

Mathematics Area
PhD course in Geometry and Mathematical Physics

Estimates for modular theory in algebraic QFT

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Abstract

The general scope of this PhD thesis is to establish relations between Tomita-Takesaki modular theory, in particular modular Hamiltonians and relative modular Hamiltonians, and physically better understood quantities, such as the stress-energy tensor, energy densities or other modular data in cases where it is known explicitly. In Chapter 1, we will present the basics of operators algebras, Tomita-Takesaki theory, symplectic spaces, and link these concepts to discuss quasi-equivalence of Gaussian states. In Chapter 2, we will discuss algebraic QFTs both in the framework of the Haag-Kastler axioms and of locally covariant QFT, to then specialize to scalar fields and present the stress-energy tensor and the Hadamard condition. In Chapter 3, focussing on Gaussian states of the Weyl-CCR algebra, we study relations between quasi-equivalence of their GNS-representations, differences of the total energy (on some Cauchy surface), and differences between functions of the modular Hamiltonians. Following qualitative relations by Araki and Yamagami, Verch and Longo, we investigate quantitative relations, including in particular estimates of differences between functions of modular Hamiltonians in terms of energy differences. These results will make use of inequalities between p -norms of operators, which we will discuss in Appendix C. In Chapter 4, generalizing the picture beyond Gaussian states, we exploit locality properties of general algebraic QFTs to construct a scheme that allows to estimate relative modular Hamiltonians for suitable pairs of states on some local algebra in terms of modular Hamiltonians of a reference state on bigger or smaller algebras, which might be better understood. For pairs of states susceptible to this scheme, there exist unitaries linking them to the reference state which do not enable superluminal signalling in the sense of Sorkin's paradox. Such unitaries may not however compose the whole class of non-signalling operators, raising the question whether the existence of a non-signalling unitary is a sufficient condition to show the applicability of our estimate. To investigate the strength of our estimates we then consider coherent states for CCR systems, focussing particularly on free scalar fields, where the difference between the upper and lower bounds can be made arbitrarily small, recovering an exact result by squeezing. This yields an independent proof for the relative entropy formula in cases where the relative modular Hamiltonian has not been computed exactly and corroborates the strength of our general estimates. For these results, we will make use of several commutation properties of operators on Fock spaces, which we will present in Appendix A. Results about operator monotone functions will be used throughout this thesis and are explained in Appendix B.

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Foreword

I think that a man without utopian aspirations, without dreams and ideals,
in other words without passion and enthusiasm,
would be a heinous beast made simply of instinct and rationality:
some kind of boar with a degree in pure mathematics.

Fabrizio De André, interview
(translation by myself)¹

During its long² history, science has seen many deep changes in the way we interpret the tools it offers to analyse the physical world we are part of. As an aspiring mathematical physicist whose interests have been mainly focused on the mathematical descriptions of the subatomic world we came to know as quantum mechanics and quantum field theory, I would argue that the one we are still struggling to come to terms with is the quantum revolution of the last century. While until the end of the 19th century there was mostly a direct correspondence between the physical phenomenon we are trying to model and the model itself, quantum mechanics has shown that this is not at all necessary to have a working physical theory. Indeed, the interpretation problem of quantum mechanics faces us with having a well-posed mathematical model, already fully formalized in 1932 by von Neumann [Neu32], but many different physical realizations that come to the same results, and thus we can treat as equivalent at least on an operative level.

This complicates an already standing debate, the one between scientific idealism versus realism: do things exist beyond our observations? Are physical models something real, something that belongs to this universe? The realist position is that things do (or may) exist beyond our observations and the data we infer from them, while the idealist would argue that those are all that exists. In the end, science will work regardless of the stance of the scientist on this matter, as its scope is to conjure up mathematical models to reproduce experimental data, and with some luck to make predictions that can be as well verified, even though the attitude towards the subject may be different.

The mathematical physicist has a tricky job on the sideline of this debate, for they are tasked to make physical models rigorous from a mathematical standpoint. While this keeps their work attached to physical reality, which a more abstract mathematician may be less inclined to give attention to, it still tends to keep them detached from the actual experimental reality of physics. This may be expressed as the old adage of ‘being a physicist to mathematicians and a mathematician to physicists’. The reason to cite such high philosophy is merely to point out the fact that there are concepts which are ‘closer to the experimenter’, like the probability of measuring some value of

¹Italian original: ‘Penso che un uomo senza utopia, senza sogno e senza ideali, vale a dire senza passioni e senza slanci, sarebbe un mostruoso animale fatto semplicemente di istinto e raziocinio: una specie di cinghiale laureato in matematica pura’. I would like to note that, while I do not agree with the sentiment portrayed here, a thesis is a good place to subvert meanings, provided a good explanation, which will hopefully follow.

²at least for human standards.

a certain observable, and others which are arguably not, such as the Lie group associated to some QFT. In the middle, we may find quantities like the energy of some state in a spacetime region, which has a clear physical meaning even though it may not be directly measurable.

While many quantities which are further away from the ‘experimental reality’ may be hard to compute directly, a useful strategy is to try to relate them to quantities that have a clearer interpretation, physical or mathematical it may be. One of such topics, to which this thesis will give a fair amount of attention, is Tomita-Takesaki modular theory. On a mathematical level, modular theory (may its two creators forgive me for often omitting their names from now on) offers a method for obtaining a kind of dynamical evolution on an abstract von Neumann algebra, whose generator is the *modular Hamiltonian*. Note that it is not an actual Hamiltonian (read: energy), however it formally performs a similar function. This is already a remarkable result, however it begs the question: what is the physical sense of this modular *Hamiltonian*? During the (almost!) 70 years of research on modular theory, an interpretation for its objects has been established only in a handful of cases, which the more technically inclined reader will find listed in the introduction that follows this foreword. However, this stands to highlight that we will be treading on the very murky terrain that is the threshold between mathematics and physics.

This thesis will not make an attempt to solve these general problems, however we will employ the most powerful tool a mathematical physicist has under their belt: estimates. While we may not be able to compute exactly the quantities I’ve been introducing, we might relate them to better understood concepts, like energy densities, or (more generally) the stress-energy tensor. To further complicate the situation, modular theory can be as well formulated in a ‘relational’ sense, which gives us *relative modular theory*. While we will go in more detail later about these concepts (not that there is any detail yet), it gives us the *relative* version of the same objects as before, like the *relative* modular Hamiltonian. Again, the few people who will be able to understand what I’m saying will find many more wonderful details in the introduction. Of course, at this point it should not come as a surprise to know that, if modular data is already very hard to compute, the situation does not get better with relative modular data, quite the opposite. We may however adopt the same strategy and estimate relative modular Hamiltonians in terms of other quantities, for example (would you able to guess?) in terms of energies.

Given these challenges, what you should expect to see in this thesis is all the physical and mathematical machinery I had to (start to) make sense of during the course of the past four long years, such as our modular Hamiltonians (relative or not), energies and energy densities and a bunch of estimates relating these quantities for different classes of physical states and different settings. Of course, more concepts which are central to discuss these topics will be introduced, such as what is a *Gaussian state* or what does it mean for Gaussian states to be *quasi-equivalent*. This will however require a deeper level of mathematical technicality that I’ve tried to keep out of this foreword. For the moment, I will argue that I do understand the physicists to whom this all does sound suspiciously close to abstract nonsense, and also the mathematicians who might find a bit funny all this struggle to make rigorous something that seemingly doesn’t want to be. At the same time, however, I find that there is something of merit in trying to connect the abstract and the concrete and working in this grey area where it is unclear how real something is. After all, both mathematics and physics have this inexplicable ability of drawing connections between different areas of knowledge which may at first sight look totally unrelated. I still find it baffling that suddenly a modular Hamiltonian can be estimated above by energy. Wouldn’t you?

Acknowledgements

I would like to thank SISSA for giving me the opportunity of pursuing the PhD project I am now concluding and for the opportunity to work both at a distance and in the same place with my supervisor, Dr. Ko Sanders, whom I thank for the general ideas behind this research and for all the help navigating many different subjects and physical and mathematical tools I encountered during these years. It would be impossible to express in only a few words how much I've learned in these years from Ko. Apart from presenting to me the many technical topics which I have tried to explain in this thesis, Ko has been an example of what it means to be both a mathematical physicist and a supervisor, for his pragmatic but never indifferent approach to research and mentoring, which I will always keep as a standard in any of my future endeavours. On this note, I would also like to thank Prof. Marcello Porta and Prof. Ludwik Dąbrowski for their support during these years, which has been essential to make my project progress despite what would have been, in other situations, problematic technical difficulties.

I would also like to thank, in chronological order, the QFT group at Friedrich-Alexander-Universität Erlangen-Nürnberg of Prof. Gandalf Lechner for their hospitality during my short stay in Erlangen in December 2023, the ITP in Leipzig and Prof. Daniela Cadamuro for my stay in April 2024, and the Institute for Analysis at Leibniz Universität Hannover and again Dr. Sanders for my stays there in March 2025 and between October 2025 and March 2026, which have all proved to be incredibly valuable for the development of the results I will present in this thesis. Talking about my time in Hannover, I also thank Christoph Minz for the discussions and our collaboration during what proved to be a very long German winter.

Also, I would like to thank again Gandalf Lechner and Daniela Cadamuro for their referee work for this thesis, which led to improving the exposition of some statements. In addition, a comment by Lechner also led to the refinement of a number of estimates in Chapter 3, improving the results presented in [CS25].

Then, I cannot fail to mention the many people that I have met during these years in SISSA and in my European academic wanderings, who have all taught me something new, may it be in mathematics, in physics, or in any of the other boundless aspects of life. Between my non-academic acquaintances, I must also thank all the people from Rome for their ever so strong presence, despite the physical distance that moving to Trieste has created. And to remember these four years, from the first person I've met in October 2022 to the last in October 2026, may you all know that your contribution is present in these pages, even if only through the mediating filter of their author.

Author's declaration

Sources for the background material and the appendices have been stated in the respective sections. Parts of Chapter 1 and the totality of Chapter 3 are taken from [CS25], written with Ko Sanders. The author has done most of the detailed work in deriving the results presented, the discussion about doubled symplectic spaces on pp. 38-40 is due to Ko Sanders. Some of the estimates in Sections 3.1 and 3.2 are however presented here in an improved form compared to those in [CS25]. Similarly, the totality of Chapter 4 (apart for minor additions) and parts of Appendix A have been taken from [CMS26], written with Christoph Minz and Ko Sanders, which has been submitted to Communications in Mathematical Physics for publication. The author's main focus has been the discussion on Sorkin's paradox of Section 4.1.1, however lesser contributions also appear in other sections. The link to the Buchholz-Fredenhagen approach to Lagrangian QFTs at the end of Section 4.1.1 is a more recent development and it is not present in the current version of [CMS26].

The figures in Chapter 4, which are taken from [CMS26], have been made by Christoph Minz. Figure 2.1 has been made by Niccolò Alfredo and has already appeared in a less refined form on the author's Master's thesis (University of Rome Tor Vergata, 2022).

Introduction

Since the advent of Tomita-Takesaki theory, a physical interpretation of the quantities coming from it has been established only in a handful of cases, all of which are characterized by the modular flow having a geometric action. On a mathematical level, modular theory allows to obtain a one-parameter group of automorphisms from a von Neumann algebra and a suitable ‘standard’ vector, which we can interpret as some kind of dynamical evolution (the modular flow) on the algebra, whose generator is the modular Hamiltonian. However, despite formally being akin to a Hamiltonian, how should a modular Hamiltonian be understood?

As a first example, a thermal (KMS) state Ω at temperature T on a stationary spacetime has $K_\Omega = H/T$ as its modular Hamiltonian, where H is the Hamiltonian, this is due to Takesaki [Tak70]. Then, considering the simple case of the vacuum state on the Minkowski spacetime for a general (algebraic) QFT, if we consider a wedge region, its corresponding modular Hamiltonian will correspond to the generator of Lorentz boosts. This is the content of the Bisognano-Wichmann theorem [BW76; BW75], which can be generalized to curved spacetimes [Sew82; San15]. In the case of massless free scalar fields, considering the Minkowski vacuum as state and double cones as regions (for which there is conformal invariance), we have that the modular flow is a subgroup of conformal transformations [HL82] and the modular Hamiltonian follows this fact [LM23]. For the future lightcone, it corresponds to dilations [Buc78], [Haa12, Thm. V.4.2.2]. For massless fermions, the modular Hamiltonian of a double cone was determined in [LM25]. We refer to [Haa12, Sec. V.4] for a review of these standard results. While these known cases show a connection between modular data and spacetime symmetries (the *geometric action* is key here), no general picture exists for what this modular data should physically mean. Already trying to compute the *massive* modular Hamiltonian for double cone regions has become one of the greatest challenges in this field, as the few techniques known to work are not sufficient to attack the problem. (A conjecture attributed to Fredenhagen from the 90s claims that the massive modular Hamiltonian should differ from the massless one by some pseudo-differential operator of order zero.)

To add to the already rich picture, modular theory can be as well formulated for pairs of states, which gives us *relative modular theory*, which can be defined for pairs of states on a von Neumann algebra [Ara75; Ara77; Tak03], leading to relative modular Hamiltonians. Modular Hamiltonians arise as a special case, where both states are equal. This special case is more commonly presented in the literature, because it is easier and it can be generalized to the setting of standard subspaces of complex Hilbert spaces [Lon08]. In QFT, the explicit expressions we have mentioned solely concern the modular Hamiltonian of a single state. Relative modular Hamiltonians are a powerful tool, as they allow to define in a very general sense relative entropy, which is indeed obtained as a suitable expectation value of the relative modular Hamiltonian [Ara75; Ara77], and it is sometimes called *Araki (relative) entropy* in this setting. Relative entropy is a central quantity in quantum information theory and in quantum field theory, which serves as a generalized notion of distance between states. Intuitively speaking, we interpret the relative entropy $H(\omega, \tilde{\omega})$ as the amount of information that we expect to gain when we learn that our system is in the state ω , where we

previously thought it was in the state $\tilde{\omega}$ [BF14].

In the endeavour to give a characterization of these modular objects, relative or not, this thesis will not generally aim at direct computations but rather at estimating such quantities, relating them to better understood concepts, like energy densities, or (more generally) the stress-energy tensor. A notable example of such an approach is the one by Bekenstein, who has argued on physical grounds that entropy can be estimated from above in terms of energies and energy densities using the Bekenstein bound [Bek81]. More recently, relative entropies have been estimated in terms of energy densities of a spacetime region of interest [Lon25; HL25]. Another idea is to estimate relative modular Hamiltonians with their non relative counterparts, with special attention to the few cases where the latter are known. In this thesis, we will explore two different ideas about estimating modular Hamiltonians, relative modular Hamiltonians and relative entropy, following the results presented in [CS25] and [CMS26].

In [CS25], the idea has been to estimate differences of (functions of) modular Hamiltonians of Gaussian states and suitable reference Gaussian states with the energy of said states, and linking these estimates with quasi-equivalence relation for Gaussian states due to Araki and Yamagami [AY82], Verch [Ver94], and Longo [Lon22]. The motivation behind quasi-equivalence, whose generalities we will review in Section 1.3.1, is that, as C^* -algebras often admit many representations, in order to express the idea that the choice of representation does not matter, one may consider representations that are pairwise quasi-equivalent. This condition, which is weaker than unitary equivalence, ensures that every state that can be described by a density operator in one representation can also be represented by a density operator in another representation. E.g. in quantum field theories, especially in curved spacetime, a theory typically admits many representations that are not unitarily equivalent, but are, at least locally, quasi-equivalent, so that the choice of a Hilbert space representation is irrelevant for describing local physics [Wit22; Ver94].

For a bosonic quantum system satisfying canonical commutation relations (CCR), the earliest investigation into the equivalence of Gaussian states of the Weyl algebra appears to be Shale's work on unitary equivalence of pure states [Sha62]. In the most general situation, allowing (degenerate) pre-symplectic forms and Gaussian states that need not be pure, necessary and sufficient conditions for quasi-equivalence were established by Araki and Yamagami [AY82]. These general conditions were verified for the class of Gaussian Hadamard states of a linear real scalar quantum field on bounded regions of any globally hyperbolic Lorentzian manifold by Verch [Ver94]. It is gratifying to see that the Hadamard condition, which we will discuss in Section 2.1.2, ensures local quasi-equivalence, because this condition has been identified as physically important and these states have finite and smoothly varying expectation values for the renormalised stress tensor. This class includes ground and thermal (KMS) states on stationary spacetimes [SV00] and is preserved under scattering against smooth perturbations in the metric [FSW78]. Because a smooth energy density on a bounded region integrates to a finite total energy, one expects that a finite change in energy is insufficient to violate quasi-equivalence.

After reviewing the conditions of Araki-Yamagami, together with a recent development by Longo [Lon22] (see also [CM24]), who found equivalent conditions in a slightly more limited setting, formulated first in terms of polarization operators and then in terms of modular Hamiltonians, we will establish in Chapter 3 quantitative relations between [AY82], [Ver94] and [Lon22], connecting the perspectives of quasi-equivalence, finite energy differences and the comparison of modular operators, focussing on easy applications rather than full generality. In particular, we supplement the existing results by explicit estimates, which allow us to estimate the difference of suitable functions of the modular Hamiltonians in two Gaussian states in terms of the difference of their energies. (For a rather different approach to estimates between modular operators and energy

see [MPV22].) The estimates that we present rely on inequalities by Powers and Størmer [PS70], van Hemmen and Ando [HA80], Kittaneh [Kit87] and Kosaki [Kos98].

In [CMS26], shifting the focus to relative modular theory, the approach has been to elaborate a scheme that allows us to estimate relative modular Hamiltonians, and hence also relative entropies, for some states ω and $\tilde{\omega}$ in terms of the modular Hamiltonian of some reference state $\hat{\omega}$, which might be better understood. Such relations are bound to depend on the operators necessary to link ω and $\tilde{\omega}$ to $\hat{\omega}$. This scheme, which we will present in Chapter 4, combines locality properties of general QFTs with general properties of relative modular operators and suitable assumptions on the states involved. For suitable pairs of states ω and $\tilde{\omega}$, it allows us to estimate the relative modular Hamiltonian $K_{\tilde{\omega},\omega}$ of some region V_2 , and hence also the relative entropy $H(\omega, \tilde{\omega})$, from above, resp. from below, in terms of the modular Hamiltonian of the reference state $\hat{\omega}$ on a larger region $V_3 \supset V_2$, resp. a smaller region $V_1 \subset V_2$.

To examine which pairs of states and choices of regions are susceptible to our scheme, it is interesting to note that its applicability is linked to Sorkin’s paradox. In [Sor93], Sorkin points out that in a naive view of QFT it seems possible to construct examples of superluminal signalling, so-called ‘impossible measurements’. In QFT, the typical setting involves three observers, Alice, Bob and Charlie, such that Alice and Charlie are localised in spacelike related regions. An impossible measurement arises if Bob can perform a unitary operation that allows Charlie to determine whether Alice has performed some unitary operation on the shared quantum system or not, apparently violating causality. For our discussion, we will adopt the point of view of [BJK21; Jub22], where conditions on the unitaries localised in Bob’s part of the system were formulated that ensure they are non-signalling, i.e. they do not allow superluminal signalling. Note that these non-signalling conditions also involve a direction (Alice to Charlie or Charlie to Alice), which is something not explicitly highlighted in the previous literature, but important in our discussion. We refer to [PF24] for a comprehensive review of the current state of research on Sorkin’s paradox. Regarding our estimates, we observe that if we choose $\omega = \hat{\omega}$ as our reference state, then there is a unitary operation that maps ω to $\tilde{\omega}$ on V_3 and that does not allow superluminal signalling from the spacelike complement V_3' to V_2 in the sense of Sorkin’s paradox, if our upper bound applies. Similarly, if our lower bound applies, then there exists a unitary that maps ω to $\tilde{\omega}$ on V_2 and that does not allow superluminal signalling from V_1 to V_2' . However, it is an open question whether the existence of a non-signalling unitary (in either direction) is a sufficient condition to show the applicability of our estimate (in the corresponding direction). We comment on this issue using a construction involving the Cuntz algebra. We also remark that the unitaries generating the dynamical algebra of Buchholz-Fredenhagen for a Lagrangian QFT [BF20a; BF20b; BF19; BF21] are non-signalling and yield excitations to which our estimates apply in both directions.

To investigate the strength of our estimates we consider applications to coherent states, first on general CCR Weyl algebras and then for free scalar fields in the Minkowski vacuum representation. In general, coherent states in a quasi-free representation are defined in terms of Weyl operators, which are always non-signalling unitaries. For a standard reference state, the coherent states are also standard, so that relative modular Hamiltonians are always well-defined. One may often express the relative modular Hamiltonian between two coherent states, and hence also their relative entropy, in terms of the modular Hamiltonian of the quasi-free reference state. However, for coherent states whose excitations have a non-zero difference at the boundary of the region the exact computation becomes non-trivial. This is why our estimates are of some interest even in this simple case. It is known that the relative entropy between all pairs of coherent states can be obtained by approximation arguments using its lower semicontinuity [BCD22; Lon19; CLR20]. (This argument does not directly apply to the relative modular Hamiltonian.) For the special case

of free scalar fields on a Rindler wedge or, in the massless case, on a double cone we show that an exact formula for the relative entropy can also be recovered from our estimates using a squeezing argument involving an appropriate choice of cutoff functions. This proof works also for excitations that do not vanish at the boundary and it differs from existing proofs, because it does not exploit the lower semicontinuity of the relative entropy. This result indicates that our general estimates may not be losing too much information.

Chapter 1

The mathematical background

Physics is mathematical, not because we know so much about the physical world, but because we know so little: it is only its mathematical properties that we can discover.

Bertrand Russell, *An Outline of Philosophy* [Rus27]

We shall start by laying the background concepts of operator algebras needed for our discussion. For general concepts about C^* -algebras and von Neumann algebras, we refer to [KR97a; KR97b; RS75; BR87; BR97], for Tomita-Takesaki modular theory to [Tak79; Tak03; Lon08] and to [HS18] for aspects related to its application to entanglement entropies.

1.1 Operator algebras: the bare minimum

We shall start with a quick rundown of the main operator algebraic tools behind the concepts we need. The main structures we will focus on in this thesis are C^* -algebras and von Neumann algebras.

1.1.1 C^* -algebras

A $*$ -algebra is an algebra $\mathcal{A}$ closed under the $*$ operation $*$: $A \mapsto A^*$, which is an antilinear and antimultiplicative involution ($(A^*)^* = A$, $A \in \mathcal{A}$). A $*$ -homomorphism between two $*$ -algebras is a homomorphism which preserves the involution $*$, and a $*$ -isomorphism is an injective and surjective $*$ -homomorphism. Then, a C^* -algebra $\mathcal{A}$ is a Banach¹ $*$ -algebra such that $\|A^*A\| = \|A\|^2$, for all $A \in \mathcal{A}$, which is called the *C^* -identity of the norm*. We will generally consider unital algebras with unit $\mathbb{1}$. Note that the involution map $*$ is isometric for any C^* -algebra, as it preserve the norm. Given any Hilbert space $\mathcal{H}$, the algebra $\mathcal{B}(\mathcal{H})$ of all bounded operators on $\mathcal{H}$ is a C^* -algebra. This is relevant as any C^* -algebra can be seen as a subalgebra of $\mathcal{B}(\mathcal{H})$, cf. [GN43].

Theorem 1.1.1 (Gelfand-Naimark). *Any C^* -algebra is isometrically $*$ -isomorphic to a C^* -subalgebra of $\mathcal{B}(\mathcal{H})$, for some Hilbert space $\mathcal{H}$.*

In other words, the Gelfand-Naimark theorem provides an isometric representation of $\mathcal{A}$ on $\mathcal{B}(\mathcal{H})$, i.e. a $*$ -homomorphism $\pi : \mathcal{A} \mapsto \mathcal{B}(\mathcal{H})$.

Notable elements of a C^* -algebra $A \in \mathcal{A}$ are the class of normal operators $[A, A^*] = 0$, to which belong the self-adjoint operators $A = A^*$. Positive elements $A \geq 0$ are self-adjoint with non-negative

¹A Banach algebra is a normed algebra which is complete with respect to the norm topology.

spectrum. We speak of strictly positive elements $A > 0$ if zero does not belong to the point spectrum of A . (Orthogonal) projections $A = A^2$ are self-adjoint as well. A will be unitary if $A^*A = AA^* = \mathbb{1}$. An operator V on $\mathcal{H}$ is a partial isometry if $V^*V = E$ is an orthogonal projection. This induces an orthogonal decomposition of $\mathcal{H}$ as $\mathcal{H} = E\mathcal{H} \oplus (\mathbb{1} - E)\mathcal{H}$. The operator V acts as an isometry on the range of the *initial projection* $E = V^*V$, mapping it isometrically onto the range of the *final projection* $F = VV^*$. On the orthogonal complement $(\mathbb{1} - E)\mathcal{H}$, the operator V is zero. Then, V is a partial isometry if and only if V^* is a partial isometry. This allows to state the following standard result, cf. [KR97b, Thm. 6.1.2].

Theorem 1.1.2 (Polar decomposition). *Let $A \in \mathcal{B}(\mathcal{H})$. Then $A = V|A|$, where*

- i. $|A|$ is a positive self-adjoint operator, defined as $|A| = (A^*A)^{\frac{1}{2}}$, the modulus of A ;
- ii. V is a partial isometry, $V : \overline{\text{range}(|A|)} \mapsto \overline{\text{range}(A)}$ such that V^*V is the projection on $\overline{\text{range}(|A|)}$ and VV^* the projection on $\overline{\text{range}(A)}$.

This decomposition with said properties is unique, i.e. if $A = WK$ such that $K \geq 0$, W^*W is the projection on $\overline{\text{range}(K)}$ and WW^* the projection on $\overline{\text{range}(A)}$, then $W = V$ and $K = |A|$.

