representation, while the independent variable z only appears in the term $R_z(\lambda) - R_z(-\lambda)$. The term $\frac{B(\alpha)}{1-\alpha}$ as well as the remaining integral contributions are of little interest in our treatment, since they are constant and therefore, they do not contribute to the Rényi entanglement entropy.

Since entanglement is essentially a quantum mechanical concept, we introduced its formal definition in Chapter 3 in the abstract framework of C^*-algebras supplied with canonical anticommutation relations to correctly describe a system of fermions. In this formalism the one-particle density operator D of the system is essentially expressed by the Hilbert operator on $L^2(\mathbb{R})$, as shown in Theorem 3.3.1. Moreover, since we restrict our treatment to massless fermions only, chirality is accounted for in the γ^3 matrix as shown in Eq. 3.6.

Splitting the whole system into two disjoint subsystems of one-particle densities D_1, D_2, we defined the Rényi entanglement entropy by $\operatorname{tr}\sigma(\alpha, D, D_1, D_2)$, whereby the operator σ is defined in Def. 3.1.11 simply as the Rényi mutual entropy of the bipartite system. For $\operatorname{tr}\sigma(\alpha, D, D_1, D_2)$ to be a suitable definition of an entanglement measure, its positivity is of course required. To this aim, in Section 3.2 we first proved that operator σ is concave and furthermore that from this property the non-negativity of its trace follows (cf. Theorem 3.2.9). As a further consequence of positiveness we could prove in Section 3.6, employing a criterion developed by Brislawn [Bri88], that operator $\sigma(\alpha, D, D_1, D_2)$ is traceable. Therefore, in conclusion, our entanglement measure $\operatorname{tr}\sigma(\alpha, D, D_1, D_2)$ is well-defined for Rényi index $\alpha \in (0, 1)$.

After this preparatory work, the explicit calculation of the Rényi entanglement entropy is a generalization of the treatment shown by Longo and Xu in Ref. [LX17]. In Section 3.5.3 we reduced our Nevanlinna-Herglotz canonical integral representation of operator $\sigma(\alpha, D, D_1, D_2)$ in a form involving the same integral kernel G studied by Longo and Xu, that is independent of the Rényi index α. In fact, this reduction allowed us to partly reuse in a more general context the techniques of the regularized entropy operator and classical results from the theory of singular integrals for the explicit analytical computation of the resolvents R_D, R_{D_1}, R_{D_2} of the one-particle density operators D, D_1, D_2, respectively.

Our final result for the entanglement entropy in Theorem 3.7.5 is completely analytical. It is proportional to the the number N of fermions in the system and moreover to a geometric factor $g(\mathcal{I}^1) + g(\mathcal{I}^2) - g(\mathcal{I})$, which simply describes the spatial domain of the system as a union of finite disjoint intervals on the real line. The only dependence on the Rényi index α appears through the entanglement coefficient $\Xi(\alpha)$, that is represented by an integral which contains the derivative $\frac{f_\alpha(\lambda)}{1-\alpha}$ of the generating function of the Nevanlinna-Herglotz integral measure explicitly. The similarity of our result with Longo and Xu's formula of the entanglement entropy in the von Neumann case is striking, and our formula reduces very naturally to theirs by replacing the derivative of the generating function above with $\lambda - \frac{1}{2}$.

In Theorem 3.8.2 we established that the entanglement coefficient $\Xi(\alpha)$ may be calculated analytically, and this yields the hyperbolic formula $\Xi(\alpha) = \frac{1}{24}\frac{1+\alpha}{\alpha}$, which is in accordance with the $\Xi(1)$ value obtained by Longo and Xu, and the $\Xi(\frac{1}{2})$ value of the logarithmic negativity entanglement, which we evaluated in Lemma 3.8.1. Moreover, our hyperbolic formula is identical to the scaling law derived in Ref. [LSS14].

Of course, our results may be extended in several directions relaxing a few of the assumptions we made in this Thesis. However, although the generalizations provide some more refined statements in more complicated cases of theoretical and practical interest, our main Theorems 3.7.5 and 3.8.2 still maintain their central theoretical validity. Since these further generalizations lie somewhat outside the main line and focus of this Thesis, we addressed them as special and advanced topics in Section 4 giving short sketches, hints and ideas about the possible extension of our method, but we refrained from formal and detailed proofs which would require further work.

The first and obvious generalization concerns the definition domain of the fermionic system. In Chapter 3 we chose a quasi-free system of fermions distributed on the real line. This is a special case of a more general picture, where the particles are confined on a closed smooth curve in $\mathbb{R}^2$. This generalization is straightforward, since our whole treatment rests on the explicit knowledge of the resolvent of the one-particle density operator, and classical results from the theory of singular integrals seamlessly extend even to domains defined on Jordan curves of constant curvature. We addressed this topic in Section 4.1.

Another interesting question concerns the behaviour of the entanglement entropy as the Rényi index moves into the $\alpha > 1$ interval. Although our hyperbolic formula from Theorem 3.8.2 extends to this α-interval, a rigorous proof of this generalization is not straightforward. Indeed, this case is subtly tricky, since the power function $\Pi_+ \to \mathbb{C}, z \mapsto z^\alpha$ in the complex upper half-plane now fails to be of Nevanlinna-Herglotz type. Therefore, the general $\alpha > 1$ problem requires a new method.

In Section 4.2 we proposed to employ the Dunford analytic functional calculus, which may be applied to a much wider function class than the Nevanlinna-Herglotz class, at the expense of being able to express the results of the entanglement entropy only through a complicated Cauchy line integral in $\mathbb{C}$. We must additionally point out that the questions of the positivity and traceability of the Rényi entanglement entropy operator σ are still open in the interval $\alpha \in (1, +\infty)$ and in fact, it has been pointed out in the literature that the operator σ may become negative, e.g. for $\alpha = 2$ and two-qubit systems. These questions require to be fully and carefully addressed separately.

The Dunford analytic functional calculus may be also applied to treat a wider class of problems. As an example, we applied it in Section 4.3 to treat yet another entropy form, namely the non-extensive entropy [GMT04], which was employed with success in the study of complex systems.

The last topic we considered in Section 4.4 was a system of quasi-free fermions distributed on a discrete lattice $\mathbb{Z}$. The main idea here is to work with the discrete version of the Hilbert transform and its inverse to build up a discretized resolvent of the one-particle density operator of the system. This reduces to the evaluation of the inverse of a matrix, which may be easily achieved numerically.

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Selbstständigkeitserklärung

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Modul: Masterarbeit

Thema: 1D Rényi Entanglement Entropy of Free Relativistic Fermions

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