Given a positive operator $A \geq 0$ in $\mathcal{B}(\mathcal{H})$, its trace is defined as

$$\text{tr}(A) = \sum_i \langle e_i, Ae_i \rangle,$$

w.r.t. some orthonormal basis $\{e_i\}$ for $\mathcal{H}$ and the scalar product $\langle \cdot, \cdot \rangle$ on $\mathcal{H}$. Standard properties of the trace are $\text{tr}(A^*A) = \text{tr}(AA^*)$, the cyclicity $\text{tr}(AB) = \text{tr}(BA)$ for $A, B \in \mathcal{B}(\mathcal{H})$, and for $U \in \mathcal{B}(\mathcal{H})$ unitary, $\text{tr}(UAU^*) = \text{tr}(A)$, so the trace does not depend on the specific orthonormal basis chosen. Relevant classes of operators $A \in \mathcal{B}(\mathcal{H})$ are trace-class operators, such that $\text{tr}(|A|) < \infty$, and Hilbert-Schmidt operators, such that $\text{tr}(A^*A) < \infty$. It follows that trace-class operators are a subset of Hilbert-Schmidt operators, and both are subsets of the compact operators $\mathcal{K}(\mathcal{H})$ on $\mathcal{H}$. Hilbert-Schmidt operators on $\mathcal{H}$ form a Hilbert space w.r.t. the inner product $\langle A, B \rangle_2 = \text{tr}(A^*B)$ for A, B Hilbert-Schmidt operators [Ped11, Thm. 3.4.9], and trace-class operators form a Banach algebra under the norm $\|A\|_1 = \text{tr}(|A|)$, for A trace-class. This algebra will be the dual² of $\mathcal{K}(\mathcal{H})$ (on the same Hilbert space) and its dual will be $\mathcal{B}(\mathcal{H})$. We refer to Appendix C for the definition of more general p -norms.

1.1.2 States and representations

Let's now talk about linear functionals on a generic C^* -algebra $\mathcal{A}$, i.e. elements φ of its dual space $\mathcal{A}^*$. We say that φ is positive ($\varphi \geq 0$) if $\varphi(A) \geq 0$ for all $A \geq 0$. Equivalently, φ is positive if and only if $\varphi(A^*A) \geq 0$ for all $A \in \mathcal{A}$. We have that $\varphi \geq 0$ iff $\varphi(\mathbb{1}) = \|\varphi\|$ [Con19, Prop. 5.11 and Cor. 5.12]. This is stating that the positivity on the dual space, which is an algebraic condition, is equivalent to a metric condition, the norm taking a certain value. Then, φ is a *state* if it is a positive, normalized linear functional, i.e. $\varphi \geq 0$ and $\|\varphi\| = 1$. It follows that $\varphi(\mathbb{1}) = 1$. A state φ is faithful if it is strictly positive, i.e. for $A \in \mathcal{A}$, $\varphi(A^*A) = 0$ iff $A = 0$. We will call $\mathcal{S}(\mathcal{A})$ the set of states on $\mathcal{A}$, which will be a convex set, i.e. for $\varphi_1, \varphi_2 \in \mathcal{S}(\mathcal{A})$ and $0 \leq \lambda \leq 1$, $\varphi = \lambda\varphi_1 + (1 - \lambda)\varphi_2 \in \mathcal{S}(\mathcal{A})$. Pure states will be the extremal elements of $\mathcal{S}(\mathcal{A})$, i.e. the ones that cannot be written as non-trivial convex combinations. For $\mathcal{A}$ unital, $\mathcal{S}(\mathcal{A})$ is weakly compact, the set of pure states is always non-empty and it will generate the whole set by convex combinations and weak closure [BR87, Thm. 2.3.15].

²i.e. the space of continuous linear functionals on some space.

We will now discuss representations of C^* -algebras. First, consider a representation $\pi : \mathcal{A} \mapsto \mathcal{B}(\mathcal{H}_\pi)$ of a C^* -algebra $\mathcal{A}$. If there exists a closed subspace $\mathcal{C} \subset \mathcal{H}_\pi$ which is invariant under π , i.e. $\pi(A)\mathcal{C} \subset \mathcal{C}$ for any $A \in \mathcal{A}$, a *subrepresentation* is a representation $\pi|_{\mathcal{C}} : \mathcal{A} \mapsto \mathcal{B}(\mathcal{C})$, taken by restricting each $\pi(A)$ to act on $\mathcal{C}$. We will notate this as $\pi|_{\mathcal{C}}(A) := \pi(A)|_{\mathcal{C}}$, for any $A \in \mathcal{A}$.

Then, we say that π is an *irreducible representation* if it is a nonzero representation which has no proper³ nontrivial subrepresentation. Otherwise, it is *reducible*. We say that π is faithful if it is injective. Also, given a state $\varphi \in \mathcal{S}(\mathcal{A})$, we say that φ is *normal with respect to π* (or π -normal) if there exists a trace-class operator ρ_φ such that $\varphi(\cdot) = \text{tr}(\rho_\varphi \pi(\cdot))$. All π -normal states on $\mathcal{A}$ form a convex set called the *folium* of π . We can also say that a π -normal state φ is a *vector state of the representation π* if, given a unit vector $\psi \in \mathcal{H}$, $\varphi(\cdot) = \langle \psi, \pi(\cdot)\psi \rangle$. This allows to define a central construction in our discussion, the GNS-representation of a state, which represents it as a vector state, cf. [Con19, Thm. 5.14].

Theorem 1.1.3 (Gelfand-Naimark-Segal). *Let φ be a state on $\mathcal{A}$. Then there exists a triple $(\mathcal{H}, \pi, \xi)$ (the GNS-triple), where $\mathcal{H}$ is a Hilbert space, π is a representation of $\mathcal{A}$ on $\mathcal{B}(\mathcal{H})$, and $\xi \in \mathcal{H}$ is cyclic for π , i.e. $\overline{\pi(\mathcal{A})\xi} = \mathcal{H}$, such that $\varphi(A) = \langle \xi, \pi(A)\xi \rangle$, for all $A \in \mathcal{A}$.*

This representation is unique up to unitary equivalence, in the sense that if $(\mathcal{H}', \pi', \xi')$ is a triple with the same properties, then there exists a unitary operator $U : \mathcal{H} \mapsto \mathcal{H}'$ such that $U\xi = \xi'$ and $\pi'(A) = U\pi(A)U^*$.

We note that the GNS-representation arising from a pure state is irreducible and vector states of an irreducible representation are pure [Haa12, Thm. 2.2.17].

We shall now discuss some notions of equivalence between representations and states. To do so, let's consider two representations $\pi : \mathcal{A} \mapsto \mathcal{B}(\mathcal{H}_\pi)$, $\pi' : \mathcal{A} \mapsto \mathcal{B}(\mathcal{H}_{\pi'})$ of a C^* -algebra $\mathcal{A}$. A bounded linear operator $R : \mathcal{H}_\pi \mapsto \mathcal{H}_{\pi'}$ is an *intertwiner* from π to π' if $R\pi(A) = \pi'(A)R$, for all $A \in \mathcal{A}$. The adjoint operator of an intertwiner R is a uniquely defined bounded operator $R^* : \mathcal{H}_{\pi'} \mapsto \mathcal{H}_\pi$, $\langle \xi, R^*\xi' \rangle = \langle R\xi, \xi' \rangle$, with $\xi \in \mathcal{H}_\pi$ and $\xi' \in \mathcal{H}_{\pi'}$, which is an intertwiner in the opposite direction, $R^*\pi'(A) = \pi(A)R^*$, for all $A \in \mathcal{A}$. Intertwiners force a decomposition of each of the two representation spaces into two invariant orthogonal subspaces $\mathcal{H}_\pi = \mathcal{H}_\pi^{(1)} \oplus \mathcal{H}_\pi^{(2)}$, $\mathcal{H}_{\pi'} = \mathcal{H}_{\pi'}^{(1)} \oplus \mathcal{H}_{\pi'}^{(2)}$, where $\mathcal{H}_\pi^{(2)}$ is the kernel of R and $\mathcal{H}_{\pi'}^{(1)}$ the norm closure of its range. This means that, when restricted to $\mathcal{H}_\pi^{(1)}$, $R : \mathcal{H}_\pi^{(1)} \mapsto \mathcal{H}_{\pi'}^{(1)}$ is an injective intertwiner from π restricted to $\mathcal{H}_\pi^{(1)}$ to π' restricted to $\mathcal{H}_{\pi'}^{(1)}$. Its polar decomposition will be $R = U(R^*R)^{\frac{1}{2}}$, where $U : \mathcal{H}_{\pi'}^{(1)} \mapsto \mathcal{H}_\pi^{(1)}$ is a unitary map which also intertwines the restrictions of the two representations, because R^*R commutes with π . In other words, an intertwiner establishes unitary equivalence between subrepresentations.

This allows to distinguish some relations between representations. We say that π and π' are *disjoint* if they contain no unitary equivalent subrepresentation, i.e. there exists no nonzero intertwiner between them, *unitarily equivalent* if there exists a unitary intertwiner between them, and *quasi-equivalent* if every subrepresentation of π contains a representation which is unitarily equivalent to a subrepresentation of π' .

The same concepts directly translate to states by the GNS-representations they generate, in the sense that two states ω, ω' on $\mathcal{A}$ are unitarily equivalent, resp. quasi-equivalent, resp. disjoint, if their GNS-representations $\pi_\omega, \pi_{\omega'}$ are unitarily equivalent, resp. quasi-equivalent, resp. disjoint. We will resume in Section 1.3.1 the discussion on quasi-equivalence of states for specific kinds of states and algebras.

³i.e. the subspace the subrepresentation refers to is a proper subspace.

1.1.3 von Neumann algebras

We will now talk about von Neumann algebras. Let $\mathcal{H}$ be a Hilbert space and $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ a unital $*$ -algebra. We say that $\mathcal{A}$ is a *von Neumann algebra* if it is weakly or strongly closed, in notation $\overline{\mathcal{A}}^w = \overline{\mathcal{A}}^s = \mathcal{A}$, denoting $\overline{\mathcal{A}}^w$, resp. $\overline{\mathcal{A}}^s$, as the closure of $\mathcal{A}$ in the weak, resp. strong, topology. (For any $*$ -subalgebra of $\mathcal{B}(\mathcal{H})$, it is the strong, weak and weak- $*$ closures coincide.) Every von Neumann algebra is also a C^* -algebra, as the weak closure implies the strong closure, the converse is only true in finite dimension. Then, the *commutant* of a generic $*$ -algebra $\mathcal{A}$ is $\mathcal{A}' = \{T \in \mathcal{B}(\mathcal{H}) \mid TA = AT, \forall A \in \mathcal{A}\}$, which will be a weakly closed unital $*$ -algebra, so it is a von Neumann algebra. If $\mathcal{A}, \mathcal{B}$ are von Neumann algebras with $\mathcal{A} \subset \mathcal{B}$, we say that $\mathcal{A}$ is a *von Neumann subalgebra* of $\mathcal{B}$. Generally, if $\mathcal{A}, \mathcal{B}$ are unital $*$ -algebras, we have that *i.* if $\mathcal{A} \subset \mathcal{B}$, then $\mathcal{B}' \subset \mathcal{A}'$ and $\mathcal{A}'' \subset \mathcal{B}''$, *ii.* $\mathcal{A} \subset \mathcal{A}''$ and *iii.* $\mathcal{A}' = \mathcal{A}'''$. $\mathcal{A}''$ is called the *double commutant* (or *bicommutant*) of $\mathcal{A}$. Since the property *iii.* tells us that the *triple commutant* $\mathcal{A}'''$ is equal to the commutant $\mathcal{A}'$ (and thus $\mathcal{A}'' = \mathcal{A}''''$, etc.), only the first two commutants of a given algebra $\mathcal{A}$ are relevant. From property *ii.*, we also note that, since $\mathcal{A}''$ is weakly closed, $\overline{\mathcal{A}}^w \subset \mathcal{A}''$. This leads to the following central result, cf. [Ped11, Thm. 4.6.7].

Theorem 1.1.4 (von Neumann bicommutant theorem).

Let $\mathcal{A}$ be a unital $*$ -algebra. Then, $\overline{\mathcal{A}}^w = \overline{\mathcal{A}}^s = \mathcal{A}''$.

The definition of a von Neumann algebra can then be seen in a topological sense ($\mathcal{A} = \overline{\mathcal{A}}^w$) or in an algebraic sense ($\mathcal{A} = \mathcal{A}''$). We can say that $\mathcal{A}''$ is the smallest von Neumann algebra generated by $\mathcal{A}$ by weak closure, i.e. including limit points of weakly convergent sequences. More generally, given $\mathcal{A}, \mathcal{B}$, we call $\mathcal{A} \vee \mathcal{B}$, the smallest von Neumann algebra containing $\mathcal{A}$ and $\mathcal{B}$, and $\mathcal{A} \wedge \mathcal{B}$, the largest von Neumann algebra contained by $\mathcal{A}$ and $\mathcal{B}$. This implies $\mathcal{A} \vee \mathcal{B} = (\mathcal{A} \cup \mathcal{B})''$ and $(\mathcal{A} \vee \mathcal{B})' = \mathcal{A}' \wedge \mathcal{B}' = \mathcal{A}' \cap \mathcal{B}'$. Also, $\mathcal{A} \wedge \mathcal{B} = \mathcal{A} \cap \mathcal{B}$.⁴ For every von Neumann algebra $\mathcal{A}$, we have $\{\lambda \mathbb{1}\} \subset \mathcal{A} \subset \mathcal{B}(\mathcal{H})$, where the former is the von Neumann algebra generated by the identity.

Then, for any von Neumann algebra $\mathcal{A}$, its centre $\mathcal{Z}(\mathcal{A}) = \{A \in \mathcal{A} \mid AB = BA, \forall B \in \mathcal{A}\} = \mathcal{A} \cap \mathcal{A}'$ is also a von Neumann algebra and we say that $\mathcal{A}$ is a (*von Neumann*) *factor* if its centre is trivial, $\mathcal{Z}(\mathcal{A}) = \{\lambda \mathbb{1} \mid \lambda \in \mathbb{C}\}$. Equivalently, $\mathcal{A} \vee \mathcal{A}' = \mathcal{B}(\mathcal{H})$, which is called a *factorization* of $\mathcal{B}(\mathcal{H})$. Factors have been initially classified through their projections content by Murray and von Neumann [MN36], this classification has been later refined by Connes [Con73; Con76] and led to Jones' theory of subfactors [Jon83]. We will present here the basic picture.

Let's start by introducing a notion of equivalence between projections, cf. [KR97b, Sec. 6.2]. For a generic von Neumann algebra $\mathcal{A}$, two projections $P_1, P_2 \in \mathcal{A}$ are equivalent, $P_1 \sim P_2$, if there exists a partial isometry $V \in \mathcal{A}$ such that $P_1 = V^*V$ and $P_2 = VV^*$. (V maps $\mathcal{H}_1 = P_1\mathcal{H}$ isometrically onto $\mathcal{H}_2 = P_2\mathcal{H}$.) We say that $P_1 \succ P_2$ or $P_2 \prec P_1$ if P_1 and P_2 are not equivalent but there exists a subspace $\mathcal{H}_{11} \subset \mathcal{H}_1$, $\mathcal{H}_{11} = P_{11}\mathcal{H}_1$, whose subprojection satisfies $P_{11} \sim P_2$. We say that P is *minimal* if it is nonzero but there does not exist $0 \neq P' \in \mathcal{A}$ such that $P' \prec P$.

These definitions can be used to define finite and infinite projections, cf. [KR97b, Sec. 6.3]. We say that P is *infinite* relative to $\mathcal{A}$ if $P \sim P' < P$, for some projection $P' \in \mathcal{A}$. (Note that $\prec, \sim, \succ$ refer to the ordering of projections defined above while $<, =, >$ refer the usual operator relations.) Otherwise, P is *finite* relative to $\mathcal{A}$. Then, P is *properly infinite* if it is infinite and $P'P$ is either zero or infinite for any central projection $P' \in \mathcal{Z}(\mathcal{A})$. If $\mathcal{A}$ is a factor, any infinite projection is properly infinite, as the only nonzero central projection is $\mathbb{1}$. We say that $\mathcal{A}$ is a finite, resp. properly infinite, von Neumann algebra if $\mathbb{1}$ is finite, resp. properly infinite. Any finite projection only has finite subprojections and any minimal projection is finite, the zero projection is also finite.

⁴Note that these relations give the structure of an *orthocomplemented lattice* w.r.t. the operations $\wedge, \vee$ and $'$ to the set of von Neumann algebras on a Hilbert space.

If $P_1 \sim P_2$ and P_1 is finite, P_2 will be as well [KR97b, Prop. 6.3.2]. If P_1 is a properly infinite projection, there will exist a projection P_2 such that $P_2 \leq P_1$ and $P_2 \sim P_1 - P_2 \sim P_1$ [KR97b, Lemma 6.3.3]. (This is the analogue for infinite projections of the possibility of ‘halving’ an infinite set.)

Now, if $\mathcal{A}$ is a factor, $P_1 \prec P_2$, $P_1 \sim P_2$ or $P_1 \succ P_2$ are the only three possible choice in ordering projections [KR97b, Prop. 6.2.4 and Prop. 6.2.6]. This allows to define a uniquely determined *relative dimension* on the set of projections in $\mathcal{A}$ up to normalization, cf. [Haa12, Sec. III.2.1]. For two projections $P_1, P_2 \in \mathcal{A}$, we may define it as $\dim P_i \in [0, \infty]$ satisfying (i) $\dim P_1 \leq \dim P_2$ if $P_1 \preceq P_2$, (ii) if $P_1 P_2 = 0$, then $\dim(P_1 + P_2) = \dim P_1 + \dim P_2$, (iii) $\dim 0 = 0$. This gives three alternatives.

- **Type I factors:** there exist minimal projections in $\mathcal{A}$, which may be chosen of dimension 1. Then, any $P \neq 0$ will have $\dim P \in \{1, 2, \dots, n\}$, and $\mathcal{A}$ is of type I_n if n is finite or of type I_∞ otherwise. Type I factors are algebraically isomorphic to $\mathcal{B}(\mathcal{H})$ for some $\mathcal{H}$.
- **Type II factors:** $\dim P$ will range through a continuum of values which either has an upper bound, so by normalization $\dim P \in [0, 1]$ and $\mathcal{A}$ is of type II_1 , or it does not, so $\dim P \in [0, \infty]$ and $\mathcal{A}$ is of type II_∞ .
- **Type III factors:** $\dim P \in \{0, \infty\}$, no other values are possible. In this case, all nonzero projections will have infinite dimension, so, if $\mathcal{H}$ is separable, they will all be equivalent.

In addition, von Neumann algebras can also be characterized as the C^* -algebras which are also dual spaces of some Banach space, called the *predual* of the algebra. The σ -weak (or ultraweak) topology on $\mathcal{B}(\mathcal{H})$ is the weak-* topology it inherits as the dual of the Banach algebra of trace-class operators. Then, for any von Neumann algebra $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ there exists a unique Banach space $\mathcal{A}_*$, the *predual* of $\mathcal{A}$, such that $\mathcal{A}$ is isometrically isomorphic to the dual space $(\mathcal{A}_*)^*$. The weak-* topology on $\mathcal{A} \cong (\mathcal{A}_*)^*$ is the σ -weak topology [Ped11, Thm. 4.6.17]. Equivalently, we can say that the predual of $\mathcal{A}$ is the space of all σ -weakly continuous functionals on $\mathcal{A}$. The σ -weak topology allows to characterize a crucial class of positive functionals on a von Neumann algebra. A positive functional φ on $\mathcal{A}$ is said to be *normal* if $\varphi(\sup_\alpha A_\alpha) = \sup_\alpha \varphi(A_\alpha)$ for all increasing nets $\{A_\alpha\}$ of positive operators $0 \leq A_\alpha \in \mathcal{A}$ with an upper bound. In particular, normal states (positive and normalized functionals) are characterized as follows, cf. [BR87, Thm. 2.4.21].

Theorem 1.1.5. *Let φ be a state on a von Neumann algebra $\mathcal{A}$ acting on a Hilbert space $\mathcal{H}$. The following are equivalent:*

- φ is normal;
- φ is σ -weakly continuous;
- there exists a density matrix ρ on $\mathcal{H}$ ($\rho \geq 0$, $\text{tr } \rho = 1$) such that $\varphi(A) = \text{tr}(\rho A)$ for any $A \in \mathcal{A}$.

This allows to link the more standard definition of a normal state as a σ -weakly continuous state with the one presented in Section 1.1.2 of a state normal w.r.t. some representation, in the sense that in both cases the state can be represented by a density matrix.

1.1.4 Isomorphisms of algebras

If $\mathcal{A}_1, \mathcal{A}_2$ are two $*$ -algebras of bounded operators acting on two Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$, we call an *isomorphism* between $\mathcal{A}_1$ and $\mathcal{A}_2$ a bijective map between the two algebras which conserves

the relevant structure. This yields several possibilities according to what structure is considered. E.g., we speak of *algebraic isomorphism* if only the algebraic structure is preserved, *complete isomorphism* if both the algebraic and topological structures are preserved, and *spatial isomorphism* (or unitary equivalence) if there exists some unitary $V : \mathcal{H}_1 \mapsto \mathcal{H}_2$ such that $\mathcal{A}_2 = V\mathcal{A}_1V^{-1}$. In the case of C^* -algebras (and thus von Neumann algebras), the first two notions are equivalent (elements of two algebraically isomorphic C^* -algebras will have the same norm). Two algebraically isomorphic von Neumann algebras are called quasi-equivalent, in correspondence to the quasi-equivalence of representations discussed in Section 1.1.2 by considering the von Neumann algebra $\pi(\mathcal{A})''$ given by a representation π of a C^* -algebra $\mathcal{A}$. In analogy, we still have that the notion of spatial isomorphism/unitary equivalence generally is a stronger requirement than quasi-equivalence, cf. [Haa12, Sec. III.2.1 and III.2.2].

Consider now a generic $*$ -algebra $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ for some Hilbert space $\mathcal{H}$. We say that a vector $\xi \in \mathcal{H}$ is *cyclic* for $\mathcal{A}$ if $\overline{\mathcal{A}\xi} = \mathcal{H}$ and *separating* for $\mathcal{A}$ if $a\xi = 0$ implies $a = 0$, $a \in \mathcal{A}$. We will then say that ξ is *standard* for $\mathcal{A}$ if it is both cyclic and separating for $\mathcal{A}$. Note that the term ‘standard’ will be used in place of ‘cyclic and separating’ throughout this thesis. (We will not specify the algebra for which the state is cyclic/separating/standard whenever it will be clear from context.) Recalling the commutant $\mathcal{A}'$ of $\mathcal{A}$, we have that a vector $\xi \in \mathcal{H}$ is cyclic for $\mathcal{A}$ iff it is separating for $\mathcal{A}'$. If $\mathcal{A}$ is a von Neumann algebra, then $\mathcal{A} = \mathcal{A}''$ and we will also have that ξ will be cyclic for $\mathcal{A}'$ iff it is separating for $\mathcal{A}$, so we have that ξ is standard for a von Neumann algebra $\mathcal{A}$ iff it is standard for its commutant $\mathcal{A}'$.

In the case when we have two different von Neumann algebras which both admit a standard vector, any $*$ -isomorphism between the two algebras can be implemented by a unitary transformation, as for the following theorem [KR97b, Thm. 7.2.9]. Note that $*$ -isomorphisms between von Neumann algebras are homeomorphisms in the weak, strong and weak- $*$ operator topologies on bounded sets [KR97b, Cor. 7.1.16], so they do not exclusively involve the norm topology.

Theorem 1.1.6 (Unitary implementation). *Let $\Phi : \mathcal{A}_1 \mapsto \mathcal{A}_2$ be a $*$ -isomorphism of a von Neumann algebra $\mathcal{A}_1$, acting on a Hilbert space $\mathcal{H}_1$, onto a von Neumann algebra $\mathcal{A}_2$, acting on a Hilbert space $\mathcal{H}_2$, and let both algebras admit a standard vector in the respective Hilbert space. Then, there will exist a unitary transformation $U : \mathcal{H}_1 \mapsto \mathcal{H}_2$ such that $\Phi(A) = UAU^{-1}$ for any $A \in \mathcal{A}_1$.*

This theorem then ensures that, in presence of standard vectors for both algebras, a $*$ -isomorphism of algebras reduces to unitary equivalence, the von Neumann algebraic structure completely determines the spatial action on the Hilbert spaces.

1.2 Tomita-Takesaki modular theory

We will now review some basic concepts about modular theory and relative modular theory, starting directly with the latter case, which is more general.

Consider two unit vectors $\xi, \xi' \in \mathcal{H}$, both standard (cyclic and separating) for a von Neumann algebra $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$, and $a \in \mathcal{A}$. Then, the *relative Tomita operator* is the operator $S_{\xi', \xi} a\xi = a^*\xi'$, which is densely defined and satisfies $S_{\xi', \xi}^{-1} = S_{\xi, \xi'}$. We can analogously define the operator $S'_{\xi', \xi}$ w.r.t. $\mathcal{A}'$, for which ξ and ξ' are also standard. Then, we can see that, for all $a \in \mathcal{A}$ and $a' \in \mathcal{A}'$

$$\langle a\xi, S_{\xi', \xi}^* a'\xi' \rangle = \langle a'\xi, S_{\xi', \xi} a\xi \rangle = \langle a'\xi, a^*\xi' \rangle = \langle a\xi, a'^*\xi' \rangle = \langle a\xi, S'_{\xi', \xi} a'\xi' \rangle,$$

i.e., $S_{\xi', \xi}^* \supset S'_{\xi', \xi}$. In particular, $S_{\xi', \xi}^*$ is densely defined and hence $S_{\xi', \xi}$ is closable. We will denote the closure by the same symbol and $S_{\xi', \xi}^{-1} = S_{\xi, \xi'}$ will still hold. Then, we may consider its unique

polar decomposition as

$$S_{\xi', \xi} = J_{\xi', \xi} \Delta_{\xi', \xi}^{1/2},$$

where $\Delta_{\xi', \xi} > 0$, the *relative modular operator*, is a strictly positive operator, and $J_{\xi', \xi}$, the *relative modular conjugation*, is anti-unitary, $J_{\xi', \xi}^* = J_{\xi', \xi}^{-1}$. The *relative modular Hamiltonian* is the self-adjoint operator

$$K_{\xi', \xi} := -\log(\Delta_{\xi', \xi}).$$

We also can see that $S_{\xi, \xi'} = S_{\xi', \xi}^{-1} = J_{\xi', \xi}^* (J_{\xi', \xi} \Delta_{\xi', \xi}^{-1/2} J_{\xi', \xi}^*)$ so by the uniqueness of the polar decomposition we have

$$\begin{aligned} J_{\xi, \xi'} &= J_{\xi', \xi}^* \\ \Delta_{\xi, \xi'}^{1/2} &= J_{\xi', \xi} \Delta_{\xi', \xi}^{-1/2} J_{\xi', \xi}^* \\ K_{\xi, \xi'} &= -J_{\xi', \xi} K_{\xi', \xi} J_{\xi', \xi}^*. \end{aligned}$$

For the adjoint we then have $S_{\xi', \xi}^* = J_{\xi, \xi'} \Delta_{\xi, \xi'}^{-1/2}$. We can define the (*Araki*) *relative entropy*, cf. [Ara75; Ara77], as⁵

$$H(\xi, \xi') = \langle \xi, K_{\xi', \xi} \xi \rangle$$

We interpret this as the amount of information that we expect to gain when we learn that our system is in the state ξ , where we previously thought it was in the state ξ' [BF14]. Note that $H(\xi, \xi') \neq H(\xi', \xi)$ in general.

The following standard example expresses the relative entropy in terms of density matrices and makes this asymmetry explicit.

Example 1.2.1. Let $\mathcal{H}_1$ be a separable complex Hilbert space and ρ, ρ' two density matrices, i.e. positive operators with trace 1. We let $\mathcal{H}$ be the Hilbert space of Hilbert-Schmidt operators on $\mathcal{H}_1$, endowed with the Hilbert-Schmidt inner product $\langle a, b \rangle := \text{tr}_{\mathcal{H}_1} a^* b$. We will write $\xi := \sqrt{\rho}$ and $\xi' := \sqrt{\rho'}$ as vectors in $\mathcal{H}$. We may identify $\mathcal{H} \simeq \mathcal{H}_1 \otimes \mathcal{H}_1^*$ in a natural way, where $\mathcal{H}_1^*$ is the dual space of $\mathcal{H}_1$. E.g., if $\{v_n\}$ is an orthonormal eigenbasis for ρ with eigenvalues $p_n \geq 0$, then $\xi = \sum_n \sqrt{p_n} v_n \otimes v_n^*$.

We let $\mathcal{R} = \mathcal{B}(\mathcal{H}_1)$ the algebra of all bounded operators on $\mathcal{H}_1$. This algebra acts on the first factor of $\mathcal{H}_1 \otimes \mathcal{H}_1^*$. The commutant $\mathcal{R}' = \mathcal{B}(\mathcal{H}_1^*)$ acts on the second factor. If ρ and ρ' are strictly positive, the vectors ξ and ξ' are cyclic and separating for $\mathcal{R}$ and we can define the relative Tomita operator. We will verify that the relative modular operator is given by

$$\Delta_{\xi', \xi} = \rho' \otimes \rho^{-1}$$

acting on $\mathcal{H}_1 \otimes \mathcal{H}_1^*$ by $\Delta_{\xi', \xi} v \otimes w^* = (\rho' v) \otimes (\rho^{-1} w)^* = \rho'(v \otimes w^*) \rho^{-1}$. Indeed, for all $a, b \in \mathcal{R}$ we have

$$\begin{aligned} \langle a\xi, \Delta_{\xi', \xi} b\xi \rangle &= \langle S_{\xi', \xi} b\xi, S_{\xi', \xi} a\xi \rangle \\ &= \langle b^* \xi', a^* \xi' \rangle \\ &= \text{tr}_{\mathcal{H}_1} (\rho' b a^*) \\ &= \text{tr}_{\mathcal{H}_1} \left(\rho (\sqrt{\rho'} a \rho^{-\frac{1}{2}})^* (\sqrt{\rho'} b \rho^{-\frac{1}{2}}) \right) \\ &= \left\langle \sqrt{\rho'} \otimes \rho^{-\frac{1}{2}} a\xi, \sqrt{\rho'} \otimes \rho^{-\frac{1}{2}} b\xi \right\rangle \\ &= \langle a\xi, \rho' \otimes \rho^{-1} b\xi \rangle, \end{aligned}$$

⁵As noted in [CMS26, Sec. 2.1], the corresponding Equation (91) in [HS18] suffers from a sign error and swapped subscripts.

where the first and last equalities hold in the sense of quadratic forms. From this we conclude that

$$K_{\xi', \xi} = -\log(\rho') \otimes \mathbb{1} + \mathbb{1} \otimes \log(\rho)$$

acting on $\mathcal{H}_1 \otimes \mathcal{H}_1^*$ and hence

$$\begin{aligned} H(\xi, \xi') &= \langle \xi, K_{\xi', \xi} \xi \rangle \\ &= \text{tr}_{\mathcal{H}_1} \left(\sqrt{\rho} [-\log(\rho') \sqrt{\rho} + \sqrt{\rho} \log(\rho)] \right) \\ &= \text{tr}_{\mathcal{H}_1} \left(\rho [\log(\rho) - \log(\rho')] \right). \end{aligned}$$

From this last expression, it is easy to see the asymmetry of the relative entropy. E.g., given an orthonormal eigenbasis $\{v_n\}$ for $\mathcal{H}_1$, consider the family of orthogonal projections P_n onto the span of each v_n and let $\rho = P_1$, $\rho' = \sum_n p_n P_n$, with $p_n > 0$ and $\sum_n p_n = 1$. Then, as $\text{tr}_{\mathcal{H}_1} \rho \log \rho = 0$, we have that $H(\xi, \xi') = -\text{tr}_{\mathcal{H}_1} \rho \log \rho' = -\log p_1 > 0$. However, $H(\xi', \xi) = +\infty$, as it involves taking the trace of $\log P_1$ and not exclusively of $P_1 \log P_1$. This is consistent with the interpretation by [BF14]. When computing $H(\xi, \xi')$, we are supposing to first have our system in the state described by ρ' and then discovering it is described by ρ , which reduces the sum over the eigenbasis to the first element only, with coefficient p_1 (in quantum mechanical terms, we go from a superposition of eigenstates to one of the possible ones). However, in the case of $H(\xi', \xi)$, we go from being certain to be in one of the eigenspaces to not knowing any more. From the point of view of relative entropy, this is an infinite increase of information.

Then, when $\xi' = \xi$ we drop the adjective ‘relative’ and we use the single subscript ξ , so the Tomita operator S_ξ , the modular operator Δ_ξ , the modular conjugation J_ξ and the modular Hamiltonian K_ξ satisfy the relations $S_\xi = J_\xi \Delta_\xi^{1/2}$, $K_\xi = -\log(\Delta_\xi)$, $J_\xi = J_\xi^* = J_\xi^{-1}$, $\Delta_\xi^{1/2} = J_\xi \Delta_\xi^{-1/2} J_\xi$, $S_\xi^* = J_\xi \Delta_\xi^{-1/2}$, and $K_\xi = -J_\xi K_\xi J_\xi$. These will satisfy the following central result, cf. [Ped79, Thm. 8.13.14]

Theorem 1.2.2 (Tomita-Takesaki). *For any $t \in \mathbb{R}$, $\Delta_\xi^{it} \mathcal{A} \Delta_\xi^{-it} = \mathcal{A}$ and $J_\xi \mathcal{A} J_\xi = \mathcal{A}'$.*

The map $t \mapsto \Delta_\xi^{it} a \Delta_\xi^{-it} = e^{-itK_\xi} a e^{itK_\xi}$, with $t \in \mathbb{R}$ and $a \in \mathcal{A}$, is called the *modular flow* and gives a one-parameter group of automorphisms of $\mathcal{A}$ generated by the modular Hamiltonian K_ξ . This serves as a justification of the name ‘modular Hamiltonian’, as it provides a sort of dynamical evolution on the von Neumann algebra $\mathcal{A}$, which solely depends on the standard vector ξ .

1.2.1 Modular theory for standard subspaces

Modular theory can be however formulated in a more general setting, the one of standard subspaces of a complex Hilbert space. Note that the same cannot be said for its relative counterpart. Following the presentation of [Lon08, Sec. 2], we may consider a complex Hilbert space $\mathcal{H}$ and a real-linear subspace $H \subset \mathcal{H}$. In analogy with the von Neumann algebra notation, we define the *symplectic complement* H' of H as

$$H' := \{ \xi \in \mathcal{H} \mid \text{Im} \langle \xi, \xi' \rangle = 0, \forall \xi' \in H \},$$

which will satisfy $H' = (iH)^\perp$, where $\perp$ indicates the real orthogonal complement w.r.t. $\text{Re} \langle \cdot, \cdot \rangle$. We get that $H \subset H''$ and $\overline{H} = H''$. Then, we say that a closed, real-linear H is *cyclic* if $H + iH \subset \mathcal{H}$ is dense, and *separating* if $H \cap iH = \{0\}$. As $(H + iH)' = H' \cap iH'$, H is cyclic iff H' is separating. Then, we can say that H is *standard* iff it is cyclic and separating and we get that H is standard iff H' is standard.

Given a standard subspace we can define the *Tomita operator* $S_H : H + iH \mapsto H + iH$ as the anti-linear operator $S(\xi + i\xi') = \xi - i\xi'$, for $\xi, \xi' \in H$, which is well-defined on a dense domain and closed. Indeed, we have that for any closed, densely defined, anti-linear involution S on $\mathcal{H}$, $H := \ker(\mathbb{1} - S)$ is a standard subspace of $\mathcal{H}$ and, conversely the map $H \mapsto S_H$ is a bijection between the set of standard subspaces of $\mathcal{H}$ and the set of closed, densely defined, anti-linear involutions on $\mathcal{H}$, which has inverse $S \mapsto \ker(\mathbb{1} - S)$ and will satisfy $S_{H_1} \subset S_{H_2}$ iff $H_1 \subset H_2$ and $S_H^* = S_{H'}$ [Lon08, Lemma 2.1.1 and Prop. 2.1.2].

The polar decomposition of the Tomita operator will be $S_H = J_H \Delta_H^{1/2}$, where $\Delta_H \geq 0$ is the *modular operator* and J_H , the *modular conjugation*, is anti-linear. From $S_H^2 = \mathbb{1}$ we see that $\Delta_H^{1/2}$ is invertible with $J_H \Delta_H^{1/2} J_H = \Delta_H^{-1/2}$. In particular, $\Delta_H > 0$ is strictly positive. Also, J_H is invertible with $J_H^{-1} = J_H^*$ and hence $S_H = \Delta_H^{-1/2} J_H^*$ and $S_H^* = J_H \Delta_H^{-1/2}$. From $\Delta_H = S_H^* S_H = J_H \Delta_H^{-1} J_H^*$ and spectral calculus one then finds $J_H \Delta_H^{1/2} J_H^* = \Delta_H^{-1/2} = J_H \Delta_H^{1/2} J_H$, which implies $J_H^* = J_H$. These operators will satisfy a Hilbert space counterpart of the Tomita-Takesaki Theorem 1.2.2, which applied to von Neumann algebras, cf. [Lon08, Thm. 2.1.4].

Theorem 1.2.3 (Longo). *For any $t \in \mathbb{R}$, $\Delta_H^{it} H = H$ and $J_H H = H'$.*

The *modular group* $t \mapsto \Delta_H^{it}$ is defined in terms of the modular operator and generated by the *modular Hamiltonian*

$$K_H := -\log(\Delta_H). \quad (1.2.1)$$

We call a standard subspace $H \subset \mathcal{H}$ *factorial* iff 1 is not in the point spectrum of Δ_H , equivalently $H \cap H' = \{0\}$.

It is then interesting to remark the relation of this formulation of modular theory to the one explained in the previous section. For any pair $(\mathcal{A}, \xi)$, where $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ is a von Neumann algebra and $\xi \in \mathcal{H}$ is a standard vector for $\mathcal{A}$, the subset $H_{\mathcal{A}, \xi}$ defined as the norm closure of $\{a\xi \mid a = a^* \in \mathcal{A}\}$ will be a standard subspace, as $H_{\mathcal{A}, \xi} + iH_{\mathcal{A}, \xi}$ is dense in $\mathcal{H}$ from the cyclicity of ξ and $H_{\mathcal{A}, \xi} \cap iH_{\mathcal{A}, \xi} = \{0\}$ from its separability. However, the map $(\mathcal{A}, \xi) \mapsto H_{\mathcal{A}, \xi}$ forgets information, as it is not possible to reconstruct $(\mathcal{A}, \xi)$ from $H_{\mathcal{A}, \xi}$. Approaches to construct von Neumann algebras from modular subspaces indeed require adding information, see e.g. [CL23].

1.3 Symplectic spaces

We will here give some generalities about (pre-)symplectic spaces and the Hilbert space constructions they give rise to. By a *pre-symplectic space* (D, σ) we speak of a real vector space D with an anti-symmetric bilinear form σ defined on it. We speak of a *symplectic space* when σ is non-degenerate, i.e. when $\sigma(f, g) = 0$ for all $g \in D$ implies $f = 0$. To any symplectic space (D, σ) , we can (uniquely up to C^* -algebraic equivalence) associate its *Weyl algebra* $\mathcal{W}[D, \sigma]$, which is the C^* -algebra obtained as the C^* -algebraic completion⁶ of the $*$ -algebra generated by the unitaries $W(f)$, $f \in D$, the *Weyl operators*, satisfying the Weyl representations of the canonical commutation relations (CCR) algebra, i.e.

$$W(f)W(g) = e^{-\frac{i}{2}\sigma(f, g)}W(f + g) \quad (1.3.1)$$

for all $f, g \in D$. We refer to Appendix A for general properties of CCR systems.

We may then consider a state (a positive, normalized linear functional) on the Weyl algebra $\mathcal{W}[D, \sigma]$ of our symplectic space and let $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ the GNS-representation of ω . If we assume that for

⁶i.e. the completion in the C^* -norm.

any $f \in D$ the unitary one-parameter group $t \mapsto \pi_\omega(W(tf))$, $t \in \mathbb{R}$, is strongly continuous and Ω_ω is in the domain of its generator $\Phi_\omega(f)$, we may then define the *two-point function* ω_2 of ω as

$$\omega_2(f, g) := \langle \Phi_\omega(f)\Omega_\omega, \Phi_\omega(g)\Omega_\omega \rangle, \quad (1.3.2)$$

for all $f, g \in D$, w.r.t. the (complex) inner product on $\mathcal{H}_\omega$, so ω_2 is a complex-valued real bilinear form, which admits a natural sesquilinear extension to the standard complexification of D .

A special class of states we will focus on is the one of *Gaussian* or *quasifree* states, which are associated to some real inner product μ_ω on D , $\mu_\omega : D \times D \mapsto \mathbb{R}$, in the following way.

Definition 1.3.1. *Let ω be a state on the Weyl algebra $\mathcal{W}[D, \sigma]$ of some pre-symplectic space (D, σ) such that there exists a two-point function ω_2 , so there exists a real scalar product μ_ω on D such that*

$$i. \quad \omega_2(f, g) = \frac{1}{2} (\mu_\omega(f, g) + i \sigma(f, g)),$$

$$ii. \quad \sigma(f, g)^2 \leq \mu_\omega(f, f) \mu_\omega(g, g),$$

for all $f, g \in D$. Then, ω is Gaussian or quasifree if

$$iii. \quad \omega(W(f)) = \exp\left(-\frac{1}{4}\mu_\omega(f, f)\right),$$

for any $f \in D$.

Gaussian states can be characterised entirely in terms of their one-particle structure [Kay78]. A *one-particle structure* for a pre-symplectic space (D, σ) is a real-linear map $\kappa : D \rightarrow \mathcal{H}$ to a complex Hilbert space $\mathcal{H}$ with inner product $(\cdot, \cdot)$ such that (i) $\kappa(D) + i\kappa(D)$ is dense in $\mathcal{H}$ and (ii) $\text{Im}(\kappa(f), \kappa(g)) = \sigma(f, g)$ for all $f, g \in D$. Given a one-particle structure we can define an inner product μ on D by setting

$$\mu(f, g) := \text{Re}(\kappa(f), \kappa(g)). \quad (1.3.3)$$

We note that $\mu(\cdot, \cdot)$ and $(\kappa(\cdot), \kappa(\cdot))$ determine the same norm $\|\cdot\|$ on D and that

$$|\sigma(f, g)| \leq \|f\| \cdot \|g\| \quad (1.3.4)$$

for all $f, g \in D$, because of $|\sigma(f, g)| \leq |(\kappa(f), \kappa(g))|$ and the Cauchy-Schwarz inequality. Conversely, given any inner product μ on D satisfying (1.3.4) there exists a one-particle structure κ such that (1.3.3) holds. This one-particle structure is unique up to unitary equivalence.

We can obtain a construction of κ with the following argument, introducing some further useful notations. Starting from (D, σ) , we can consider a real inner product μ on D and take the completion $\mathcal{K}_{\mathbb{R}, \mu} := \overline{D}_\mu$ of D with respect to μ , which will be a real Hilbert space. Under these assumptions [Ver94, Sec. 3], we can consider the *polarization operator* associated to the symplectic form σ in the real Hilbert space $\mathcal{K}_{\mathbb{R}, \mu}$, i.e. a bounded anti-self-adjoint linear operator $R_\mu : \mathcal{K}_{\mathbb{R}, \mu} \mapsto \mathcal{K}_{\mathbb{R}, \mu}$, $(R_\mu)^* = -R_\mu$ and $\|R_\mu\| \leq 1$, such that

$$\sigma(f, g) = \langle f, R_\mu g \rangle_{\mathcal{K}_{\mathbb{R}, \mu}}, \quad (1.3.5)$$

for all $f, g \in D$, which will be unique. Note that in (1.3.5) and later in this section, we will generally consider elements of D as elements of the spaces $\mathcal{K}_{\mathbb{R}, \mu}$ and other spaces containing D with abuse of notation, as these should be interpreted as their injections on these larger spaces.

Then, for any real Hilbert space $\mathcal{K}_{\mathbb{R}}$ there is a standard complexification $\mathcal{K} = \mathcal{K}_{\mathbb{R}} \oplus i\mathcal{K}_{\mathbb{R}}$ with multiplication by i given by the matrix $\begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$, where the real inner product is extended to a Hermitian inner product. $\mathcal{K}$ also carries a canonical complex conjugation Γ such that $\Gamma(f + ig) = f - ig$ when $f, g \in \mathcal{K}_{\mathbb{R}}$. Any real-linear operator A on $\mathcal{K}_{\mathbb{R}}$ can be extended to a complex-linear operator on $\mathcal{K}$ that we will denote by the same symbol. We then have $\Gamma A \Gamma = A$ and we note that the extension does not increase the operator norm. In particular, if R is a polarization operator on $\mathcal{K}_{\mathbb{R}}$, then its extension is also anti-selfadjoint with $\|R\| \leq 1$ on $\mathcal{K}$ and we will write $\Sigma := iR$, which is a self-adjoint operator with $\|\Sigma\| \leq 1$ and $\Gamma \Sigma \Gamma = -\Sigma$. (When the real Hilbert space and the polarization operator are derived from an inner product μ on a symplectic space (D, σ) satisfying (1.3.4), we will put a subscript μ on the Hilbert spaces and the operators.)

Given a polarization operator R_{μ} on a real Hilbert space $\mathcal{K}_{\mathbb{R}, \mu}$ we let $\mathcal{N}_{\mu} := \ker(\mathbb{1} + \Sigma_{\mu})$ and $\mathcal{H}_{\mu} := \mathcal{N}_{\mu}^{\perp}$ in $\mathcal{K}_{\mu}$. Furthermore, we define the real-linear map $\kappa : D \rightarrow \mathcal{H}_{\mu}$ by

$$\kappa(f) := \sqrt{\mathbb{1} + \Sigma_{\mu}} f. \quad (1.3.6)$$

Then, κ is a one-particle structure for (D, σ) satisfying (1.3.3).

1.3.1 Quasi-equivalence of Gaussian states

We will recall here some general results about quasi-equivalence of Gaussian states, following [AY82; Ver94; Lon22]. Following from the previous notations, consider two Gaussian states φ_1, φ_2 on the Weyl algebra $\mathcal{W}[D, \sigma]$ of a pre-symplectic space (D, σ) , defined by two inner products μ_1, μ_2 on D .⁷ Then, Araki and Yamagami [AY82] give necessary and sufficient conditions for the two Gaussian states to be quasi-equivalent. Indeed, we have the following result.

Theorem 1.3.2 (Araki-Yamagami). *Two Gaussian states φ_1, φ_2 on $\mathcal{W}[D, \sigma]$ with inner products μ_1, μ_2 have quasi-equivalent GNS-representations π_1, π_2 iff the following two conditions hold:*

- i. *the inner products μ_1, μ_2 are equivalent, i.e. there exists a bounded positive operator B with bounded inverse such that $\mu_1(f, f) = \mu_2(f, Bf)$, $f \in D$;*
- ii. *$\sqrt{B + iR_2} - \sqrt{\mathbb{1} + iR_2}$ is Hilbert-Schmidt, where R_2 is the polarization operator on the complex Hilbert space $\mathcal{K}_{\mu_2} \cong \mathcal{K}_{\mu_1}$.*

When these two conditions are satisfied, [AY82] extend the quasi-free states to pure states on the Weyl algebra of a doubled symplectic space and show that these are unitarily equivalent.

In particular, if we consider the states φ_i to be primary, $i = 1, 2$, i.e. $\pi_i(\mathcal{W}[D, \sigma])''$ are factors, we get the following corollary, due to Verch [Ver94, Cor. 3.5].

Corollary 1.3.3. *The GNS-representations π_1, π_2 of two primary quasifree states φ_1, φ_2 satisfying condition i. of Theorem 1.3.2 are quasi-equivalent if $\mathbb{1} - R_1 R_2^{-1}$ is a trace-class operator on the complex Hilbert space $\mathcal{K}_{\mu_1} \cong \mathcal{K}_{\mu_2}$.*

In addition, the Araki-Yamagami conditions of Theorem 1.3.2 have been expressed in a more explicit fashion by Longo in [Lon22], under more restrictive assumptions, cf. [Lon22, Cor. 4.4].

Corollary 1.3.4 (Longo). *Let H be a real Hilbert space w.r.t. two equivalent norms μ_k , $k = 1, 2$, and let R_k be corresponding polarization operators such that $\mu_1(f, R_1 g) = \mu_2(f, R_2 g)$ for all $f, g \in H$. Assume that $\mathbb{1} + R_1^2 > 0$, $\mathbb{1} + R_2^2 > 0$ and that R_1 and R_2 are invertible with $R_1^{-1} - R_2^{-1} \in \mathcal{L}^2(H)$,*

⁷We will avoid using the letter ω to denote states here, to avoid confusion with the two-point function ω_2 .

the set of Hilbert-Schmidt operators on H . Then, the Gaussian states determined by μ_1 and μ_2 are quasi-equivalent iff both

$$R_1^{-1}\sqrt{\mathbb{1} + R_1^2} - R_2^{-1}\sqrt{\mathbb{1} + R_2^2} \in \mathcal{L}^2(H) \quad (1.3.7)$$

and

$$\sqrt{\mathbb{1} + R_1^2} - \sqrt{\mathbb{1} + R_2^2} \in \mathcal{L}^2(H). \quad (1.3.8)$$

Remark. The invertibility of the R_k means that H is a factorial standard subspace in each of the one-particle Hilbert spaces $\mathcal{H}_k$ as constructed in Section 1.3. The square root of $\mathbb{1} + R_1^2$ is the positive square root w.r.t. the inner product of μ_1 and the square root of $\mathbb{1} + R_2^2$ is the positive square root w.r.t. the inner product of μ_2 . If $\mu_2(.,.) = \mu_1(., B^2.)$ for a bounded positive operator B with bounded inverse, then $R_2 = B^{-2}R_1$ and $\sqrt{\mathbb{1} + R_2^2} = B^{-1}\sqrt{\mathbb{1} + (B^{-1}R_1B^{-1})^2}B$ in terms of the positive square root w.r.t μ_1 , cf. [AY82].

Also notice that condition (1.3.8) appears to be redundant. Indeed, as R_1 and R_2 are bounded and $R_1^{-1} - R_2^{-1} \in \mathcal{L}^2(H)$, condition (1.3.7) already implies (1.3.8). Vice versa, if we assume that, say, R_2^{-1} is bounded, then (1.3.8) implies (1.3.7), because

$$R_1^{-1}\sqrt{\mathbb{1} + R_1^2} - R_2^{-1}\sqrt{\mathbb{1} + R_2^2} = (R_1^{-1} - R_2^{-1})\sqrt{\mathbb{1} + R_1^2} + R_2^{-1}\left(\sqrt{\mathbb{1} + R_1^2} - \sqrt{\mathbb{1} + R_2^2}\right) \quad (1.3.9)$$

will be Hilbert-Schmidt.

We will resume this discussion about quasi-equivalence of Gaussian states in Section 3.1, where we will apply Corollary 1.3.4 to a more special class of Gaussian states.

1.3.2 Modular theory and polarization operators

We can relate modular theory as presented in Section 1.2.1 to polarization operators as follows. Given a standard subspace $H \subset \mathcal{H}$ we can view $\mathcal{K}_{\mathbb{R}} = H$ as a real Hilbert space with inner product $\langle, \rangle = \text{Re}(\langle, \rangle)$. Furthermore, we can define a polarization operator R on H by $\langle v, Rw \rangle = \text{Im}(v, w)$ for all $v, w \in \mathcal{K}_{\mathbb{R}}$. We let $\mathcal{K}$ denote the standard complexification of $\mathcal{K}_{\mathbb{R}}$ as before and we note that for all $v, w \in H$ we have $\|v + iw\|_{\mathcal{H}}^2 = \|\sqrt{\mathbb{1} + \Sigma}(v + iw)\|_{\mathcal{K}}^2$ by a short computation. Because H is a standard subspace, both sides must be non-zero, unless $v = w = 0$. This means that $\mathbb{1} + \Sigma$ is strictly positive and consequently $\mathcal{N} = \{0\}$, so we can identify $\mathcal{H} \simeq \mathcal{K}$ using the unitary map

$$U : \mathcal{H} \rightarrow \mathcal{K} : v + iw \mapsto \sqrt{\mathbb{1} + \Sigma}(v + iw) \quad (1.3.10)$$

for all $v, w \in H$. Note that -1 is not in the point spectrum of Σ and neither is $+1$, because $\Sigma = -\Gamma\Sigma\Gamma$. Equivalently we have

$$\mathbb{1} + R^2 = \mathbb{1} - R^*R > 0. \quad (1.3.11)$$

We can express the modular operator in terms of Σ using the following computation for all $v, w \in H$:

$$\begin{aligned}
\|\Delta_H^{\frac{1}{2}}(v + iw)\|_{\mathcal{H}} &= \|S_H(v + iw)\|_{\mathcal{H}} \\
&= \|v - iw\|_{\mathcal{H}} \\
&= \|\sqrt{\mathbb{1} + \Sigma}(v - iw)\|_{\mathcal{K}} \\
&= \|\Gamma\sqrt{\mathbb{1} + \Sigma}\Gamma(v + iw)\|_{\mathcal{K}} \\
&= \|\sqrt{\mathbb{1} - \Sigma}(v + iw)\|_{\mathcal{K}} \\
&= \left\| \sqrt{\frac{\mathbb{1} - \Sigma}{\mathbb{1} + \Sigma}} U(v + iw) \right\|_{\mathcal{K}} \\
&= \left\| U^* \sqrt{\frac{\mathbb{1} - \Sigma}{\mathbb{1} + \Sigma}} U(v + iw) \right\|_{\mathcal{H}}
\end{aligned}$$

which implies $\Delta_H^{\frac{1}{2}} = U^* \sqrt{\frac{\mathbb{1} - \Sigma}{\mathbb{1} + \Sigma}} U$ by the uniqueness of the polar decomposition of $\Delta_H^{\frac{1}{2}}$. Hence we find, cf. also [Lon22, Prop. 2.4] or [CM24, Prop. 2.1],

$$\begin{aligned}
U\Delta_H U^* &= \frac{\mathbb{1} - \Sigma}{\mathbb{1} + \Sigma} = \frac{\mathbb{1} - iR}{\mathbb{1} + iR}, \\
U^* \Sigma U &= -i U^* R U = \frac{\mathbb{1} - \Delta_H}{\mathbb{1} + \Delta_H}.
\end{aligned} \tag{1.3.12}$$

When $\kappa : D \rightarrow \mathcal{H}$ is a one-particle structure for a pre-symplectic space (D, σ) , then the closed range $H := \overline{\kappa(D)}$ has a dense complexification $H + iH$ in $\mathcal{H}$. H is a standard subspace iff R_μ satisfies (1.3.11). In this case, we will use a subscript μ also on the modular operator.

Chapter 2

Algebraic QFTs

Reality is quite Euclidean, and every day this expedition
demonstrates its tendency to present itself in figures,
which despite their intangibility insist on repeating
themselves over and over again [...]

Carol Dunlop and Julio Cortázar, *Autonauts of the Cosmoroute*

We will now discuss how the operator algebraic formalism of Chapter 1 applies to quantum physics through the formalism of algebraic QFT (AQFT). For the concepts we will discuss, we refer to [Haa12; BFV03; Dim80; Ver94], more specific references will be highlighted in the text.

2.1 Locally covariant QFTs

We shall start by defining the operator content of a general algebraic QFT. Typically, this is formulated for finite, open regions $\mathcal{O}$ of the Minkowski spacetime, which are endowed with a standard set of axioms, the *Haag-Kastler axioms*, which associates suitable algebras to them. Algebraic QFTs may however be formulated in greater generality for a smooth, globally hyperbolic Lorentzian manifolds thanks to the locally covariant QFT approach by Brunetti, Fredenhagen and Verch [BFV03], of which we will review the main aspects.

Let $M = (\mathcal{M}, g)$ be a spacetime, where $\mathcal{M}$ is a $(d+1)$ -dimensional manifold and g is a pseudo-Riemannian metric with signature $(-, +, \dots, +)$. We generally assume M to be orientable and time-orientable, i.e. there exists a smooth vector field u on $\mathcal{M}$ such that $g(u, u) < 0$. Then, given a connected interval $I \subset \mathbb{R}$, we say that a smooth curve $\gamma : I \rightarrow M$ is *causal* if $g(\gamma', \gamma') \leq 0$, where γ' is the tangent vector of γ . Then, given the global timelike vector field u , we say that γ is future-directed, resp. past-directed, if $g(u, \gamma) < 0$, resp. $g(u, \gamma) > 0$, along γ . This allows to define for any point $x \in \mathcal{M}$, its *causal future* $J^+(x)$, resp. its *causal past* $J^-(x)$, as the set of all points in $\mathcal{M}$ which can be connected to x by a future-directed, resp. past-directed, causal curve starting from x . Given a subset $\mathcal{O}$ of $\mathcal{M}$, we can then consider the subsets

$$J^\pm(\mathcal{O}) := \{J^\pm(x) \mid x \in \mathcal{O}\} \quad (2.1.1)$$

and also $J(\mathcal{O}) := J^+(\mathcal{O}) \cup J^-(\mathcal{O})$. This allows to define $\mathcal{D}^+(\mathcal{O})$, resp. $\mathcal{D}^-(\mathcal{O})$, as the set of all $x \in J^+(\mathcal{O})$, resp. $x \in J^-(\mathcal{O})$, such that every past, resp. future, inextendible curve starting at x passes through $\mathcal{O}$. Then, $\mathcal{D}(\mathcal{O}) = \mathcal{D}^+(\mathcal{O}) \cup \mathcal{D}^-(\mathcal{O})$ will be the *domain of dependence* of $\mathcal{O}$. Two subset $\mathcal{O}_1, \mathcal{O}_2$ of $\mathcal{M}$ will be *causally separated* if no causal curve exists connecting their closures, i.e.

$J^\pm(\overline{\mathcal{O}_1}) \cap \overline{\mathcal{O}_2} = \emptyset$. The *causal complement* $\mathcal{O}^\perp$ of $\mathcal{O}$ will be the largest set in $\mathcal{M}$ which is causally separated from $\mathcal{O}$.

Then, M (orientable and time-orientable) is *globally hyperbolic* if for any $x, y \in \mathcal{M}$, $J^-(y) \cap J^+(x)$ is compact whenever it is non-empty. This is equivalent to the modern standard definition of a globally hyperbolic manifold as admitting a foliation in smooth Cauchy surfaces, which in turn ensures that the Cauchy problem for linear hyperbolic wave equations, like the Klein-Gordon equation we will later discuss, is well-posed and allows unique advanced and retarded solutions to such equations.

We now want to define general properties for QFTs without committing to any specific choice of spacetime. To do so, we shall establish relations between different spacetimes, for this purpose it is useful to first recall some elementary notions of category theory. A category $\mathfrak{C}$ consists of a class of *objects*, $\text{Obj}(\mathfrak{C})$ and a class of *morphisms* $\text{Mor}(\mathfrak{C})$, which can be thought as arrows between objects. Each morphism f has a domain $\text{dom}(f) \in \text{Obj}(\mathfrak{C})$ and a codomain $\text{cod}(f) \in \text{Obj}(\mathfrak{C})$. We call $\text{Hom}(a, b)$ the class of morphisms with domain a and codomain b . Also, for any object a , there exists an *identity morphism* $\text{id}_a \in \text{Hom}(a, a)$ and for any two morphisms $f \in \text{Hom}(a, b)$ and $g \in \text{Hom}(b, c)$, there will be a composition $g \circ f \in \text{Hom}(a, c)$. Given a third morphism $h \in \text{Hom}(c, d)$, we will also require that $h \circ (g \circ f) = (h \circ g) \circ f$ and $f \circ \text{id}_a = f = \text{id}_b \circ f$. Different categories can be then linked by *functors*. Let $\mathfrak{C}, \mathfrak{D}$ be categories, a functor F is a mapping that associates each $a \in \text{Obj}(\mathfrak{C})$ to $F(a) \in \text{Obj}(\mathfrak{D})$ and each $f \in \text{Mor}(\mathfrak{C})$ to $F(f) \in \text{Mor}(\mathfrak{D})$, so if $f \in \text{Hom}_{\mathfrak{C}}(a, b)$, $F(f) \in \text{Hom}_{\mathfrak{D}}(F(a), F(b))$. We also require that $F(\text{id}_a) = \text{id}_{F(a)}$, for any $a \in \text{Obj}(\mathfrak{C})$, and given $f \in \text{Hom}_{\mathfrak{C}}(a, b)$ and $g \in \text{Hom}(b, c)$, the composition will respect $F(g \circ f) = F(g) \circ F(f)$. Such functors are also called *covariant functors*, to distinguish them from contravariant functors, which we will not discuss.

Back to our discussion, we may consider two globally hyperbolic spacetimes $M_1 = (\mathcal{M}_1, g_1)$, $M_2 = (\mathcal{M}_2, g_2)$. An *isometric embedding* of M_1 into M_2 is a map $\psi : \mathcal{M}_1 \mapsto \mathcal{M}_2$ which is a diffeomorphism onto its range $\psi(\mathcal{M}_1)$ and an isometry, i.e. $\psi_* g_1 = g_2|_{\psi(\mathcal{M}_1)}$. This allows to define the following categories, $\mathfrak{Loc}$, for localisation regions, and $\mathfrak{Alg}$, for (local) algebras.

$\mathfrak{Loc}$ consists of

- $\text{Obj}(\mathfrak{Loc})$ which is composed of all $(d + 1)$ -dimensional, globally hyperbolic, oriented and time-oriented spacetimes $M = (\mathcal{M}, g)$;
- $\text{Mor}(\mathfrak{Loc})$ which is composed of isometric embeddings $\psi \in \text{Hom}_{\mathfrak{Loc}}(M_1, M_2)$ of M_1 into M_2 , with the following assumptions:
 - i. if $\gamma : [a, b] \mapsto \mathcal{M}_2$ is a causal curve and $\gamma(a), \gamma(b) \in \psi(\mathcal{M}_1)$, then $\gamma(t) \in \psi(\mathcal{M}_1)$ for any $t \in [a, b]$;
 - ii. ψ preserves orientation and time-orientation of the embedded spacetime.

Such maps compose as one may expect, if $\psi \in \text{Hom}_{\mathfrak{Loc}}(M_1, M_2)$ and $\psi' \in \text{Hom}_{\mathfrak{Loc}}(M_2, M_3)$, then $\psi' \circ \psi \in \text{Hom}_{\mathfrak{Loc}}(M_1, M_3)$ is a diffeomorphism onto its range $\psi'(\psi(\mathcal{M}_1))$ and will satisfy the above properties, this composition will be associative and there will exist an identity morphism $\text{id}_M \in \text{Hom}_{\mathfrak{Loc}}(M, M)$ such that $\text{id}_M : x \mapsto x$ for any $x \in \mathcal{M}$.

$\mathfrak{Alg}$ consists of

- $\text{Obj}(\mathfrak{Alg})$ which is composed of all unital C^* -algebras $\mathcal{A}$;

- $\text{Mor}(\mathfrak{Alg})$ which is composed of injective unit-preserving $*$ -homomorphisms. As before, given $\alpha \in \text{Hom}_{\mathfrak{Alg}}(\mathcal{A}_1, \mathcal{A}_2)$ and $\alpha' \in \text{Hom}_{\mathfrak{Alg}}(\mathcal{A}_2, \mathcal{A}_3)$, they will compose as $\alpha' \circ \alpha \in \text{Hom}_{\mathfrak{Alg}}(\mathcal{A}_1, \mathcal{A}_3)$ and the identity morphism $\text{id}_{\mathcal{A}} \in \text{Hom}_{\mathfrak{Alg}}(\mathcal{A}, \mathcal{A})$ will be given by the identity map $\text{id}_{\mathcal{A}} : A \mapsto A$, for any $A \in \mathcal{A}$.

Recalling the concepts of Section 1.1.2, we have that a state is a positive, normalized linear functional on a C^* -algebra $\mathcal{A} \in \text{Obj}(\mathfrak{Alg})$, and the set of states on $\mathcal{A}$ will be denoted by $\mathcal{S}(\mathcal{A})$. While not all states will be of physical interest (and we will indeed discuss specific classes of states in this thesis), it is relevant to note that states on $\mathcal{A}$ form a category themselves, $\mathfrak{States}$, which consists of

- $\text{Obj}(\mathfrak{States})$ which is composed of all convex subsets $\mathcal{S} \subset \mathcal{S}(\mathcal{A})$, which are closed under operations from $\mathcal{A}$, i.e. $\frac{\omega(A^* \cdot A)}{\omega(A^* A)} \in \mathcal{S}$ for $\omega \in \mathcal{S}$ and $A \in \mathcal{A}$ such that $\omega(A^* A) \neq 0$;
- $\text{Mor}(\mathfrak{States})$ which is composed of all affine maps $\sigma : \mathcal{S}_1 \mapsto \mathcal{S}_2$, i.e. maps which satisfy $\sigma(\lambda\omega_1 + (1-\lambda)\omega_2) = \lambda\sigma(\omega_1) + (1-\lambda)\sigma(\omega_2)$ for all $0 \leq \lambda \leq 1$ and $\omega_1, \omega_2 \in \mathcal{S}_1$. As before, the composition of morphisms is given by the composition of maps and the identity map $\text{id}_{\mathcal{S}}$ on $\mathcal{S} \in \text{Obj}(\mathfrak{States})$ is the identity morphism.

Any $\mathcal{S} \in \text{Obj}(\mathfrak{States})$ is in principle a candidate for a state space of a system in $\mathfrak{Alg}$, the category $\mathfrak{States}$ allows to consider them as a whole and not submit to a specific choice of state space.

With these concepts defined, we can give the definition of a locally covariant quantum field theory, cf. [BFV03, Def. 2.1].

Definition 2.1.1. *A locally covariant quantum field theory is a covariant functor F between the two categories $\mathfrak{Loc}$ and $\mathfrak{Alg}$ which, for any $M_i = (\mathcal{M}_i, g_i) \in \text{Obj}(\mathfrak{Loc})$, $i = 1, 2, 3$, and $\psi \in \text{hom}_{\mathfrak{Loc}}(M_1, M_2)$, $\psi' \in \text{hom}_{\mathfrak{Loc}}(M_2, M_3)$, acts as*

$$\begin{array}{ccc} M & \xrightarrow{\psi} & M' \\ F \downarrow & & \downarrow F \\ F(M) & \xrightarrow{F(\psi)} & F(M') \end{array}$$

with the covariance properties $F(\psi') \circ F(\psi) = F(\psi' \circ \psi)$, $F(\text{id}_M) = \text{id}_{F(M)}$.

We say that F is causal if for any two morphisms $\psi_i \in \text{hom}_{\mathfrak{Loc}}(M_i, M)$, $i = 1, 2$ so that the sets $\psi_1(\mathcal{M}_1)$ and $\psi_2(\mathcal{M}_2)$ are causally separated in M ,

$$[F_{\psi_1}(F(M_1)), F_{\psi_2}(F(M_2))] = 0,$$

i.e. they commute, indicating as F_{ψ} the morphism $F(\psi)$.

We say that F obeys the time-slice axiom if

$$F_{\psi}(F(M)) = F(M')$$

for any $\psi \in \text{hom}_{\mathfrak{Loc}}(M, M')$ such that $\psi(\mathcal{M})$ contains a Cauchy surface for M' .

We can see from this definition how we are performing an association of algebras to spacetimes together with an identification of algebras relative to isometric spacetimes. We may however want to see a more standard AQFT formulation, which typically involves some fixed spacetime, like the Minkowski spacetime, and open, bounded regions $\mathcal{O}$ in it, to which we associate a C^* -algebra

$\mathcal{A}(\mathcal{O})$, giving a net of algebras $\mathcal{O} \mapsto \mathcal{A}(\mathcal{O})$, describing operators that act ‘locally’ in $\mathcal{O}$. Then, we ask for *isotony*, i.e. if $\mathcal{O}_1 \subset \mathcal{O}_2$, then $\mathcal{A}(\mathcal{O}_1) \subset \mathcal{A}(\mathcal{O}_2)$. We may then define the algebra of ‘all local observables’ as $\mathcal{A}_{\text{loc}} = \cup \mathcal{A}(\mathcal{O})$, and its closure in the norm topology as $\mathcal{A} = \overline{\mathcal{A}_{\text{loc}}}$, which may be called the ‘algebra of all quasilocal observables’ or the ‘ C^* -inductive limit’ of the system $\{\mathcal{A}(\mathcal{O})\}$. Then, we ask for *causality*, i.e. if $\mathcal{O}_1$ and $\mathcal{O}_2$ are spacelike separated, then $[\mathcal{A}(\mathcal{O}_1), \mathcal{A}(\mathcal{O}_2)] = 0$. Lastly, we have (special relativistic) *covariance*, which asks, for any element L of the isometry group of our spacetime (e.g. the proper, orthochronous Poincaré group in the case of Minkowski) for a C^* -algebra an automorphism $\alpha_{\mathcal{A}} : \mathcal{A} \mapsto \mathcal{A}$ to exist, such that $\alpha_{L_1} \circ \alpha_{L_2} = \alpha_{L_1 \circ L_2}$, for any pair of transformations L, L' w.r.t. their composition, cf. [Dim80].

The link with Definition 2.1.1 is the following. Let $M = (\mathcal{M}, g) \in \text{Obj}(\mathfrak{Loc})$ and let $\mathcal{K}(M)$ be the set of all the relatively compact subsets of $\mathcal{M}$, which are causally complete, i.e. contain all g -causal curves connecting any pair of points. Then, $\mathcal{O} \in \mathcal{K}(M)$ and the restricted metric $g_{\mathcal{O}} := g|_{\mathcal{O}}$ define $O := (\mathcal{O}, g_{\mathcal{O}}) \in \text{Obj}(\mathfrak{Loc})$, with the induced orientation and time-orientation. Then, we can see its inclusion in M as an injection $\iota_{\mathcal{M}, \mathcal{O}} : O \mapsto M$, so $\iota_{\mathcal{M}, \mathcal{O}} \in \text{Hom}_{\mathfrak{Loc}}(O, M)$. This gives the following connection, which shows the generalization of the usual Haag-Kastler axioms, cf. [BFV03, Prop. 2.3].

Proposition 2.1.2. *Let F be a covariant functor with the properties of Definition 2.1.1 and define a net of algebras*

$$\mathcal{K}(M) \ni \mathcal{O} \mapsto \mathcal{A}(\mathcal{O}) := F_{\iota_{\mathcal{M}, \mathcal{O}}}(F(O)) \subset F(M).$$

Then, this net will have the following properties.

- i. (isotony) *if $\mathcal{O}_1 \subset \mathcal{O}_2$, then $\mathcal{A}(\mathcal{O}_1) \subset \mathcal{A}(\mathcal{O}_2)$, $\mathcal{O}_1, \mathcal{O}_2 \in \mathcal{K}(M)$;*
- ii. (covariance) *if there exists a group G of isometric diffeomorphisms $\kappa : \mathcal{M} \mapsto \mathcal{M}$, $\kappa_* g = g$, preserving orientation and time-orientation, then it admits a representation $G \ni \kappa \mapsto \alpha_{\kappa}$ by C^* -algebra automorphism $\alpha_{\kappa} : \mathcal{A} \mapsto \mathcal{A}$ (where $\mathcal{A} = \overline{\cup \mathcal{A}(\mathcal{O})}$ is the quasi-local limit) such that, for $\mathcal{O} \in \mathcal{K}(M)$,*

$$\alpha_{\kappa}(\mathcal{A}(\mathcal{O})) = \mathcal{A}(\kappa(\mathcal{O}));$$

- iii. (causality) *if the theory defined by F is causal, then for any causally separated $\mathcal{O}_1, \mathcal{O}_2 \in \mathcal{K}(M)$, $[\mathcal{A}(\mathcal{O}_1), \mathcal{A}(\mathcal{O}_2)] = 0$;*
- iv. (time-slice) *if the theory defined by F obeys the time-slice axiom, for any Cauchy surface Σ in M , $S \subset \Sigma$ open and connected and $\mathcal{O} \in \mathcal{K}(M)$ such that $S \subset \mathcal{O}$, it holds that*

$$\mathcal{A}(S^{\perp\perp}) \subset \mathcal{A}(\mathcal{O}),$$

where $S^{\perp\perp}$ is the double causal complement of S and $\mathcal{A}(S^{\perp\perp})$ is the smallest C^* -algebra formed by all the $\mathcal{A}(\mathcal{O}')$, with $\mathcal{K}(M) \ni \mathcal{O}' \subset S^{\perp\perp}$. (Note that if we further restrict $\mathcal{O}$ such that $\mathcal{O} \subset S^{\perp\perp}$, the reverse inclusion $\mathcal{A}(\mathcal{O}) \subset \mathcal{A}(S^{\perp\perp})$ follows trivially from isotony, yielding the equality $\mathcal{A}(\mathcal{O}) = \mathcal{A}(S^{\perp\perp})$.)

2.1.1 The Klein-Gordon field

The simplest example we can consider of a quantum field theory both in the Minkowski spacetime and in general curved spacetimes is the free Klein-Gordon (scalar) field. This is indeed the main example we will take in later sections to apply general arguments to more specific cases.

Given a spacetime $M = (\mathcal{M}, g) \in \text{Obj}(\mathfrak{Loc})$, we can write the Klein-Gordon equation for smooth, real-valued φ as

$$(-\square + m^2 + \xi R) \varphi = 0, \tag{2.1.2}$$

where $\square$ is the d'Alembert operator relative to g , $m \geq 0$, $\xi \in \mathbb{R}$ and R is the scalar curvature of g . As we are considering globally hyperbolic spacetimes, we know that there will exist unique advanced $(-)$ and retarded $(+)$ solutions to the Klein-Gordon equation, i.e. continuous linear maps $E^\pm : C_0^\infty(\mathcal{M}, \mathbb{R}) \mapsto C^\infty(\mathcal{M}, \mathbb{R})$ such that

$$(-\square + m^2 + \xi R) E^\pm f = f = E^\pm (-\square + m^2 + \xi R) f \quad (2.1.3)$$

for all $f \in C_0^\infty(\mathcal{M}, \mathbb{R})$ and

$$\text{supp}(E^\pm f) \subset J^\pm(\text{supp}(f)).$$

Then, $E := E^+ - E^-$ is called the *(causal) propagator* of the Klein-Gordon equation and it will similarly satisfy

$$(-\square + m^2 + \xi R) E f = 0 = E (-\square + m^2 + \xi R) f$$

for all $f \in C_0^\infty(\mathcal{M}, \mathbb{R})$. In this sense, the propagator E maps smooth functions onto the set of smooth solutions of (2.1.2) which have compact support on Cauchy surfaces [Dim80; Ver94]. Fixing any Cauchy surface Σ of $M = (\mathcal{M}, g)$ and some open subset $\tilde{\Sigma}$ of Σ , we may define $D_{\tilde{\Sigma}} := C_0^\infty(\tilde{\Sigma}, \mathbb{R}) \oplus C_0^\infty(\tilde{\Sigma}, \mathbb{R})$ and the symplectic form

$$\sigma_{\tilde{\Sigma}}((f_0, f_1), (g_0, g_1)) := \int_{\tilde{\Sigma}} (f_0 g_1 - f_1 g_0) d\mu_{\tilde{\Sigma}},$$

where $d\mu_{\tilde{\Sigma}}$ is the induced measure on $\tilde{\Sigma}$. Indeed, we can see that $(D_{\tilde{\Sigma}}, \sigma_{\tilde{\Sigma}})$ is a symplectic space, the symplectic space of smooth initial data. Alternatively, we may define $K := C_0^\infty(\mathcal{M}, \mathbb{R}) / \ker E$, with the quotient map $[\cdot] : C_0^\infty(\mathcal{M}, \mathbb{R}) \mapsto K$, and $K_{\tilde{\Sigma}} := [C_0^\infty(\text{int } \mathcal{D}(\tilde{\Sigma}))]$, where $\mathcal{D}(\tilde{\Sigma})$ is the domain of dependence of $\tilde{\Sigma}$. For any $[f], [g] \in K_{\tilde{\Sigma}}$, we can again define a symplectic form

$$\zeta_{\tilde{\Sigma}}([f], [g]) := \int_{\mathcal{M}} f E h d\mu$$

where $d\mu_{\Sigma}$ is the metric-induced volume form on $\mathcal{M}$. Note that this is independent of the choice of Cauchy surface Σ . Again, we get that $(K_{\tilde{\Sigma}}, \zeta_{\tilde{\Sigma}})$ is a symplectic space, which will be symplectomorphic to the previous one, $(D_{\tilde{\Sigma}}, \sigma_{\tilde{\Sigma}})$ [Ver94, Prop. 2.2].

As discussed in Section 1.3, to any symplectic space we can associate its Weyl algebra generated by the Weyl relations (1.3.1). In the case of the Klein-Gordon field, we may keep the constants m, ξ fixed in (2.1.2), consider the symplectic space of solutions of the Klein-Gordon equation $(K_{\tilde{\Sigma}}, \zeta_{\tilde{\Sigma}})$ and take $\tilde{\Sigma} = \Sigma$. As this is independent of the specific Cauchy surface Σ , we may drop the subscripts and consider (K, ζ) defining the Weyl algebra $\mathcal{W}[K, \zeta]$ of the Klein-Gordon field in the spacetime $M = (\mathcal{M}, g)$. We may see this construction in the locally covariant setting by defining the covariant functor as $F(M) = \mathcal{W}[K, \zeta]$, which will satisfy the properties of Definition 2.1.1 [BFV03, Sec. 2.3], making the free scalar theory a locally covariant quantum field theory. Indeed, considering two spacetimes $M, M' \in \text{Obj}(\mathfrak{Loc})$ and $\psi \in \text{hom}_{\mathfrak{Loc}}(M, M')$, we can define a spacetime $M^\psi = (\psi(\mathcal{M}), \psi_* g)$ which will be isomorphic to M via the map ψ_* (so the corresponding symplectic spaces will be symplectomorphic) and will define a C^* -algebraic isomorphism $\alpha_\psi : \mathcal{W}[K, \zeta] \mapsto \mathcal{W}[K^\psi, \zeta^\psi]$, such that

$$\alpha_\psi(W(f)) = W^\psi(\psi_*(f)),$$

$f \in K$, where the quantities with the superscript ψ will be relative to M^ψ . Similarly, we indicate with a prime the quantities relative to M' . Now, we have that $\psi : \mathcal{M} \mapsto \psi(\mathcal{M}) \subset \mathcal{M}'$ is an isometry, so $\psi_* g = g'|_{\psi(\mathcal{M})}$ and the uniqueness of the propagators of the Klein-Gordon equation

yields $E^\psi = \chi_{\psi(\mathcal{M})} E'|_{C_0^\infty(\psi(\mathcal{M}), \mathbb{R})}$, where $\chi_{\psi(\mathcal{M})}$ is the characteristic function of $\psi(\mathcal{M})$ and we may identify K^ψ with $E'(C_0^\infty(\psi(\mathcal{M}), \mathbb{R}))$ and ζ^ψ with $\zeta'|_{K^\psi}$.

Then, defining the symplectic map $T^\psi : (K^\psi, \zeta^\psi) \mapsto (K', \zeta')$ by $T^\psi E h := E' \psi_* h$, $h \in C_0^\infty(\mathcal{M}, \mathbb{R})$, this yields a C^* -algebraic endomorphism $\alpha'_\psi : \mathcal{W}[K^\psi, \zeta^\psi] \mapsto \mathcal{W}[K', \zeta']$ as

$$\alpha'_\psi(W^\psi(f)) = W'(T^\psi f),$$

for $f \in K^\psi$. It follows that $\alpha'_\psi \circ \alpha_\psi : F(M) \mapsto F(M')$ is a C^* -algebraic endomorphism, which will satisfy the assumptions in Definition 2.1.1 as for the following theorem, cf. [BFV03, Thm. 2.2].

Theorem 2.1.3. *Consider $M = (\mathcal{M}, g) \in \text{Obj}(\mathfrak{Loc})$, $F(M) = \mathcal{W}[K, \zeta]$, w.r.t. the Klein-Gordon equation (2.1.2) with m, ξ fixed for all M , and, for any $\psi \in \text{hom}_{\mathfrak{Loc}}(M, M')$, the C^* -algebraic endomorphism $\alpha'_\psi \circ \alpha_\psi : F(M) \mapsto F(M')$ as defined above. Then, F is a covariant functor defining a locally covariant quantum field theory as for Definition 2.1.1, which is causal and obeys the time-slice axiom.*

2.1.2 The stress-energy tensor and the Hadamard condition

Given our spacetime $M = (\mathcal{M}, g)$, the theory we have obtained will describe the expectation values of all observables contained in the Weyl algebra $\mathcal{W}[D, \sigma]$ of the Klein-Gordon field¹, these will compose a large class of physically relevant quantities. In addition, when considering a spacetime with a preferred time flow and in the GNS-representations of states that are stationary w.r.t. this flow, the Hamiltonian may be also represented by the fact that the classical time evolution generated by the Hamiltonian gives rise to a linear mapping $\tau_t : D \mapsto D$ preserving σ . Then, τ_t will induce an automorphism $\alpha_t : \mathcal{W}[D, \sigma] \mapsto \mathcal{W}[D, \sigma]$ of the Weyl algebra, which we can associate to the transformation of observables in the Heisenberg picture, whose generator can be seen as the Hamiltonian (up to a multiple of the identity), cf. [Wal94, Sec. 4.6].

The Weyl algebra $\mathcal{W}[D, \sigma]$ will not however include many field observables present in the classical theory, namely ones which are quadratic in the field operators like the stress-energy tensor. Considering the Klein-Gordon field 2.1.2, in which we will take for simplicity the the minimally coupled case $\xi = 0$, the classical stress tensor takes the form

$$T_{ab}[\varphi] = \partial_a \varphi \partial_b \varphi - \frac{1}{2} g_{ab} \left(\eta^{cd} \partial_c \varphi \partial_d \varphi + m^2 \varphi^2 \right), \quad (2.1.4)$$

where η is the Minkowski metric. The energy density will be its (00)-component. The stress-energy tensor is of central importance as it describes the local energy, momentum and stress properties of the field. In addition, it also describes the back-reaction of the field on the spacetime geometry, the idea being that matter classically influences the geometry via the (classical) stress-energy tensor in the Einstein equations $G_{ab} = 8\pi T_{ab}$, so we would expect something analogous on a quantum level. At a semiclassical level, the back-reaction is given by the *semiclassical Einstein equation*

$$G_{ab} = 8\pi \langle T_{ab} \rangle, \quad (2.1.5)$$

where the expectation value is taken w.r.t some physically relevant state, e.g. the vacuum in the case of the Minkowski spacetime.

This immediately raises some mathematical concerns. First, as the stress-tensor (2.1.4) is quadratic in the field φ , which is a distribution, it will involve taking products of distributions on the same

¹We will refer here and in the following to the symplectic space of the Klein-Gordon field (D, σ) instead of (K, ζ) , keeping in mind that the two are symplectomorphic.

point, which will be ill-defined and requires a regularization procedure. The easier approach to this issue is to disregard the problem of including observables like the stress tensor in the algebras under consideration and instead define the expectation value of the stress tensor $\langle T_{ab} \rangle_\omega$ in some state ω , or better the difference $\langle T_{ab} \rangle_\omega - \langle T_{ab} \rangle_{\omega_0}$ w.r.t. some suitable reference state ω_0 so that this difference is well-behaved. We will follow here this approach and discuss a different one in Section 2.1.3. (For an overview of the literature on extended algebras, we refer to [HW15].) For example, in the case of the Minkowski spacetime, the natural choice for ω_0 is the vacuum and this ‘point-splitting’ procedure is defined as follows. As the stress-energy tensor, $\langle \varphi(x)^2 \rangle$ is not a well-defined concept, however $\langle \varphi(x)\varphi(x') \rangle$ does make sense as a bi-distribution. Then, we expect physically reasonable states to give bi-distributions $\langle \varphi(x)\varphi(x') \rangle$ which show the same singular behaviour for $x' \rightarrow x$ as $\langle \varphi(x)\varphi(x') \rangle_0 = \langle \varphi(x)\varphi(x') \rangle_{\omega_0}$, in the sense that

$$F(x, x') := \langle \varphi(x)\varphi(x') \rangle - \langle \varphi(x)\varphi(x') \rangle_0 \quad (2.1.6)$$

is a smooth function of x and x' . Then, the coincidence limit $x' \rightarrow x$ exists and we can define

$$\langle \varphi^2 \rangle_{\text{reg}}(x) = \lim_{x' \rightarrow x} F(x, x'), \quad (2.1.7)$$

as to denote a regularized version of the expectation value $\langle \varphi(x)^2 \rangle$. The same logic can be then applied to the stress tensor and define

$$\langle T_{ab} \rangle_{\text{reg}}(x) = \lim_{x' \rightarrow x} \left[\partial_a^{(x)} \partial_b^{(x')} F(x, x') - \frac{1}{2} g_{ab} \left(\left(\eta^{cd} \partial_c^{(x)} \partial_d^{(x')} + m^2 \right) F(x, x') \right) \right], \quad (2.1.8)$$

where again this goes to denote a regularized version of $\langle T_{ab}(x) \rangle$.

From the case of the Minkowski spacetime, it becomes apparent that for general spacetimes we should consider differences in the expectation values of the stress tensor for pairs of states ω_1, ω_2 such that $\langle \varphi(x)\varphi(x') \rangle_1 - \langle \varphi(x)\varphi(x') \rangle_2$ is smooth. Before we discuss what kind of states do satisfy this behaviour, we have the question of how $\langle T_{ab} \rangle$ should be defined from this assumption. A list of properties one would expect it to hold are the following, which are known as Wald’s axioms, cf. [Wal77], [Wal94, Sec. 4.6].

- i. when $\langle \varphi(x)\varphi(x') \rangle_1 - \langle \varphi(x)\varphi(x') \rangle_2$ is a smooth function, $\langle T_{ab} \rangle_1 - \langle T_{ab} \rangle_2$ should be given by the point-splitting procedure (2.1.8);
- ii. the expectation value of the stress-energy tensor should be local w.r.t. to the state of the field, in the following sense. Let $M = (\mathcal{M}, g), M' = (\mathcal{M}', g') \in \text{Obj}(\mathfrak{Loc})$ and consider globally hyperbolic, open neighbourhoods $\mathcal{O}, \mathcal{O}'$ of $x \in \mathcal{M}, x' \in \mathcal{M}'$ such that there exists an isometry $\iota : \mathcal{O} \rightarrow \mathcal{O}'$ with $\iota(x) = x'$. Then, assume that $\tilde{\Sigma}$ is a smooth spacelike Cauchy surface for $\mathcal{O}$ and $\tilde{\Sigma}' = \iota(\tilde{\Sigma})$ for $\mathcal{O}'$. Under the isometry, we may identify the Weyl subalgebras $\mathcal{W}[D_{\tilde{\Sigma}}, \sigma_{\tilde{\Sigma}}] \subset \mathcal{W}[D, \sigma]$ for M and $\mathcal{W}[D'_{\tilde{\Sigma}'}, \sigma'_{\tilde{\Sigma}'}] \subset \mathcal{W}[D', \sigma']$ for M' . Suppose now that the states ω on $\mathcal{W}[D, \sigma]$ and ω' on $\mathcal{W}[D', \sigma']$ have equal restrictions to $\mathcal{W}[D_{\tilde{\Sigma}}, \sigma_{\tilde{\Sigma}}]$ and $\mathcal{W}[D'_{\tilde{\Sigma}'}, \sigma'_{\tilde{\Sigma}'}]$ under this identification. Then, the requirement is that under the identification of $\mathcal{O}$ and $\mathcal{O}'$ given by ι , $\langle T_{ab}(x) \rangle_\omega = \langle T_{ab}(x') \rangle_{\omega'}$;
- iii. for all states, $\partial^a \langle T_{ab} \rangle = 0$;
- iv. in Minkowski spacetime, $\langle T_{ab} \rangle_0 = 0$ w.r.t. the vacuum.

In particular, the first two properties determine $\langle T_{ab} \rangle$ up to local curvature terms [Wal94, Thm. 4.6.1]. Indeed, if $\langle T_{ab} \rangle, \langle \tilde{T}_{ab} \rangle$ both satisfy i. and ii., for any two states ω_1, ω_2 on a fixed spacetime $M = (\mathcal{M}, g)$, i. gives

$$\langle T_{ab} \rangle_1 - \langle T_{ab} \rangle_2 = \langle \tilde{T}_{ab} \rangle_1 - \langle \tilde{T}_{ab} \rangle_2,$$

which in turn implies that

$$t_{ab} = \langle T_{ab} \rangle_\omega - \langle \tilde{T}_{ab} \rangle_\omega$$

is independent of the state ω . While property i. does not restrict the way in which t_{ab} depends on M , property ii. implies that t_{ab} at $x \in \mathcal{M}$ only depends on the geometry in an arbitrary open neighbourhood of p , which may be taken be arbitrarily small. In this sense, the difference t_{ab} of different prescriptions of $\langle T_{ab} \rangle$ is a ‘local curvature term’. Note that point iii. further implies that $\partial^a t_{ab} = 0$ and point iv. that in Minkowski spacetime $t_{ab} = 0$. Indeed, if the geometry in a neighbourhood of x is flat, we get $t_{ab}(x) = 0$.

These axioms do not, however, immediately provide a concrete prescription for $\langle T_{ab} \rangle$ on a generic globally hyperbolic spacetime, nor do they address the question of what would be a class of states to which such a scheme is well-posed. If we attempt to naively apply the point-splitting procedure by subtracting from $\langle \varphi(x)\varphi(x') \rangle$ its expectation value in some arbitrary reference state (as is done with the vacuum in Minkowski spacetime), we get a prescription which satisfies property i. but not ii., it is not local. As a reference state intrinsically depends on the global properties of the spacetime, its subtraction is neither local nor covariant. To satisfy property ii., we must instead subtract a ‘locally constructed’ bi-distribution that depends purely on the local geometry and possesses the correct short-distance singularity structure, so that it yields a suitably regular coincidence limit. However, constructing a purely local bi-distribution that also exactly satisfies the wave equation in both x and x' is not generally possible. As a result, this local subtraction will inevitably produce a tensor that is not automatically conserved, so that to satisfy property iii., an additional geometric correction is required.

The way in which this locally constructed bi-distribution is achieved is through Hadamard’s algorithm, originally developed by Hadamard for constructing bi-distributional solutions to elliptic and hyperbolic equations [Had23]. For the purpose of this thesis, we only need that their two-point distributions of the states under consideration differ by a smooth, symmetric function, however we will discuss the main ideas behind this construction. Considering our spacetime $M = (\mathcal{M}, g) \in \text{Obj}(\mathfrak{Loc})$, we say that a *convex normal neighbourhood* is an open set $\mathcal{U}$ of $\mathcal{M}$ such that for any $x, x' \in \mathcal{U}$, there exists a unique geodesic contained in $\mathcal{U}$ which connects x and x' . A *causal normal neighbourhood* is an open neighbourhood $\mathcal{N}$ of a Cauchy surface Σ of M for which Σ is a Cauchy surface for $\mathcal{N}$ and for $x, x' \in \mathcal{N}$ with $x \in J^+(x')$, there exists a convex normal neighbourhood $\mathcal{O}$ in $\mathcal{M}$ such that $J^-(x) \cap J^+(x') \subset \mathcal{O}$. Any Cauchy surface Σ will have such a neighbourhood [KW91, Lemma 2.2]. The *(signed) square of the geodesic distance* from x to x' in a convex normal neighbourhood $\mathcal{U}$ is

$$s(x, x') = \pm \left(\int_{\tau_0}^{\tau_1} \left| g_{ab}(y(\tau)) \frac{dy^a(\tau)}{d\tau} \frac{dy^b(\tau)}{d\tau} \right|^{\frac{1}{2}} d\tau \right)^2, \quad (2.1.9)$$

where $y(\tau)$ is a parametrization of the unique geodesic in $\mathcal{U}$ connecting x and x' , so that $y(\tau_0) = x$ and $y(\tau_1) = x'$. The sign plus, resp. minus, corresponds to $y(\tau)$ being spacelike, resp. causal. (E.g., on Minkowski spacetime $(\mathbb{R}, \eta)$, we have $s(x, x') = (x - x')^2$.)

Then, let $\mathcal{V} \subset \mathcal{M} \times \mathcal{M}$ be the set of all causally related points (x, x') such that $J^+(x) \cap J^-(x')$ and $J^-(x) \cap J^+(x')$ are contained within a causal normal neighbourhood. Then, there will exist

an open neighbourhood $\mathcal{O}$, in $\mathcal{M} \times \mathcal{M}$, of $\mathcal{V}$ on which $s(x, x')$ is well-defined and smooth [Rad96, Lemma 3.1], this $\mathcal{O}$ can be chosen to be a union of sets of the form $\mathcal{U} \times \mathcal{U}$, where the $\mathcal{U}$ are convex normal neighbourhoods.

Remark. Note that, in [KW91], the structures involved in the Hadamard construction, including the square of the geodesic distance s , are assumed to be well-defined in an open neighbourhood of the diagonal of $\mathcal{M} \times \mathcal{M}$ that is larger than $\mathcal{U} \times \mathcal{U}$. This however creates an ambiguity, because two points $x, x' \in \mathcal{M}$ may belong to many convex normal neighbourhoods and different choices of such a neighbourhood may lead to different values for $s(x, x')$ and to different singularity structures, affecting this whole construction. Moretti in [Mor21] resolves this ambiguity by slightly reformulating definitions in [KW91] and exploiting topological consequences of the manifold's paracompactness property to rigorously construct a suitable, well-defined open neighbourhood of the diagonal where the needed structures hold. This reformulation is in agreement with Radzikowski's microlocal version of the Hadamard condition [Rad96].

Fixing a smooth time function $\mathcal{T} : \mathcal{M} \mapsto \mathbb{R}$ increasing towards the future, we can define for all $\varepsilon > 0$ and $(x, x') \in \mathcal{O}$, the complex-valued functions

$$Q_{\mathcal{T}}(x, x'; \varepsilon) := s(x, x') - 2i\varepsilon(\mathcal{T}(x) - \mathcal{T}(x')) - \varepsilon^2 \quad (2.1.10)$$

and, for $n \geq 1$ integer,

$$G_{\varepsilon}^{\mathcal{T}, n}(x, x') := \frac{1}{4\pi^2} \left(\frac{U(x, x')}{Q_{\mathcal{T}}(x, x'; \varepsilon)} + V^{(n)}(x, x') \log(Q_{\mathcal{T}}(x, x'; \varepsilon)) \right), \quad (2.1.11)$$

where $V^{(n)}(x, x') := \sum_{m=0}^n V_m(x, x') s(x, x')^m$ and the branch cut for the logarithm is chosen to be on the negative real axis. The functions U and V_m , $m \geq 0$ integer, are smooth and defined on $\mathcal{O}$. U is the square root of the Van Vleck-Morette determinant, and does not vanish where s does, while V_m is the sequence determined by the Hadamard recursion relations. Such quantities, for fixed mass m , are solely determined by the spacetime metric g , cf. [Ver94, App. C]. (We refer to [Gar64] for the general theory behind these objects and to [San15, Sec. 4] for the explicit construction of the coefficients of these series.)

Now, consider the set $\mathcal{C} \supset \mathcal{V}$ of all causally related pairs of points $(x, x') \in \mathcal{M} \times \mathcal{M}$ and an open neighbourhood $\mathcal{O}$ of $\mathcal{V}$ on which s is well-defined and smooth. For any causal normal neighbourhood on some Cauchy surface Σ , we have that in $\mathcal{N} \times \mathcal{N}$ there is an open neighbourhood $\mathcal{O}'$ of $\mathcal{C} \cap (\mathcal{N} \times \mathcal{N})$ such that the closure of $\mathcal{O}'$ in $\mathcal{N} \times \mathcal{N}$ is contained in $\mathcal{O} \cap (\mathcal{N} \times \mathcal{N})$ [Rad96, Lemma 3.3]. Then, choose a smooth function $\chi(x, x') \in C^\infty(\mathcal{N} \times \mathcal{N})$ such that $\chi(x, x') = 0$ when $(x, x') \notin \mathcal{O}$ and $\chi(x, x') = 1$ whenever $(x, x') \in \overline{\mathcal{O}'}$. Then, we have the following definition, cf. [KW91].

Definition 2.1.4. Let ω_2 be a two-point distribution on $D \times D$ and let $\mathcal{T}$ be a choice of a smooth global time function on $\mathcal{M}$, increasing towards the future. Given a causal normal neighbourhood $\mathcal{N}$ of a Cauchy surface Σ of M , ω_2 is (globally) Hadamard on $\mathcal{N} \times \mathcal{N}$ if for any integer $n \geq 0$ there exists a function $H^n \in C^n(\mathcal{N} \times \mathcal{N})$ such that for all $f, g \in C_0^\infty(\mathcal{N})$,

$$\omega_2(f, g) = \lim_{\varepsilon \rightarrow 0^+} \int_{\mathcal{N} \times \mathcal{N}} \Lambda_{\varepsilon}^{\mathcal{T}, n}(x, x') f(x) g(x') d\mu_g(x) d\mu_g(x'), \quad (2.1.12)$$

where $d\mu_g(x) = \sqrt{|\det g_{ab}(x)|} d^{d+1}x$ on coordinate patches and

$$\Lambda_{\varepsilon}^{\mathcal{T}, n}(x, x') := \chi(x, x') G_{\varepsilon}^{\mathcal{T}, n}(x, x') + H^n(x, x'),$$

with χ defined as before.

Note that this definition is independent of the choice of $\Sigma, \mathcal{N}, \mathcal{T}$ and χ . It follows that if ω_2 is Hadamard in a causal normal neighbourhood $\mathcal{N}$ of Σ , it will be Hadamard in some causal normal neighbourhood $\mathcal{N}'$ of any other Cauchy surface Σ' (*causal propagation property*) [Ver94, Prop. C.2]. Also, if ω_2 is Hadamard, it is locally a distribution, i.e. for any $x \in \mathcal{M}$, there will exist a neighbourhood $\mathcal{O}$ of x such that the real and imaginary parts of ω_2 can be identified with distributions on $C^\infty(\mathcal{O} \times \mathcal{O})$. Then, we can speak of Hadamard states.

Definition 2.1.5. *Let ω be a state on the Weyl algebra $\mathcal{W}[D, \sigma]$ of the Klein-Gordon field in M . Then, ω is called an Hadamard state if its two-point function exists and it is of Hadamard form.*

Note that this approach to Hadamard two-point functions, based on their singularity structure, can be equivalently formulated with microlocal analysis in terms of *wavefront sets*, this is due to Radzikowski [Rad96]. Generally speaking, the wavefront set of a distribution is a characterization of its singularity structure. (This concept is due to Hörmander, cf. [Hör70].) Let f be a distribution on $\mathcal{M}$ and let the pair (x, k) be given by a point $x \in \mathcal{M}$ and a nonzero element k of the cotangent bundle $T^*\mathcal{M}$. Then, we say that (x, k) is not in the wavefront set of f if there exist (i) a smooth test function with compact support (a bump function) $g \in C_0^\infty(\mathcal{M})$ such that $g(x) \neq 0$, and (ii) an open conic² neighbourhood V of k . For (x, k) to satisfy this regularity condition, the Fourier transform $\widehat{gf}$ of the localized distribution gf must exhibit rapid decay within the cone V , i.e. for every positive integer N , there exists a constant $C_N > 0$ such that $|\widehat{gf}(\xi)| \leq C_N(1 + |k|)^{-N}$, for all $k \in V$. Then, the *wavefront set* $\text{WF}(f)$ of f is the closed, conic subset of the cotangent bundle $T^*\mathcal{M} \setminus 0$ of points which do not satisfy this regularity condition. In this approach, recalling the advanced $(-)$ and retarded $(+)$ solutions to the Klein-Gordon equation $E^\pm : C_0^\infty(\mathcal{M}, \mathbb{R}) \mapsto C^\infty(\mathcal{M}, \mathbb{R})$ satisfying (2.1.3), we may see these as distributions on $\mathcal{M} \times \mathcal{M}$ with support

$$\text{supp}(E^\pm) \subset \{(x, x') \in \mathcal{M} \times \mathcal{M} \mid x \in J^\pm(x')\},$$

and in fact they will satisfy $E^\pm(x, x') = E^\mp(x', x)$. Then, their wavefront set is

$$\text{WF}(E^\pm) = \{((x, x'), (k, -k')) \mid x \in J^\pm(x') \text{ and either } ((x, k) \sim (x, k')) \text{ or } (x = x' \text{ and } k = -k')\},$$

where $(x, k) \sim (x, k')$ means that there exists a lightlike geodesic from x to x' with cotangent vector k at x and k' at x' . Then, we get that for the causal propagator $E = E^+ - E^-$ we have

$$\text{WF}(E) = \{((x, x'), (k, -k')) \mid (x, k) \sim (x, k')\}.$$

Then, Radzikowski's definition of a Hadamard distribution is the following, which is equivalent to Definition 2.1.4, cf. [Rad96].

Definition 2.1.6. *Let $M = (\mathcal{M}, g)$ a time-oriented globally hyperbolic spacetime. Then, a two-point distribution ω_2 on $\mathcal{M} \times \mathcal{M}$ is Hadamard for the free scalar field on M if, for all $x, x' \in \mathcal{M}$,*

- i. *the anti-symmetric part of ω_2 is E , i.e. $\omega_2(x, x') - \omega_2(x', x) = iE(x, x')$;*
- ii. *its wave front set is one causal half that of the causal propagator, i.e.*

$$\text{WF}(\omega_2) = \{((x, x'), (k, -k')) \mid (x, k) \sim (x', k') \text{ and } k \in V_x^+\},$$

where V_x^+ is the closed future light cone in the cotangent space $T_x^*\mathcal{M}$ at the point x (this is called the wavefront set spectral condition, cf. [Rad96, Thm. 5.1 and Def. 6.1]);

²A set V is conic if $k \in V$ implies $tk \in V$, for all $t > 0$.

iii. ω_2 is a bi-solution of the Klein-Gordon equation, i.e.

$$(-\square + m^2)\omega_2(\cdot, x) = 0 = \omega_2(x, \cdot)(-\square + m^2) :$$

iv. ω_2 is positive semi-definite, i.e. for any complex-valued bump function g , we have that

$$\int_{\mathcal{M} \times \mathcal{M}} g^*(x)\omega_2(x, y)g(y)d\text{vol}(x)d\text{vol}(y) \geq 0.$$

Circling back to our discussion on the stress-energy tensor, we can then generalize the point-splitting procedure on Minkowski spacetime given by (2.1.8). As discussed, generalizing the point-splitting procedure by subtracting a global reference state fails Wald's covariance and locality axioms. Instead, it is physically reasonable to restrict the discussion to Hadamard states and define the point-splitting procedure as before, however substituting (2.1.6) with a distribution

$$F(x, x') := \langle \varphi(x)\varphi(x') \rangle - G(x, x'), \quad (2.1.13)$$

where $G(x, x')$ is a bi-distribution of the form (2.1.11), which will encode the short-distance singularity structure of any Hadamard state and is constructed purely from local spacetime geometry, so axioms i. and ii. will be satisfied by this subtraction. However, as $G(x, x')$ only satisfies the Klein-Gordon equation up to smooth terms, the naive stress-energy tensor constructed directly from $F(x, x')$ w.r.t. any Hadamard state as in (2.1.8) will not be automatically conserved. To satisfy Wald's conservation axiom iii., an additional, local, and covariant geometric correction term must be explicitly added to the point-splitting prescription. With this necessary conservation correction, $\langle T_{ab} \rangle$ is rigorously defined for all Hadamard states, satisfying all of Wald's axioms up to the standard local curvature ambiguities.

If we now consider Hadamard states which are also Gaussian, as for Definition 1.3.1, we obtain a large class of states. Indeed, the set of Gaussian Hadamard states on $\mathcal{W}[D, \sigma]$ spans an infinite-dimensional subspace of the topological dual space of $\mathcal{W}[D, \sigma]$ [Ver94, Thm. C.4]. Recalling the discussion on quasi-equivalence of Section 1.3.1, we may also consider quasi-equivalence of such states, which has been characterised by Verch [Ver94, Thm. 3.9].

Theorem 2.1.7. *Let φ_1, φ_2 be two Gaussian Hadamard states on the Weyl algebra $\mathcal{W}[D, \sigma]$ of the Klein-Gordon field in $M = (\mathcal{M}, g) \in \text{Obj}(\mathfrak{Loc})$ and let π_1, π_2 be their associated GNS-representations. Then, $\pi_1|_{\mathcal{A}(\mathcal{O})}$ and $\pi_2|_{\mathcal{A}(\mathcal{O})}$ are quasi-equivalent for every open subset $\mathcal{O}$ of $\mathcal{M}$ with compact closure.*

In other terms, two such Gaussian Hadamard states are *locally* quasi-equivalent for any choice of region. Given an open spacetime region $\mathcal{O}$ with compact closure, two states φ_1, φ_2 are *locally quasi-equivalent* if $\pi_1|_{\mathcal{A}(\mathcal{O})}$ and $\pi_2|_{\mathcal{A}(\mathcal{O})}$ are quasi-equivalent, i.e. there exists a $*$ -isomorphism³ $\beta_{\mathcal{O}} : \pi_1(\mathcal{A}(\mathcal{O})'') \mapsto \pi_2(\mathcal{A}(\mathcal{O})'')$ such that $\beta_{\mathcal{O}} \circ \pi_1(A) = \pi_2(A)$ for any $A \in \mathcal{A}(\mathcal{O})$. This concept is of great physical relevance, as two locally quasi-equivalent states will give rise to isomorphic local von Neumann algebras through their GNS-representations.

2.1.3 Lagrangian scalar QFTs

Following the discussion of Section 2.1.2, we will now discuss the idea of extending the algebras under consideration beyond the Weyl algebra, to include operators like the stress tensor, following the approach recently pursued by Buchholz and Fredenhagen [BF20a; BF20b; BF19; BF21] for

³As discussed before Theorem 1.1.6, a $*$ -isomorphism between von Neumann algebras is also a homeomorphism in the weak- $*$ topology.

Lagrangian QFTs. We will follow here notations and the presentation of these topics in [San25, Sec. 2.2 and 2.3], to which we refer for more details.

Given a spacetime $M = (\mathcal{M}, g) \in \text{Obj}(\mathfrak{Loc})$, the general idea is to consider a theory described by some reference Lagrange density $\mathcal{L} = \mathcal{L}[g, \varphi]$, which will depend on some quantum field φ and the spacetime metric g , and then consider dynamics given by equations of motion derived from a Lagrange density $\mathcal{L}'[g', \varphi]$, w.r.t. a spacetime metric g' , which in principle is different from g , which possibly contains a different interaction potential than the one in $\mathcal{L}[g, \varphi]$. This ‘perturbation’ of the dynamics of $\mathcal{L}[g, \varphi]$ will be encoded by functionals F (with suitable properties), which will compose a set $\mathcal{F}(M, \mathcal{L})$. Elements $F \in \mathcal{F}(M, \mathcal{L})$ will generate a C^* -algebra $\mathcal{A}_M^{(\mathcal{L})}$, the *dynamical algebra*, by first defining the group generated by these elements modulo some relations, and then taking $\mathcal{A}_M^{(\mathcal{L})}$ as its group C^* -algebra.

To be more concrete, we will specialize to the Klein-Gordon field and consider Lagrangian densities of the form

$$\mathcal{L}[g', \varphi] = \left(\frac{1}{2}(g')^{ab} \partial_a \varphi \partial_b \varphi + \frac{1}{2} m^2 \varphi^2 + \frac{1}{2} \xi R' \varphi^2 + V(\varphi) \right) \text{dvol}_{g'} , \quad (2.1.14)$$

with a polynomial potential function $V(\varphi)$ defined by arbitrary $n \in \mathbb{N}$ and $c_n \in C^\infty(\mathcal{M}, \mathbb{R})$ as

$$V(\varphi) := \sum_{n=0}^N c_n(x) \varphi(x)^n , \quad (2.1.15)$$

and the metric g'_{ab} is such that the difference $\delta g_{ab} := g'_{ab} - g_{ab}$ is compactly supported and smooth, so we will have that $\text{dvol}_{g'}(x) = \mu_{g'} \text{dvol}_g(x)$ for some $\mu_{g'} \in C_0^\infty(\mathcal{M}, \mathbb{R}_{>0})$ with $\mu_{g'} - 1$ compactly supported. The action functional corresponding to (2.1.14) will then be

$$S[g', \varphi] = \int_{\mathcal{M}} f \mu_{g'} \left(\frac{1}{2}(g')^{ab} \partial_a \varphi \partial_b \varphi + \frac{1}{2} m^2 \varphi^2 + \frac{1}{2} \xi R' \varphi^2 + V(\varphi) \right) \text{dvol}_g . \quad (2.1.16)$$

By considering compactly supported variations of the form (2.1.14), of $\mathcal{L}[g, \varphi]$, with the reference metric g , we can now define differences of the form $\lambda[\varphi] := \mathcal{L}[g', \varphi] - \mathcal{L}[g, \varphi]$, where the coefficients only vary on compact sets. Then, the terms with m and ξ will stay the same on both Lagrangians and $\mu_{g'} - 1, \mu_{g'} R' - R \in C_0^\infty(\mathcal{M}, \mathbb{R})$, so by redefining the coefficients $c_n \in C_0^\infty(\mathcal{M}, \mathbb{R})$ and considering the compactly supported, smooth, symmetric tensor field $\gamma^{ab} = \mu_{g'}(g')^{ab} - g^{ab}$, we can get

$$\lambda[\varphi] = \left(\frac{1}{2} \gamma^{ab} \partial_a \varphi \partial_b \varphi + \sum_{n=0}^N c_n \varphi(x)^n \right) \text{dvol}_g . \quad (2.1.17)$$

This allows to construct functionals of the form

$$F[\varphi] := \int_{\mathcal{M}} \lambda[\varphi] = c + \int_{\mathcal{M}} \left(\frac{1}{2} \gamma^{ab}(x) \partial_a \varphi(x) \partial_b \varphi(x) + \sum_{n=1}^N c_n \varphi(x)^n \right) \text{dvol}_g(x) , \quad (2.1.18)$$

where the $n = 0$ term of the sum, i.e. $\int_{\mathcal{M}} c_0(x) \text{dvol}_g(x)$, has been absorbed into the constant c . Note that the quantities c , $c_n(x)$ and $\gamma^{ab}(x)$ are all uniquely determined by $F[\varphi]$.

We will consider here spacetimes of dimension $d > 2$, the reason being that in dimension $d = 2$, all Lorentzian metrics are conformally equivalent, i.e. locally $g'_{ab} = \nu^2 g_{ab}$ with smooth $\nu > 0$, so $\mu_{g'} = \nu^2$, $(g')^{ab} = \nu^{-2} g^{ab}$, and $\gamma^{ab} = 0$, perturbations of our form are not described by local degrees

of freedom. In dimension $d > 2$, if we have that $(g^{-1} + \gamma)_{ab}^{-1}$ defines a Lorentzian metric, which is justified if γ is ‘small enough’, we may instead consider perturbations of the metric of the form

$$g'_{ab} = \mu_{(g^{-1} + \gamma)^{-1}}^{-\frac{2}{d-2}} (g^{-1} + \gamma)_{ab}^{-1}.$$

This allows to define the following class of functionals.

Definition 2.1.8. $\mathcal{F}(M, \mathcal{L})$ is the class of functionals $F \in C^\infty(\mathcal{M}, \mathbb{R})$ of the form (2.1.18) such that $(g_F)_{ab} = g^{ab} + \gamma^{ab}$ defines an inverse Lorentzian metric, making M globally hyperbolic.

Note that $\mathcal{F}(M, \mathcal{L})$ is not a vector space, however it contains as a subspace the vector space of functionals with $\gamma^{ab} = 0$, so sums of its elements must be checked for admissibility case by case. (This issue is already present in the flat spacetime treatment of kinetic perturbations in [BF21].) Since each F fixes γ^{ab} uniquely, the metric g_F is well-defined and agrees with g outside a compact set. The *spacetime support* of F is the union of the supports of γ^{ab} and of the coefficients c_n with $n \geq 1$, so constant functionals have empty support. The coefficient c_0 is not relevant as it does not alter the equations of motion. Then, we have the following definition.

Definition 2.1.9. For $\varphi_0 \in C_0^\infty(\mathcal{M}, \mathbb{R})$ the relative action is

$$\delta S(\varphi_0)[g, \varphi] := S(f)[g, \varphi + \varphi_0] - S(f)[g, \varphi],$$

where $f \in C_0^\infty(\mathcal{M})$ satisfies $f \equiv 1$ on $\text{supp}(\varphi_0)$.

Under these hypotheses, the relative action depends only on the field perturbation φ_0 and not on the cutoff function f . Note that $\delta S(\varphi_0)[g, \varphi] \in \mathcal{F}(M, \mathcal{L})$ with the reference metric staying unchanged, $g_{\delta S} = g$, as the terms quadratic in $\partial_a \varphi$ coming from the kinetic part cancel, and those linear in $\partial_a \varphi$ may be integrated by parts. The same argument shows that the shifted functional $\varphi \mapsto F[\varphi + \varphi_0]$ belongs to $\mathcal{F}(M, \mathcal{L})$ with the same γ^{ab} . These closure properties are what permit the dynamics to be expressed within the algebra itself [BF20a]. Then, we can define the dynamical algebra as follows.

Definition 2.1.10. Given a Lagrange density $\mathcal{L}$ on M , we define the dynamical algebra $\mathcal{A}_M^{(\mathcal{L})}$ as the algebra generated by a unit $\mathbf{1}$ together with operators $U(F)$ and their adjoints, for each $F \in \mathcal{F}(M, \mathcal{L})$, subject to

- i. (unitarity) $U(F)^* = U(F)^{-1}$ for every $F \in \mathcal{F}(M, \mathcal{L})$;
- ii. (normalisation) $U(c) = e^{ic} \mathbf{1}$ for constant functionals $c[\varphi] = c$, $c \in \mathbb{R}$;
- iii. (dynamics) $U(F) = U(F[\cdot + \varphi_0] + \delta S(\varphi_0))$ for every $F \in \mathcal{F}(M, \mathcal{L})$ and every $\varphi_0 \in C_0^\infty(\mathcal{M}, \mathbb{R})$;
- iv. (causal factorization) whenever $F_1 + F_2 + F_3$, $F_1 + F_3$ and $F_2 + F_3$ all lie in $\mathcal{F}(M, \mathcal{L})$ and $\text{supp}(F_1)$ does not intersect $J_{(M, g_{F_3})}^-(\text{supp}(F_2))$,

$$U(F_1 + F_3 + F_2) = U(F_1 + F_3) U(F_3)^{-1} U(F_3 + F_2).$$

The interpretation of the properties required in Definition 2.1.10 goes as follows.

Regarding point i., reading unitaries as operations performed on the system is the classic interpretive stance of quantum mechanics. In this setting, a change of the Lagrangian is an intervention that alters the dynamics, and it is therefore represented by a unitary. It is argued in [BF20b] that taking operations as the starting point, together with the fact that they can be ordered in time, already

forces the algebra to be non-commutative, with the particular form of the commutation relations being fixed afterwards by the Lagrangian. A general element of $\mathcal{A}_M^{(\mathcal{L})}$ is a finite linear combination of products $U(F_1)^{s_1} \cdots U(F_N)^{s_N}$ with $s_j \in \{\pm 1\}$, so that each term is a multiple of a unitary. This yields a $*$ -algebra, and setting $\|A\| := \sup_{\omega} \|\pi_{\omega}(A)\|$ over states ω of the dynamical algebra, the completion in this norm gives a C^* -algebra [BF20a].

Point *ii.* works as a normalization, even without assuming it, point *iv.* already implies that $c \mapsto U(c)$ is a homomorphism from $(\mathbb{R}, +)$ into the unitaries of the centre of $\mathcal{A}_M^{(\mathcal{L})}$.

Point *iii.* is an integrated form of the Schwinger-Dyson equation from perturbative QFT, in this sense the classical field equation enters the algebra. Note that in [BF20a] this identity is not postulated but derived, as within algebraic perturbation theory the Schwinger-Dyson equation is imposed as a renormalisation condition and then integrated, yielding our relation. Note however that *iii.* does not determine the dynamics completely, it fixes $U(F)$ for functionals at most linear in φ , and the remaining freedom is the subject of the time-slice axiom, cf. [Bru+23].

Point *iv.* (causal factorization) expresses time ordering, but with respect to the deformed metric g_{F_3} rather than the reference metric. This dependence is unavoidable once kinetic perturbations are admitted, since these alter the causal structure itself, cf. [BF21].⁴ For $F_3 = 0$ the relation collapses to $U(F_1 + F_2) = U(F_1)U(F_2)$ whenever $\text{supp}(F_1)$ is later than $\text{supp}(F_2)$ in g . In particular, spacelike separated functionals give commuting $U(F_1)$ and $U(F_2)$, this is an expression of Einstein causality. The product $U(F_1 + F_2)$ then behaves like the time-ordered exponential of perturbation theory, whose identities indeed motivate the axiom. Note also that points *iii.* and *iv.* are what survives of the Feynman path integral once one retains only the invariance of the formal measure under compactly supported deformations of the orbits and the time ordering built into the scattering operators, cf. [BF19].

Finally, the dependence of the construction on the choice of Lagrangian is weaker than one might expect. If $\mathcal{L}'$ is a second Lagrange density with the same reference metric, then $\mathcal{F}(M, \mathcal{L}') = \mathcal{F}(M, \mathcal{L})$. Then, setting $H[\varphi] := \int_{\mathcal{M}} (\mathcal{L}'[g, \varphi] - \mathcal{L}[g, \varphi])$ we have that the operators $U_H(F) := U(H)^{-1}U(H+F)$, defined for all $F, H \in \mathcal{F}(M, \mathcal{L})$ such that $F + H \in \mathcal{F}(M, \mathcal{L})$, satisfy the defining relations of $\mathcal{A}_M^{(\mathcal{L}')}$. Since $U(F)$ can be recovered as $U_H(-H)^{-1}U_H(-H+F)$, the two algebras are isomorphic. This is the local interaction picture of [BF20a], where it is shown further that the residual dependence on the cutoff is only given by internal unitary operators and that the local isomorphisms can be patched into a global embedding, so the physical content of a theory resides not in the algebra but in the assignment of subalgebras to regions. Note that the isomorphism fails if the difference of the Lagrange densities is not compactly supported, or if the kinetic term is modified, since in either case $\mathcal{F}(M, \mathcal{L}') \neq \mathcal{F}(M, \mathcal{L})$. In the first case the argument can however still be applied locally by means of suitable cutoff functions [BF20a].

As an example of this construction, we will briefly discuss the case of the free scalar field whose details we have presented in Section 2.1.1, whose Lagrange density will be

$$\mathcal{L}_{\text{fsf}}[g, \varphi] = \frac{1}{2}(g^{ab}\partial_a\varphi\partial_b\varphi + m^2\varphi^2 + \xi R\varphi^2) \text{dvol}_g \quad (2.1.19)$$

To build the dynamical algebra $\mathcal{A}_M^{(\mathcal{L}_{\text{fsf}})}$, we consider functionals of the simple form $F = c + L_f$ with $L_f[\varphi] = \int_{\mathcal{M}} f\varphi \text{dvol}_g$. Constants factor out, since $U(L_f + c) = e^{ic}U(L_f)$ by normalisation and causal factorization. Defining the Klein-Gordon operator as $P = -\square + m^2 + \xi R$, we can see that the relative action of the free field is itself of this form, $\delta S_{\text{fsf}}(\varphi_0) = L_{P\varphi_0} + S_{\text{fsf}}(h)[\varphi_0]$, so the

⁴Note that this is discussed in [BF21] but not in [BF20a].

dynamical relation gives $U(\delta S_{\text{fsf}}(\varphi_0)) = \mathbb{1}$ and hence

$$U(L_{P\varphi_0}) = e^{-iS_{\text{fsf}}(h)[\varphi_0]} \mathbb{1}.$$

Combining this with a decomposition $f = f_+ + P\varphi_+$, we can see that the support of f may be translated to that of f_+ at the cost of an explicit phase, this makes causal factorization applicable. Choosing f_+ to the future of a compact set containing the support of F , one obtains $U(L_f)U(F) = U(L_f + F[\cdot + E^+f])$ and symmetrically $U(F)U(L_f) = U(L_f + F[\cdot + E^-f])$, from which $U(L_f)U(F) = U(F[\cdot + Ef])U(L_f)$.

Then, we may define the Weyl operators as $W(f) := e^{\frac{i}{2}\langle f, E^-f \rangle} U(L_f)$ for $f \in C_0^\infty(M, \mathbb{R})$. Then

$$W(h)W(f) = e^{-\frac{i}{2}\langle h, Ef \rangle} W(f+h) = e^{-i\langle h, Ef \rangle} W(f)W(h),$$

and in particular $W(0) = \mathbb{1}$ and $W(-f) = W(f)^{-1} = W(f)^*$. Specialising this to $F = L_h$ gives $U(L_h)U(L_f) = e^{i\langle h, E^-f \rangle} U(L_{f+h})$, in which the phase disappears when the supports are causally ordered, as time ordering requires. The symmetrised choice of phase in the definition of W , or equivalently the replacement of E^- by the Dirac propagator $E_D = \frac{1}{2}(E^+ + E^-)$, trades this asymmetry for a relation that is antisymmetric under reversal of the time orientation.

Remark. These are the same Weyl relations (1.3.1) which arise if $W(f)$ is interpreted as the exponential of a smeared field satisfying the canonical commutation relations, cf. Section 1.3 and Appendix A. Here, they have been recovered without having been assumed. Indeed, the algebra was defined by two relations abstracted from perturbation theory, and the commutation relations of the free field are a consequence rather than an input [BF20a]. The same computation carried out in Minkowski space is what establishes that the dynamical algebra is non-trivial [BF20a], for perturbations at most quadratic in the field it is known in addition that these operators admit Fock space representations, although the argument is cohomological rather than constructive [BF21].

2.2 Some general properties of QFTs

A standard result in QFT which we have not up to this point discussed is the Reeh-Schlieder theorem. We shall start with a general formulation. Recall from Section 1.2 that, if we have a complex Hilbert space $\mathcal{H}$ and a von Neumann algebra $\mathcal{A}$ acting on it, a vector $\xi \in \mathcal{H}$ is cyclic for $\mathcal{A}$ if $\mathcal{A}\xi$ is dense in $\mathcal{H}$. This means that, given any cyclic vector ξ , we can approximate arbitrarily well in norm any element of $\mathcal{H}$ with $A\xi$, with some $A \in \mathcal{A}$. In the context of AQFT, considering a spacetime $M = (\mathcal{M}, g) \in \text{Obj}(\mathfrak{Loc})$ and relatively compact subsets $\mathcal{O} \in \mathcal{K}(M)$, we have local algebras $\mathcal{A}(\mathcal{O})$ and the C^* -inductive limit $\mathcal{A} = \cup \mathcal{A}(\mathcal{O})$.

Let's start by considering the Minkowski spacetime $M = (\mathbb{R}^{d+1}, \eta)$. In this case, the Haag-Kastler axioms require the existence of the vacuum state ω_0 , which is invariant under the automorphisms that implement the Poincaré group and yields a positive energy representation, meaning it satisfies the 'spectrum condition', i.e. the joint spectrum of the spacetime translation generators is restricted to the closed forward light cone. Through its GNS-representation $(\mathcal{H}_0, \pi_0, \Omega_0)$, we can consider a local net of von Neumann algebras $\pi_0(\mathcal{A}(\mathcal{O}))''$ acting on $\mathcal{H}_0$, which will still satisfy the axioms. From the GNS-construction, Ω_0 is cyclic for π_0 , so $\pi_0(\mathcal{A})\Omega_0$ is dense in $\mathcal{H}_0$. This may not look surprising, as $\mathcal{A}$ comes from the union of all local algebras. However, the same generally holds for any local algebra. We say that the vacuum representation π_0 of a net of local algebras $\mathcal{A}(\mathcal{O})$ satisfies *weak additivity* if

$$\mathcal{B}(\mathcal{H}_0) = \left(\bigcup_{x \in \mathbb{R}^{d+1}} \pi_0(\mathcal{A}(\mathcal{O} + x)) \right)'' , \quad (2.2.1)$$

for any causally complete region $\mathcal{O}$. (This is expected to be a general property, it is satisfied by all known models.) Then, we have the following standard result, cf. [RS61], [Ara99, Thm. 4.14].

Theorem 2.2.1 (Reeh-Schlieder). *For any causally complete region $\mathcal{O}$ and a net of local algebras $\mathcal{A}(\mathcal{O})$ which satisfies weak additivity, we have that the vacuum vector Ω_0 is cyclic for $\pi_0(\mathcal{A}(\mathcal{O}))$ and it is separating for $\pi_0(\mathcal{A}(\mathcal{O}))''$.*

Note that this is also true for any finite-energy vector, in place of the vacuum [HS18, Thm. 1]. More generally, the Reeh-Schlieder Theorem can be formulated for states on globally hyperbolic spacetimes under additional assumptions on the state. For example, considering the Klein-Gordon field, states are required to satisfy an analytic microlocal spectrum condition which is equivalent to the Hadamard condition of Section 2.1.2, cf. [SVW02], this further highlights the role of Hadamard states as ‘generalizations’ of the Minkowski vacuum. More generally, one may define Reeh-Schlieder states (on generic spacetimes) as states satisfying the property. While such states (algebraically) always exist on any globally hyperbolic spacetime, it is not guaranteed that they will be physically reasonable and the property may have to be weakened [San09].

Then, talking about ‘localized states’ in QFT is a rather tricky business, as for any state vector ψ , we can always find an operator $A \in \pi_0(\mathcal{A}(\mathcal{O}))$ which, applied to any finite-energy vector, approximates ψ arbitrarily well, no matter the region $\mathcal{O}$. In this sense, there will always exist long-range correlations between local observables w.r.t. the cyclic vector which yield this result. The question may then become whether it is reasonable to consider states for which the length of vectors $A\Omega_0$, $A \in \mathcal{A}(\mathcal{O})$, decreases fast enough with increasing delocalization, or that have appropriately damped energy, so as to suppress long-range correlations. Intuitively, we could say that the set of states localized in a region $\mathcal{O}$, with energy below a certain value E , is ‘essentially finite-dimensional’, in the sense that its extension is limited in energy and volume. More rigorously, this is formulated as *nuclearity conditions*, of which we will briefly discuss the one due to Buchholz and Wichmann [BW86].

First, given two Banach spaces X, Y and a linear operator $T : X \rightarrow Y$, we define the *1-nuclear norm* of T as

$$\|T\|_1 = \inf \sum_i \|y_i\| \|\varphi_i\|, \quad (2.2.2)$$

where the infimum is taken over all the possible realizations of T as a norm-convergent sum $T(\cdot) = \sum_i y_i \varphi_i(\cdot)$, with $\varphi_i \in X^*$ and $y_i \in Y$. If this is not possible, $\|T\|_1 = \infty$. We say that T is *nuclear* if $\|T\|_1 < \infty$. If X and Y are Hilbert spaces, then $\|T\|_1 = \text{tr}|T|$.

This allows us to formulate the *Buchholz-Wichmann (BW) nuclearity* as an additional assumption to add to the standard Haag-Kastler axioms. Let $\mathcal{O}_r$ be a standard double cone of radius $r > 0$ and let $\Theta_{\beta,r}$ be the map $\Theta_{\beta,r} : \mathcal{A}(\mathcal{O}_r) \mapsto \mathcal{H}_0$, $A \mapsto e^{-\beta H} \pi_0(A) \Omega_0$, where $\beta > 0$ and H is the Hamiltonian. Then, we assume that there exist positive constants $n > 0$ and $c = c(r) > 0$ such that

$$\|\Theta_{\beta,r}\|_1 \leq e^{\left(\frac{c}{\beta}\right)^n}. \quad (2.2.3)$$

The vectors $e^{-\beta H} \pi_0(A) \Omega_0$, with $\|A\| \leq 1$, form a set (an ellipsoid) in the Hilbert space $\mathcal{H}_0$ and $\|\Theta_{\beta,r}\|_1$ quantifies the extension of this set. Vectors of this type are localized in $\mathcal{O}_r$ and have their energy exponentially damped by the factor β^{-1} . In d spatial dimensions, we expect to have $c(r) \propto r$ and $n = d$, cf. [HS18, Sec. 2.3].

BW-nuclearity implies a notion of statistical independence between local algebras, which is the *split property*. Consider two spacelike separated regions $\mathcal{O}_A, \mathcal{O}_B$, then we may redefine their respective local algebras as the von Neumann algebras $\mathcal{A} = \pi_0(\mathcal{A}(\mathcal{O}_A))''$, $\mathcal{B} = \pi_0(\mathcal{A}(\mathcal{O}_B))''$. By locality,

these will commute, but if we assume that ‘they do not touch’, i.e. $\mathcal{O}_A$ is contained in a larger region $\tilde{\mathcal{O}}_A$ which is spacelike to $\mathcal{O}_B$ (we will say that $\mathcal{O}_A$ and $\mathcal{O}_B$ are *strictly* spacelike separated, see Figure 2.1), they will also be *statistically independent*. Two normal states φ_A, φ_B respectively on $\mathcal{A}, \mathcal{B}$ will be statistically independent if there exists an extension of the two states to a normal state φ on $\mathcal{A} \vee \mathcal{B}$ such that

$$\varphi(A \otimes B) = \varphi_A(A) \varphi_B(B) , \quad (2.2.4)$$

with $A \in \mathcal{A}, B \in \mathcal{B}$. Physically speaking, this means that there are no correlations between results of measurements of observables relative to $\mathcal{O}_A$ and $\mathcal{O}_B$ in the state φ .

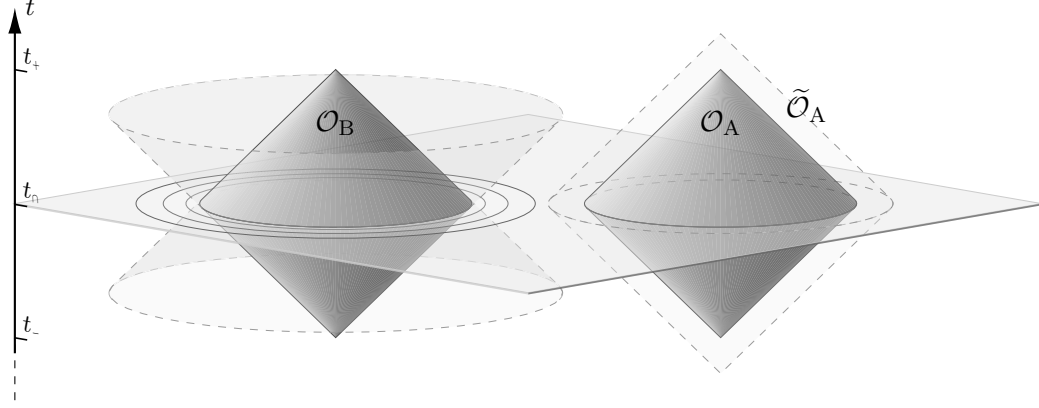


Figure 2.1: ‘Strictly’ spacelike double cones in two spatial dimensions.

To understand statistical independence of von Neumann algebras, we shall start with a weaker condition, which is that if $AB = 0$, then either $A = 0$ or $B = 0$, with $A \in \mathcal{A}, B \in \mathcal{B}$. (This is referred to as *algebraic independence*.) Note that this is always the case if $\mathcal{A}$ and $\mathcal{B}$ are factors [Haa12, Lemma 2.1.10]. This is often the case, as all known AQFTs present type III factors as local algebras $\mathcal{A}(\mathcal{O})$, for relatively compact regions $\mathcal{O}$ (this holds under general assumptions, cf. [BDF87]). Then we may consider the algebraic tensor product $\mathcal{C}$ of $\mathcal{A}, \mathcal{B}$, i.e. the algebra formed by finite linear combinations of products AB , with $A \in \mathcal{A}, B \in \mathcal{B}$, which will admit a representation $\pi : \mathcal{C} \rightarrow \mathcal{B}(\mathcal{H})$ defined as $\pi(AB) = AB$. However, if algebraic independence holds, we can also define a representation $\pi_p : \mathcal{C} \rightarrow \mathcal{B}(\mathcal{H} \otimes \mathcal{H})$ such that $\pi_p(AB) = A \otimes B$, where A acts on the first copy of $\mathcal{H}$ and B on the second one. This leads to the definition of a *standard split inclusion* by Doplicher and Longo [DL84], cf. also [Haa12, Prop. V.5.2.1].

Proposition 2.2.2. *Let $\mathcal{H}$ be a Hilbert space and $\mathcal{A}_1, \mathcal{A}_2 \subset \mathcal{B}(\mathcal{H})$ factors such that $\mathcal{A}_1 \subset \mathcal{A}_2$. Let $\xi \in \mathcal{H}$ be a standard (cyclic and separating) vector for $\mathcal{A}_1, \mathcal{A}_2$, and $\mathcal{A}_2 \wedge \mathcal{A}'_1$. Then, the following properties are equivalent:*

- i. $\mathcal{A}_1$ and $\mathcal{A}'_2$ are statistically independent;
- ii. there exists a vector $\chi \in \mathcal{H}$, which is cyclic and separating for $\mathcal{A}_1 \vee \mathcal{A}'_2$ such that

$$\langle \chi, A_1 A'_2 \chi \rangle = \langle \xi, A_1 \xi \rangle \langle \xi, A'_2 \xi \rangle , \quad (2.2.5)$$

with $A_1 \in \mathcal{A}_1, A'_2 \in \mathcal{A}'_2$;

- iii. there exists a unitary operator $U : \mathcal{H} \rightarrow \mathcal{H} \otimes \mathcal{H}$ such that

$$U \pi(A_1 A'_2) U^* = \pi_p(A_1 A'_2) , \quad (2.2.6)$$

with $A_1 \in \mathcal{A}_1, A'_2 \in \mathcal{A}'_2$;

iv. there exists an ‘interpolating’ type I factor $\mathcal{N}$ such that

$$\mathcal{A}_1 \subset \mathcal{N} \subset \mathcal{A}_2. \quad (2.2.7)$$

A triple $(\mathcal{A}_1, \mathcal{A}_2, \xi)$, with these properties defines a *standard split inclusion*; ξ is a *standard vector for the split* as it is cyclic and separating for $\mathcal{A}_1$, $\mathcal{A}'_2$ and $\mathcal{A}_1 \vee \mathcal{A}'_2$. The unitary operator U defines the unitary equivalence relations

$$\begin{cases} \mathcal{A}_1 \otimes \mathbb{1} = U \mathcal{A}_1 U^*, \\ \mathbb{1} \otimes \mathcal{A}'_2 = U \mathcal{A}'_2 U^*, \end{cases} \quad (2.2.8)$$

and, observing that $\mathcal{B}(\mathcal{H}) \otimes \mathbb{1}$ is a type I factor on $\mathcal{H} \otimes \mathcal{H}$ and that $\mathbb{1} \otimes \mathcal{B}(\mathcal{H})$ is its commutant,

$$\begin{cases} \mathcal{B}(\mathcal{H}) \otimes \mathbb{1} = U \mathcal{N} U^*, \\ \mathbb{1} \otimes \mathcal{B}(\mathcal{H}) = U \mathcal{N}' U^*. \end{cases} \quad (2.2.9)$$

This leads us to say that the algebras are statistically independent if and only if

$$\mathcal{A}_1 \vee \mathcal{A}_2 \cong \mathcal{A}_1 \otimes \mathcal{A}_2, \quad (2.2.10)$$

where we may interpret the tensor product of von Neumann algebras $\mathcal{A}_1 \otimes \mathcal{A}_2$ as $(\mathcal{A}_1 \otimes \mathbb{1}) \vee (\mathbb{1} \otimes \mathcal{A}_2)$ on $\mathcal{H} \otimes \mathcal{H}$.⁵ As $\mathcal{N}$ is a factor, $\mathcal{B}(\mathcal{H}) \cong \mathcal{N} \vee \mathcal{N}'$, and we also get the factorization

$$\mathcal{B}(\mathcal{H}) \cong \mathcal{N} \vee \mathcal{N}' \cong \mathcal{B}(\mathcal{H}) \otimes \mathcal{B}(\mathcal{H}), \quad (2.2.11)$$

so we can see $\mathcal{A}_1$ as a subalgebra of the first copy of $\mathcal{B}(\mathcal{H})$ and $\mathcal{A}_2$ of the second one.

Remark. Note that in the terminology of [DL84], we say that ξ is a *semi-standard*, resp. *standard*, vector for the inclusion $\mathcal{A}_1 \subset \mathcal{A}_2$ if it is a standard vector for $\mathcal{A}_2 \wedge \mathcal{A}'_1$, resp. for $\mathcal{A}_1$, $\mathcal{A}_2$, and $\mathcal{A}_2 \wedge \mathcal{A}'_1$.⁶ A state ω of $\mathcal{A}_2$ is called a semi-standard, resp. standard, state for the inclusion if it is normal, has central cover⁷ $\mathbb{1}$ and, in its GNS-representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$, yields a semi-standard, resp. standard, vector Ω_ω for the inclusion $\pi_\omega(\mathcal{A}_1) \subset \pi_\omega(\mathcal{A}_2)$. Correspondingly, a semi-standard, resp. standard, inclusion is a triple $(\mathcal{A}_1, \mathcal{A}_2, \omega)$ where ω is a semi-standard, resp. standard, state for the inclusion $\mathcal{A}_1 \subset \mathcal{A}_2$. So, we recover a triple $(\pi_\omega(\mathcal{A}_1), \pi_\omega(\mathcal{A}_2), \Omega_\omega)$ through the GNS-representation of ω , where we may neglect to indicate the representation. Then, these inclusions are called *split* if point iv. of Proposition 2.2.2 holds [DL84, Def. 1.4].

Going back to local algebras, consider the vacuum Hilbert space $\mathcal{H}_0$ and two strictly spacelike regions $\mathcal{O}_A, \mathcal{O}_B$. As for Proposition 2.2.2, if the local algebras $\mathcal{A} = \mathcal{A}(\mathcal{O}_A)$, $\mathcal{B} = \mathcal{A}(\mathcal{O}_B)$ are factors, we have that $\mathcal{A}$ and $\mathcal{B}'$ are split, as we have that $\mathcal{A} \subset \mathcal{B}'$ and the vacuum is standard for the required algebras by the Reeh-Schlieder Theorem 2.2.1. Then, there will exist a type I factor $\mathcal{N}$ such that $\mathcal{A} \subset \mathcal{N} \subset \mathcal{B}'$ and thus

$$\begin{cases} \mathcal{A} \vee \mathcal{B} \cong \mathcal{A} \otimes \mathcal{B} \\ \mathcal{B}(\mathcal{H}_0) \cong \mathcal{N} \vee \mathcal{N}' \cong \mathcal{B}(\mathcal{H}_0) \otimes \mathcal{B}(\mathcal{H}_0) \end{cases} \implies \mathcal{A} \otimes \mathcal{B} \subset \mathcal{B}(\mathcal{H}_0) \otimes \mathcal{B}(\mathcal{H}_0). \quad (2.2.12)$$

Note that if the split property holds and an interpolating type I factor $\mathcal{N}$ exists, it will not be unique, in fact, an infinite number of them will exist. Suppose to have two double cones $\mathcal{O}_A, \mathcal{O}_B$ such that $\overline{\mathcal{O}_A} \subset \mathcal{O}_B$. Then, for their corresponding local algebras the split property holds,

$$\mathcal{A}(\mathcal{O}_A) \subset \mathcal{N} \subset \mathcal{A}(\mathcal{O}_B). \quad (2.2.13)$$

⁵Here, the tensor product $\mathcal{A}_1 \otimes \mathcal{A}_2$ will be the *spatial tensor product*, i.e. the von Neumann-algebraic completion of the algebraic tensor product in the representation on $\mathcal{H} \otimes \mathcal{H}$ obtained through this construction.

⁶Also note that Doplicher and Longo refer to inclusions of von Neumann algebras as W^* -inclusions.

⁷i.e. the smallest projection P in the centre of the algebra such that $\omega(P) = 1$.

Also, we have that

$$\overline{\mathcal{O}_A} \subset \tilde{\mathcal{O}} \subset \overline{\tilde{\mathcal{O}}} \subset \mathcal{O}_B, \quad (2.2.14)$$

where $\tilde{\mathcal{O}}$ is another region strictly included in $\mathcal{O}_B$. Then, the split property will also hold for both pairs $\mathcal{O}_A, \tilde{\mathcal{O}}$ and $\tilde{\mathcal{O}}, \mathcal{O}_B$, so there will exist two type I factors $\mathcal{N}_1, \mathcal{N}_2$ such that

$$\mathcal{A}(\mathcal{O}_A) \subset \mathcal{N}_1 \subset \mathcal{A}(\tilde{\mathcal{O}}) \subset \mathcal{N}_2 \subset \mathcal{A}(\mathcal{O}_B), \quad (2.2.15)$$

by isotony. Both $\mathcal{N}_1$ and $\mathcal{N}_2$ are valid interpolating factors for the pair $\mathcal{O}_A, \mathcal{O}_B$, but generally $\mathcal{N}_1 \neq \mathcal{N}_2$. If e.g. $\mathcal{N}_1$ was unique and thus independent from the choice of $\tilde{\mathcal{O}}$, we would have

$$\mathcal{A}(\mathcal{O}_A) \subset \mathcal{N}_1 \subset \bigcap_{\overline{\mathcal{O}_A} \subset \tilde{\mathcal{O}}} \mathcal{A}(\tilde{\mathcal{O}}) = \mathcal{A}(\mathcal{O}_A), \quad (2.2.16)$$

so $\mathcal{A}(\mathcal{O}_A) = \mathcal{N}_1$, would be a type I factor, the same would hold for $\mathcal{N}_2$ and $\mathcal{A}(\mathcal{O}_B)$. As this is not the case in QFT, we are left with arbitrariness in the choice of $\mathcal{N}$.

Remark. Proposition 2.2.2 will not hold if the two regions under consideration ‘touch’, i.e. if their boundaries intersect. In this case, an interpolating type I factor does not exist and the two local algebras cannot be statistically independent [HS18, Thm. 2].

While the choice of the interpolating type I factor $\mathcal{N}$ may not be generally unique, there exists a ‘canonical’ interpolating type I factor, defined through the following construction, cf. the proof of [DL84, Thm 2.1]. Denote by $\Lambda = (\mathcal{A}, \mathcal{B}, \Omega)$ a (semi-standard) inclusion, where Ω is the GNS-vector of some state ω . We want to construct a specific choice of the unitary U implementing the split as for Proposition 2.2.2. Let E_1 be the orthogonal projection onto the closure of $\mathcal{A}\Omega$ and E'_2 the one onto the closure of $\mathcal{B}'\Omega$. Note that $E_1 \in \mathcal{A}'$ and $E'_2 \in \mathcal{B}$. Then, let $\mathcal{H}_1$, resp. $\mathcal{H}'_2$, be the range of E_1 , resp. E'_2 . As E_1, E'_2 commute with their respective algebras, we may define $\mathcal{A}_{E_1}$ as the von Neumann algebra $\mathcal{A}$ restricted to act only on $\mathcal{H}_1$, and $\mathcal{B}'_{E'_2}$, as the von Neumann algebra $\mathcal{B}'$ restricted to act only on $\mathcal{H}'_2$. Similarly, for any $A \in \mathcal{A}$ and $B' \in \mathcal{B}'$, we define $A_{E_1} := E_1 A E_1 \in \mathcal{A}_{E_1}$ and $B'_{E'_2} := E'_2 B' E'_2 \in \mathcal{B}'_{E'_2}$. Then, as Λ splits, there will exist a $*$ -isomorphism

$$\varphi_\Lambda : \mathcal{A} \vee \mathcal{B}' \mapsto \mathcal{A}_{E_1} \otimes \mathcal{B}'_{E'_2} \subset \mathcal{B}(\mathcal{H}_1) \otimes \mathcal{B}(\mathcal{H}'_2),$$

such that $\varphi_\Lambda(AB') = A_{E_1} \otimes B'_{E'_2}$, for $A \in \mathcal{A}$ and $B' \in \mathcal{B}'$. Now, as Ω is standard for $\mathcal{A}_{E_1}$ and $\mathcal{B}'_{E'_2}$, we get that $\Omega \otimes \Omega \in \mathcal{H}_1 \otimes \mathcal{H}'_2$ is standard for $\mathcal{A}_{E_1} \otimes \mathcal{B}'_{E'_2}$. Thanks to Theorem 1.1.6, this allows to implement the $*$ -isomorphism φ_Λ with a unitary operator $U_\Lambda : \mathcal{H} \mapsto \mathcal{H}_1 \otimes \mathcal{H}'_2$, where $\mathcal{H}$ is the GNS-Hilbert space associated to Ω , as $U_\Lambda A B' U_\Lambda^* = A_{E_1} \otimes B'_{E'_2}$ for $A \in \mathcal{A}$ and $B' \in \mathcal{B}'$. Then, we may fix U_Λ by requiring that it maps the standard cone⁸ of the first algebra onto the standard cone of the second,

$$U_\Lambda P_\Omega^\natural(\mathcal{A}' \wedge \mathcal{B}) = P_{\Omega \otimes \Omega}^\natural(\mathcal{A}'_{E_1} \otimes \mathcal{B}_{E'_2}),$$

where $\mathcal{A}'_{E_1}$ and $\mathcal{B}_{E'_2}$ are restricted algebras defined in analogy as the ones before. Note that this makes the choice of U_Λ unique, cf. [DL84, App. A.4]. The unitary will satisfy the relations

$$\begin{aligned} U_\Lambda \mathcal{A} U_\Lambda^* &= \mathcal{A}_{E_1} \otimes \mathbb{1}_{\mathcal{H}'_2}, \\ U_\Lambda \mathcal{B}' U_\Lambda^* &= \mathbb{1}_{\mathcal{H}_1} \otimes \mathcal{B}'_{E'_2}, \\ U_\Lambda \mathcal{B} U_\Lambda^* &= (U_\Lambda \mathcal{B}' U_\Lambda^*)' = \mathcal{B}(\mathcal{H}_1) \otimes \mathcal{B}_{E'_2}. \end{aligned}$$

⁸Given a von Neumann algebra $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ and $\Omega \in \mathcal{H}$ standard for $\mathcal{A}$, its *standard cone* $P_\Omega^\natural(\mathcal{A}) \subset \mathcal{H}$ is defined as the norm closure of $\{\Delta^{1/4} A \Omega \mid A \in \mathcal{A}\}$, w.r.t. the modular operator Δ .

Then, we define the *canonical interpolating type I factor* $\mathcal{N}_\Lambda$ for the semi-standard split inclusion Λ

$$\mathcal{N}_\Lambda := U_\Lambda^* \left(\mathcal{B}(\mathcal{H}_1) \otimes \mathbb{1}_{\mathcal{H}'_2} \right) U_\Lambda, \quad (2.2.17)$$

which will indeed be a type I factor such that $\mathcal{A} \subset \mathcal{N}_\Lambda \subset \mathcal{B}$, by the previous construction.

If Λ, Λ' are two semi-standard inclusions, an isomorphism $\Phi : \Lambda \mapsto \Lambda'$ is a $*$ -isomorphism of von Neumann algebras φ of $\mathcal{A}_{2,\Lambda}$ onto $\mathcal{A}_{2,\Lambda'}$ such that $\varphi(\mathcal{A}_{1,\Lambda}) = \mathcal{A}_{1,\Lambda'}$ and $\omega_\Lambda = \omega_{\Lambda'} \circ \varphi$. Then, the canonical interpolating type I factors $\mathcal{N}_\Lambda$ relative to Λ , as for (2.2.17), will be functorially associated to Λ , in the sense that if $\Phi : \Lambda \mapsto \Lambda'$ is an isomorphism of semi-standard split inclusions, then $\Phi(\mathcal{N}_\Lambda) = \mathcal{N}_{\Lambda'}$, where $\mathcal{N}_{\Lambda'}$ is the canonical factor of Λ' [DL84, Thm. 2.1]. We refer to [DL84] for other properties of $\mathcal{N}_\Lambda$.

In particular, if $\mathcal{A}_1 = \mathcal{A}_{1,\Lambda}$ and $\mathcal{A}_2 = \mathcal{A}_{2,\Lambda}$ are factors, there exists a more explicit expression for $\mathcal{N}_\Lambda$ obtained through modular theory, given by the following theorem, cf. [DL84, Thm. 4.1].

Theorem 2.2.3. *Let $\Lambda = (\mathcal{A}_1, \mathcal{A}_2, \Omega)$ be a semi-standard split inclusion and let J be the modular conjugation of $\mathcal{A}'_1 \wedge \mathcal{A}_2$ w.r.t. Ω . If both $\mathcal{A}_1$ and $\mathcal{A}_2$ are factors, then*

$$\mathcal{N}_\Lambda = \mathcal{A}_1 \vee J\mathcal{A}_1J = \mathcal{A}_2 \wedge J\mathcal{A}_2J, \quad (2.2.18)$$

and $\mathcal{N}_\Lambda$ is the only von Neumann algebra between $\mathcal{A}_1$ and $\mathcal{A}_2$ which is globally invariant under the action implemented by J .

Physical applications of the canonical interpolating type I factor are for example found in computing entanglement entropies, see e.g. [LX18; LX21; OT18].

To conclude this section, we shall discuss the implied link between the BW-nuclearity condition and the split property. The argument revolves around the relationship between nuclear maps and modular data explored in [BDF87; BDL90a; BDL90b], we will follow [Haa12, Sec. V.5.2] for this exposition. Consider the strict inclusion of two standard double cones $\mathcal{O}_1 \subset \mathcal{O}_2$ with radii $r_1 < r_2$, with $\delta := r_2 - r_1 > 0$. Then, consider a continuous unitary representation $t \mapsto U(t)$ of $\mathbb{R}$ implementing the time translations on Minkowski space, in the sense that for some region $\mathcal{O}$, we have $U(t)\mathcal{A}(\mathcal{O})U(t)^* \subset \mathcal{A}(\mathcal{O} + te)$, where e is a vector fixing the time direction and let the Hamiltonian H be the generator of the time translations $U(t)$. Then, we get the following result, cf. [BDF87, Lemma 2.3].

Lemma 2.2.4. *Let $A \in \mathcal{A}(\mathcal{O}_1)$, $B' \in \mathcal{A}(\mathcal{O}_2)'$ be such that $[U(t)AU(t)^*, B'] = 0$ for $|t| < \delta$. Then, there exists some continuous real-valued function $f(x)$, $x \in \mathbb{R}$, which will decrease almost exponentially, i.e.*

$$\sup_x |f(x)|e^{|x|^k} < \infty$$

for every $0 < k < 1$, such that

$$\langle \Omega_0, AB'\Omega_0 \rangle = \langle \Omega_0, Af(H)B'\Omega_0 \rangle + \langle \Omega_0 B'f(H)A\Omega_0 \rangle. \quad (2.2.19)$$

This lemma allows to prove that the BW-nuclearity condition 2.2.3 implies the split property.

Theorem 2.2.5. *Let $\mathcal{O}_1 \subset \mathcal{O}_2$ be two standard double cones with radii $r_1 < r_2$, and let for $r > 0$ the map $\Theta_{\beta,r} : \mathcal{A}(\mathcal{O}_r) \mapsto \mathcal{H}_0$, $\Theta_{\beta,r}A = e^{-\beta H}\pi_0(A)\Omega_0$, with $A \in \mathcal{A}(\mathcal{O}_r)$, satisfy the BW-nuclearity condition 2.2.3. Then, $\mathcal{A}(\mathcal{O}_1)$ and $\mathcal{A}(\mathcal{O}_2)'$ are split.*

Proof. We will give the main ideas of the proof and refer to [BDF87; BY91] for some of the details. The main point is that Lemma 2.2.4 implies that the nuclearity of the map $\Theta_{\beta,r}$ with the properties required implies the nuclearity of the map $\Theta_f : \mathcal{A}(\mathcal{O}_r) \mapsto \mathcal{H}_0$, $\Theta_f A = f(H)A\Omega_0$, with $A \in \mathcal{A}(\mathcal{O}_r)$, where f satisfies the condition of Lemma 2.2.4. The argument is the following. Consider the spectral projection P_k of H for the interval $[k-1, k]$ and write $\Theta_f = \sum_k \Theta_k$, with $\Theta_k := P_k f(H) e^{\beta H} \Theta_{\beta,r}$. Each Θ_k is nuclear and, with $f_k := \sup_{k-1 \leq x \leq k} |f(x)|$, we get $\|\Theta_k\|_1 \leq f_k \exp(\beta k + (c/\beta)^n)$. As this holds for any $\beta > 0$, for each k we can choose β so as to minimize these exponents. This happens for $\beta = c(n/(ck))^{1/(n+1)}$, which yields $\|\Theta_k\|_1 \leq f_k \exp(c_n(ck)^{n/(n+1)})$, where $c_n := n^{1/(n+1)} + n^{-n/(n+1)} \leq 2$ for $n > 0$. It follows that $\|\Theta_f\|_1 \leq \sum_k \|\Theta_k\|_1 < \infty$. Then, as Θ_f is nuclear, we have $F(H)A\Omega_0 =: \Theta_f A = \sum_i \varphi_i(A) y_i$, $A \in \mathcal{A}(\mathcal{O}_r)$, with $y_i \in \mathcal{H}_0$ and φ_i is a linear form on $\mathcal{A}(\mathcal{O}_r)$ such that $\sum_i \|y_i\| \|\varphi_i\| < \infty$. Now, since Θ_f is a nuclear map from a von Neumann algebra into a Hilbert space, we may choose the linear forms φ_i to be normal linear functionals, i.e. elements of the predual $\mathcal{A}(\mathcal{O}_r)_*$ of the algebra, cf. Theorem 1.1.5. This means that $\langle \Omega_0, B' f(H) A \Omega_0 \rangle = \sum_i \varphi_i(A) \langle \Omega_0, B' y_i \rangle$. Furthermore, utilizing the self-adjointness of $f(H)$ and the fact that $A^* \in \mathcal{A}(\mathcal{O}_r)$, we have $\langle \Omega_0, A f(H) B' \Omega_0 \rangle = \langle f(H) A^* \Omega_0, B' \Omega_0 \rangle = \langle \Theta_f(A^*), B' \Omega_0 \rangle = \sum_i \overline{\varphi_i(A^*)} \langle y_i, B' \Omega_0 \rangle$. Choosing $r = r_1$ and substituting in (2.2.19), this implies that the vacuum state ω_0 is an absolutely convergent sum of normal linear forms that factorize over the algebraic tensor product $\mathcal{C}$ of $\mathcal{A}(\mathcal{O}_1)$ and $\mathcal{A}(\mathcal{O}_2)'$, so ω_0 is normal in the representation π_p , so π and π_p are not disjoint representations. In fact, π and π_p are unitarily equivalent, we refer to [BDF87; BY91] for more details on this fact. Then, point *iii.* of Proposition 2.2.2 holds and the algebras $\mathcal{A}(\mathcal{O}_1)$ and $\mathcal{A}(\mathcal{O}_2)'$ are split. $\square$

Chapter 3

Energy estimates for functions of modular Hamiltonians

In this chapter, we will present the results in [CS25], which involve relations between the quasi-equivalence conditions for the Gaussian states of Section 1.3.1 and the energy of states constructed as perturbations of a given reference Gaussian state. We should note that the results presented here are sharper than the ones in [CS25], thanks to a refinement in the proof of (3.1.11) in Theorem 3.1.2 (which improved the estimate by a factor $\frac{1}{2}$), which also led to improving (3.1.12) and the corresponding estimates in Corollary 3.1.3 and Theorem 3.2.2.

3.1 Perturbed states and quasi-equivalence

We will start by specializing the general quasi-equivalence conditions for Gaussian states by Araki-Yamagami [AY82] (Theorem 1.3.2) and Longo [Lon22] (Corollary 1.3.4), presented in Section 1.3.1, to a more specific class of states, obtained as perturbations of a suitable reference Gaussian state, and consider the quasi-equivalence of the corresponding Gaussian states. We then supplement these investigations with some explicit estimates that will be useful for our applications in Section 3.2.

We can do so through the following construction. Let (D, σ) be a pre-symplectic space and let μ_0 be a real inner product on D fixing a Gaussian reference state, as for Definition 1.3.1. Hilbert spaces and other constructions from μ_0 as in Section 1.3 will be indicated by a subscript 0. Then, we can consider perturbations μ_δ of μ_0 of the following form:

$$\mu_\delta(f, g) := \mu_0(f, (\mathbb{1} + \delta)g), \quad (3.1.1)$$

where we assume that δ is a self-adjoint operator on $\mathcal{K}_{\mathbb{R},0}$ whose form domain contains D . To ensure that μ_δ is an inner product we require that $\mathbb{1} + \delta > 0$ is strictly positive. We extend δ by complex linearity to $\mathcal{K}_0$, where we note that $\Gamma_0 \delta \Gamma_0 = \delta$.

We want to ensure that the inner product μ_δ on D dominates the pre-symplectic form σ as in (1.3.4). This means, equivalently, that $\mathbb{1} + \delta + \Sigma_0$ defines a Hermitean inner product on $D + iD \subset \mathcal{K}_0$, i.e. $\mathbb{1} + \delta + \Sigma_0 \geq 0$. A sufficient condition for this to hold is $\delta \geq 0$.

In line with our notations in Section 1.3 we let $\mathcal{K}_{\mathbb{R},\delta}$ denote the Hilbert space completion of D in the inner product μ_δ and $\mathcal{K}_\delta$ its complexification. There is a unitary map $V_\delta : \mathcal{K}_\delta \rightarrow \mathcal{K}_0$ defined by $V_\delta f := \sqrt{\mathbb{1} + \delta} f$ for all $f \in D$. If R_δ denotes the polarization operator on $\mathcal{K}_\delta$, then we must have $\sigma(f, g) = \mu_0(f, R_0 g) = \mu_\delta(f, R_\delta g)$ and hence

$$V_\delta R_\delta V_\delta^* = (\mathbb{1} + \delta)^{-\frac{1}{2}} R_0 (\mathbb{1} + \delta)^{-\frac{1}{2}}$$

and similarly

$$V_\delta \Sigma_\delta V_\delta^* = (\mathbb{1} + \delta)^{-\frac{1}{2}} \Sigma_0 (\mathbb{1} + \delta)^{-\frac{1}{2}}. \quad (3.1.2)$$

Note that $V_\delta \Sigma_\delta V_\delta^*$ is self-adjoint and has norm ≤ 1 , because $\mathbb{1} + \delta + \Sigma_0 \geq 0$.

The perturbed state defined by μ_δ has a well-defined modular operator iff $\mathbb{1} + \Sigma_\delta > 0$, which is equivalent to $\mathbb{1} + \delta + \Sigma_0 > 0$. (A sufficient condition for this to hold is $\delta > 0$.) Denoting the unitary map relating $\mathcal{H}_\delta$ and $\mathcal{K}_\delta$ by U_δ , we then have

$$V_\delta U_\delta \Delta_\delta U_\delta^* V_\delta^* = \frac{\mathbb{1} - V_\delta \Sigma_\delta V_\delta^*}{\mathbb{1} + V_\delta \Sigma_\delta V_\delta^*}$$

by (1.3.12) and hence

$$V_\delta U_\delta K_\delta U_\delta^* V_\delta^* = -\log \left(\frac{\mathbb{1} - V_\delta \Sigma_\delta V_\delta^*}{\mathbb{1} + V_\delta \Sigma_\delta V_\delta^*} \right) = 2 \operatorname{artanh} (V_\delta \Sigma_\delta V_\delta^*)$$

by an identity for the inverse hyperbolic tangent.

Now we turn to the question of quasi-equivalence of the two Gaussian states on the Weyl algebra $\mathcal{W}[D, \sigma]$ determined by μ_0 and μ_δ . The general conditions by Araki and Yamagami given in Theorem 1.3.2 can be adapted in terms of our perturbation operator δ . The bounded positive operator linking the two inner products will be $B = \mathbb{1} + \delta$ and the two conditions become the following ones. Firstly, the norms determined by the inner products μ_0 and μ_δ should be equivalent, which means that

$$\mathbb{1} + \delta, (\mathbb{1} + \delta)^{-1} \in \mathcal{B}(\mathcal{K}_0) \quad (3.1.3)$$

must both be in the space $\mathcal{B}(\mathcal{K}_0)$ of bounded operators on $\mathcal{K}_0$. Secondly, the difference

$$\sqrt{\mathbb{1} + \delta + \Sigma_0} - \sqrt{\mathbb{1} + \Sigma_0} \in \mathcal{L}^2(\mathcal{K}_0) \quad (3.1.4)$$

must be in the space $\mathcal{L}^2(\mathcal{K}_0)$ of Hilbert-Schmidt operators on $\mathcal{K}_0$. Note that this implies that

$$\delta = \frac{1}{2} \sum_{\pm} (\sqrt{\mathbb{1} + \delta + \Sigma_0} \mp \sqrt{\mathbb{1} + \Sigma_0}) (\sqrt{\mathbb{1} + \delta + \Sigma_0} \pm \sqrt{\mathbb{1} + \Sigma_0}) \quad (3.1.5)$$

is also Hilbert-Schmidt.

This construction simplifies in the case where the states μ_0 and μ_δ have invertible polarization operators satisfying the additional condition (1.3.11). In this case, we may identify $H_0 := \mathcal{K}_{0, \mathbb{R}}$ as a factorial standard subspace of the one-particle Hilbert space $\mathcal{H}_0$. Following [Lon22], the doubled symplectic space can then be identified as $H_0 + H'_0$ endowed with the inner product $\operatorname{Re}(\cdot, \cdot)_{\mathcal{H}_0}$ and with the symplectic form $\operatorname{Im}(\cdot, \cdot)_{\mathcal{H}_0}$, which extends the symplectic form on H_0 . (This is called the symplectic dilation in [Lon22].) The completion of this doubled symplectic space w.r.t. its inner product is $\mathcal{H}_0$ as a real Hilbert space. Analogous identifications hold for the perturbed state.

Remark. The idea is the following. Consider the direct sum Hilbert space $\hat{H}_0 = H_0 \oplus H_0$. Araki-Yamagami endow this space with the symplectic form $\beta \oplus -\beta$ and inner product given by the matrix

$$M_0 := \begin{pmatrix} \mathbb{1} & \sqrt{\mathbb{1} + R_0^2} \\ \sqrt{\mathbb{1} + R_0^2} & \mathbb{1} \end{pmatrix}.$$

Identifying the second copy of H_0 with H'_0 using J_0 we find for all $h_i \in H_0$ and $k_i \in H'_0$ that $J_0 k_i \in H_0$ and

$$\operatorname{Im}(h_1 + k_1, h_2 + k_2) = \operatorname{Im}(h_1, h_2) + \operatorname{Im}(k_1, k_2) = \operatorname{Im}(h_1, h_2) - \operatorname{Im}(J_0 k_1, J_0 k_2)$$

which reproduces the symplectic form. Using $\mathbb{1} + R_0^2 = \frac{4\Delta_0}{(\mathbb{1} + \Delta_0)^2}$ we also find

$$\begin{aligned} \operatorname{Re}(h_1 + J_0 k_1, M_0(h_2 + J_0 k_2)) &= \operatorname{Re}(h_1, h_2) + \operatorname{Re}(J_0 k_1, J_0 k_2) \\ &\quad + \operatorname{Re}(h_1, \sqrt{\mathbb{1} + R_0^2} J_0 k_2) + \operatorname{Re}(J_0 k_1, \sqrt{\mathbb{1} + R_0^2} h_2). \end{aligned}$$

Note that

$$\begin{aligned} \operatorname{Re}\left(h_1, \sqrt{\mathbb{1} + R_0^2} J_0 k_2\right) &= 2 \operatorname{Re}\left(h_1, \frac{\sqrt{\Delta_0}}{\mathbb{1} + \Delta_0} J_0 k_2\right) \\ &= \operatorname{Re}\left(h_1, \frac{\sqrt{\Delta_0}}{\mathbb{1} + \Delta_0} J_0 k_2\right) + \operatorname{Re}\left(J_0 h_1, \frac{\sqrt{\Delta_0}}{\mathbb{1} + \Delta_0} k_2\right) \\ &= \operatorname{Re}\left(h_1, \frac{\mathbb{1} + \Delta_0}{\mathbb{1} + \Delta_0} k_2\right) \\ &= \operatorname{Re}(h_1, k_2), \end{aligned}$$

because $k_2 = J_0 \Delta_0^{-\frac{1}{2}} k_2$ and $h_1 = J_0 \Delta_0^{\frac{1}{2}} h_1$, respectively. A similar argument for the term with k_1 and h_2 then shows that

$$\operatorname{Re}(h_1 + J_0 k_1, M_0(h_2 + J_0 k_2)) = \operatorname{Re}(h_1 + k_1, h_2 + k_2)$$

as desired.

Using the modular conjugations, indicated with the appropriate subscripts, there is a bijection

$$\begin{aligned} T : H_0 + H'_0 &\rightarrow H_\delta + H'_\delta \\ \xi + J_0 \eta &\mapsto \xi + J_\delta \eta \end{aligned}$$

for all $\xi, \eta \in H_0$. This bijection is symplectic, $\operatorname{Im}(T(\xi_1 + J_0 \eta_1), T(\xi_2 + J_0 \eta_2))_{\mathcal{H}_\delta} = \sigma(\xi_1, \xi_2) - \sigma(\eta_1, \eta_2) = \operatorname{Im}(\xi_1 + J_0 \eta_1, \xi_2 + J_0 \eta_2)_{\mathcal{H}_0}$, as

$$\begin{aligned} \operatorname{Im}(T(\xi_1 + J_0 \eta_1), T(\xi_2 + J_0 \eta_2))_{\mathcal{H}_\delta} &= \operatorname{Im}(\xi_1 + J_\delta \eta_1, \xi_2 + J_\delta \eta_2)_{\mathcal{H}_\delta} \\ &= \operatorname{Im}(\xi_1, \xi_2)_{\mathcal{H}_\delta} - \operatorname{Im}(\eta_1, \eta_2)_{\mathcal{H}_\delta} \\ &= \sigma(\xi_1, \xi_2) - \sigma(\eta_1, \eta_2) \\ &= \operatorname{Im}(\xi_1, \xi_2)_{\mathcal{H}_0} - \operatorname{Im}(\eta_1, \eta_2)_{\mathcal{H}_0} \\ &= \operatorname{Im}(\xi_1 + J_0 \eta_1, \xi_2 + J_0 \eta_2)_{\mathcal{H}_0}, \end{aligned}$$

and it allows us to transport the structure of the perturbed system to the Hilbert space $\mathcal{H}_0$, where we have

$$\operatorname{Re}(T\xi, T\eta)_{\mathcal{H}_\delta} = \operatorname{Re}(\xi, T^* T \eta)_{\mathcal{H}_0}$$

for all $\xi, \eta \in H_0 + H'_0$. As T is symplectic we have

$$\begin{aligned} \operatorname{Re}(\xi, \hat{R}_0 \eta)_{\mathcal{H}_0} &= \operatorname{Im}(\xi, \eta)_{\mathcal{H}_0} \\ &= \operatorname{Im}(T\xi, T\eta)_{\mathcal{H}_\delta} \\ &= \operatorname{Re}(T\xi, \hat{R}_\delta T\eta)_{\mathcal{H}_\delta} \\ &= \operatorname{Re}(\xi, T^* \hat{R}_\delta T\eta)_{\mathcal{H}_0}, \end{aligned}$$

i.e. $\hat{R}_0 = T^* \hat{R}_\delta T$, where we denote the polarization operators for the doubled systems with a hat. Because the polarization operators are given by multiplication by $-i$ on $\mathcal{H}_0$, respectively $\mathcal{H}_\delta$, we see that $\hat{R}_0^2 = -\mathbb{1}$ and $\hat{R}_\delta^2 = -\mathbb{1}$ and hence

$$T^* = -\hat{R}_0 T^{-1} \hat{R}_\delta.$$

The results of [AY82] show that the states determined by μ_0 and μ_δ are quasi-equivalent iff the states determined by $\text{Re}(\cdot, \cdot)$ and $\text{Re}(\cdot, T^* T \cdot)$ on $H_0 + H'_0$ are unitarily equivalent, which, by the results of Shale [Sha62], is equivalent to¹

$$T^* T - \mathbb{1} \in \mathcal{L}^2(\mathcal{H}_0).$$

Longo then shows that this condition is equivalent to

$$C := T \hat{R}_0 (T^* T - \mathbb{1}) = \hat{R}_\delta T - T \hat{R}_0$$

being in $\mathcal{L}^2(\mathcal{H}_0, \mathcal{H}_\delta)$ (as real Hilbert spaces), cf. [Lon22, Prop. 3.10]. Decomposing C as operators between H_0 , H_δ and their real orthogonal complements, and exploiting the intertwining properties of C with the polarization operators and modular conjugations, [Lon22, Thm. 4.2] finds an equivalent expression for the conditions for quasi-equivalence in terms of the polarization operators R_0 and R_δ , which may be re-expressed in terms of modular operators.

A more special case of these general results is then given by Corollary 1.3.4, which we will use instead of aiming for the most general setting, as it can be directly applied to our perturbed Gaussian states. To simplify our treatment for μ_δ and μ_0 we will make the stronger assumptions

$$\delta \geq 0 \tag{3.1.6}$$

and

$$\text{tr } \delta < \infty. \tag{3.1.7}$$

These conditions have the advantage that they do not depend on Σ and they will be general enough for our applications in Section 3.2. They imply that both $\mathbb{1} + \delta$ and $(\mathbb{1} + \delta)^{-1}$ are bounded and, by the Powers-Størmer inequality, Theorem C.2.1, we have

$$\left\| \sqrt{\mathbb{1} + \delta + \Sigma_0} - \sqrt{\mathbb{1} + \Sigma_0} \right\|_{\text{HS}}^2 \leq \text{tr } |(\mathbb{1} + \delta + \Sigma_0) - (\mathbb{1} + \Sigma_0)| = \text{tr } |\delta|, \tag{3.1.8}$$

so condition (3.1.4) is also verified. (This observation has been made before, cf. [Buc74, App. B] or [CM24, Sec. 2.1].) Note that our conditions on δ may not be strong enough to have a well-defined modular operator.

Now, we want to supplement the above results on quasi-equivalence with some explicit estimates on the Hilbert-Schmidt norms of the operators involved. For this purpose, we will use some of the inequalities discussed in Appendix C. To avoid confusion, we will take all square roots w.r.t. the reference inner product μ_0 and we use the notation R_δ as introduced at the beginning of this section, but omitting the unitary V_δ , which should not lead to any confusion. We then start with the following basic estimate.

¹More precisely, Shale [Sha62] assumes the existence of a bounded Bogolyubov transformation with a bounded inverse, i.e. a bounded real linear map $B : \mathcal{H}_0 \rightarrow \mathcal{H}_0$ with a bounded inverse which preserves the symplectic form ($B^* \hat{R}_0 B = \hat{R}_0$) and such that $B^* B = T^* T$ gives the change in the inner product. If T is not bounded, then condition (3.1.3) of [AY82] is violated, so quasi-equivalence (and hence unitary equivalence) must fail for the purified states. However, assuming (3.1.3) one can show that T is bounded [AY82; AS71] with a bounded inverse. Furthermore, if T is bounded, [AY82] prove the existence of the desired Bogolyubov transformation.

Lemma 3.1.1. *Let μ_0 be an inner product on a pre-symplectic space (D, σ) , defining a Gaussian state, and μ_δ a perturbation of μ_0 of the form (3.1.1). If $\delta \geq 0$ and $\|\delta\|_p < \infty$ for some $p \in [1, \infty]$, then*

$$\|R_\delta - R_0\|_p \leq \|\delta\|_p. \quad (3.1.9)$$

Proof. Using $\|R_0\| \leq 1$, $\|(\mathbb{1} + \delta)^{-\frac{1}{2}}\| \leq 1$, $\|AX\|_p \leq \|A\|\|X\|_p$ and the triangle inequality for the p -norm, we find

$$\begin{aligned} \|R_\delta - R_0\|_p &= \left\| ((\mathbb{1} + \delta)^{-\frac{1}{2}} - \mathbb{1})R_0(\mathbb{1} + \delta)^{-\frac{1}{2}} - R_0(\mathbb{1} - (\mathbb{1} + \delta)^{-\frac{1}{2}}) \right\|_p \\ &\leq 2 \left\| \mathbb{1} - (\mathbb{1} + \delta)^{-\frac{1}{2}} \right\|_p \\ &\leq 2 \left\| (\mathbb{1} + \delta)^{-\frac{1}{2}} \right\| \left\| \sqrt{\mathbb{1} + \delta} - \mathbb{1} \right\|_p \\ &\leq \|\delta\|_p \end{aligned}$$

by Theorem C.2.4 with $\alpha = 2$. □

If we only assume $\mathbb{1} + \delta > 0$ instead of $\delta \geq 0$, then we can still apply Theorem C.2.4 with $\alpha = 1$, showing that $\|R_\delta - R_0\|_p \leq 2\|(\mathbb{1} + \delta)^{-\frac{1}{2}}\|\|\delta\|_p$.

Sometimes we will also assume that R_0^{-1} is bounded, which is not implied by our previous assumptions, but, as we will discuss in Section 3.2, this holds in some relevant cases. Regarding some of the functions that appear in Longo's analysis, cf. Corollary 1.3.4, we then get the following results.²

Theorem 3.1.2. *Let μ_0 be an inner product on a pre-symplectic space (D, σ) , defining a Gaussian state, and μ_δ a perturbation of μ_0 of the form (3.1.1). If $\delta \geq 0$ and $\text{tr } \delta < \infty$, then,*

$$\left\| \sqrt{\mathbb{1} + R_\delta^2} - \sqrt{\mathbb{1} + R_0^2} \right\|_{\text{HS}}^2 \leq 2 \text{tr } \delta. \quad (3.1.10)$$

If we also assume R_0^{-1} to be bounded, then

$$\text{tr} |R_\delta^{-1} - R_0^{-1}| \leq \|R_0^{-1}\| \text{tr } \delta, \quad (3.1.11)$$

$$\left\| R_\delta^{-1} \sqrt{\mathbb{1} + R_\delta^2} - R_0^{-1} \sqrt{\mathbb{1} + R_0^2} \right\|_{\text{HS}}^2 \leq 2 \|R_0^{-1}\|^2 \left(2 \text{tr } \delta + (\text{tr } \delta)^2 \right). \quad (3.1.12)$$

Proof. Let's start with condition (1.3.8). By applying Theorem C.2.1,

$$\left\| \sqrt{\mathbb{1} + R_\delta^2} - \sqrt{\mathbb{1} + R_0^2} \right\|_{\text{HS}}^2 \leq \text{tr} |\mathbb{1} + R_\delta^2 - (\mathbb{1} + R_0^2)| = \text{tr} |R_\delta^2 - R_0^2|. \quad (3.1.13)$$

Writing $R_\delta^2 - R_0^2 = \frac{1}{2}(R_\delta - R_0)(R_\delta + R_0) + \frac{1}{2}(R_\delta + R_0)(R_\delta - R_0)$ and using $\|R_\delta + R_0\| \leq 2$ and the triangle inequality for the trace norm gives

$$\text{tr} |R_\delta^2 - R_0^2| \leq 2 \text{tr} |R_\delta - R_0|.$$

²Strictly speaking, to compare with the results in [Lon22] we would need to replace all functions $X(R_\delta)$ by $(\mathbb{1} + \delta)^{-\frac{1}{2}} X(R_\delta) (\mathbb{1} + \delta)^{\frac{1}{2}}$ in order to account for the change in inner product. Note, however, that $(\mathbb{1} + \delta)^{\frac{1}{2}} - \mathbb{1}$ is trace-class in our setting.

Together with (3.1.13) and Lemma 3.1.1 for $p = 1$, this proves the estimate (3.1.10).

Now, assuming R_0^{-1} to be bounded, to prove (3.1.11), we have

$$\begin{aligned}
\operatorname{tr} |R_\delta^{-1} - R_0^{-1}| &= \operatorname{tr} \left| \sqrt{\mathbb{1} + \delta} R_0^{-1} \sqrt{\mathbb{1} + \delta} - R_0^{-1} \right| \\
&= \operatorname{tr} \left| \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right) R_0^{-1} \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right) \right. \\
&\quad \left. + R_0^{-1} \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right) + \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right) R_0^{-1} \right| \\
&\leq \operatorname{tr} \left| \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right) R_0^{-1} \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right) \right| \\
&\quad + 2 \|R_0^{-1}\| \operatorname{tr} \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right),
\end{aligned} \tag{3.1.14}$$

as $\sqrt{\mathbb{1} + \delta} - \mathbb{1} \geq 0$. We can estimate the first term by Theorem C.2.6,

$$\begin{aligned}
&\operatorname{tr} \left| \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right) R_0^{-1} \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right) \right| \\
&\leq \frac{1}{2} \operatorname{tr} \left| \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right)^2 R_0^{-1} + R_0^{-1} \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right)^2 \right| \\
&\leq \|R_0^{-1}\| \operatorname{tr} \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right)^2.
\end{aligned} \tag{3.1.15}$$

Then, combining (3.1.14) and (3.1.15), we get

$$\begin{aligned}
\operatorname{tr} |R_\delta^{-1} - R_0^{-1}| &\leq \|R_0^{-1}\| \left[\operatorname{tr} \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right)^2 + 2 \operatorname{tr} \left(\sqrt{\mathbb{1} + \delta} - \mathbb{1} \right) \right] \\
&= \|R_0^{-1}\| \operatorname{tr} \left((\mathbb{1} + \delta) - 2\sqrt{\mathbb{1} + \delta} + \mathbb{1} + 2\sqrt{\mathbb{1} + \delta} - 2\mathbb{1} \right) \\
&= \|R_0^{-1}\| \operatorname{tr} \delta,
\end{aligned} \tag{3.1.16}$$

which gives us (3.1.11).

As noted in Remark 1.3.1, (3.1.12) is already implied by (3.1.10), (3.1.11) and the boundedness of R_0^{-1} . We get

$$\begin{aligned}
&\left\| R_\delta^{-1} \sqrt{\mathbb{1} + R_\delta^2} - R_0^{-1} \sqrt{\mathbb{1} + R_0^2} \right\|_{\text{HS}}^2 \\
&= \left\| (R_\delta^{-1} - R_0^{-1}) \sqrt{\mathbb{1} + R_\delta^2} + R_0^{-1} \left(\sqrt{\mathbb{1} + R_\delta^2} - \sqrt{\mathbb{1} + R_0^2} \right) \right\|_{\text{HS}}^2 \\
&\leq 2 \left\| \sqrt{\mathbb{1} + R_\delta^2} \right\|^2 \|R_\delta^{-1} - R_0^{-1}\|_{\text{HS}}^2 + 2 \|R_0^{-1}\|^2 \left\| \sqrt{\mathbb{1} + R_\delta^2} - \sqrt{\mathbb{1} + R_0^2} \right\|_{\text{HS}}^2,
\end{aligned} \tag{3.1.17}$$

where $\left\| \sqrt{\mathbb{1} + R_\delta^2} \right\|^2 \leq 1$ (since $R_\delta^2 \leq 0$) and $\left\| \sqrt{\mathbb{1} + R_\delta^2} - \sqrt{\mathbb{1} + R_0^2} \right\|_{\text{HS}}^2 \leq 2 \operatorname{tr} \delta$ by equation (3.1.10).

The Hilbert-Schmidt norm of $R_\delta^{-1} - R_0^{-1}$ can be obtained from its trace norm (3.1.11),

$$\|R_\delta^{-1} - R_0^{-1}\|_{\text{HS}}^2 \leq (\operatorname{tr} |R_\delta^{-1} - R_0^{-1}|)^2 \leq \|R_0^{-1}\|^2 (\operatorname{tr} \delta)^2. \tag{3.1.18}$$

Together with (3.1.17), we get (3.1.12). $\square$

Remark. These estimates were made in terms of $\operatorname{tr} \delta$, avoiding $\|\delta\|$, but this is not the only possible approach. E.g., one could also estimate the left-hand side of equation (3.1.18) from above by $(1 + \|\mathbb{1} + \delta\|) \|R_0^{-1}\|^2 \operatorname{tr} \delta$, which avoids the square of the trace of δ , but introduces its norm.

It is relevant to note that up to this point we did not make use of condition (1.3.11), or, equivalently, $\mathbb{1} + \Sigma_\delta > 0$, necessary to have a well-defined modular operator. Indeed, the class of quasi-equivalent states we have considered contains states which admit modular operators as well as states which do not. If we require the Gaussian state μ_δ to satisfy the condition $\mathbb{1} + R_\delta^2 > 0$, the estimate of Lemma 3.1.1 for $p = 1$ can equivalently be written as

$$\mathrm{tr} |-i \tanh(K_\delta/2) - R_0| \leq \mathrm{tr} \delta. \quad (3.1.19)$$

Similarly, we can express the estimates of Theorem 3.1.2 in terms of modular Hamiltonians.

Corollary 3.1.3. *Let μ_0, μ_δ satisfy the hypotheses of Theorem 3.1.2, with $\delta \geq 0$, $\mathrm{tr} \delta < \infty$ and $\mathbb{1} + R_\delta^2 > 0$. Then,*

$$\left\| \frac{1}{\cosh(K_\delta/2)} - \sqrt{\mathbb{1} + R_0^2} \right\|_{\mathrm{HS}}^2 \leq 2 \mathrm{tr} \delta. \quad (3.1.20)$$

If R_0^{-1} is bounded,

$$\mathrm{tr} |i \coth(K_\delta/2) - R_0^{-1}| \leq \|R_0^{-1}\| \mathrm{tr} \delta, \quad (3.1.21)$$

$$\left\| i \frac{1}{\sinh(K_\delta/2)} - R_0^{-1} \sqrt{\mathbb{1} + R_0^2} \right\|_{\mathrm{HS}}^2 \leq 2 \|R_0^{-1}\|^2 \left(2 \mathrm{tr} \delta + (\mathrm{tr} \delta)^2 \right). \quad (3.1.22)$$

Proof. Note that $\mathbb{1} + R_\delta^2 > 0$ iff $\mathbb{1} + \Sigma_\delta > 0$ (using $\Gamma \Sigma \Gamma = -\Sigma$), so we see from (1.3.12) that $R_\delta = -i \tanh(K_\delta/2)$ is well-defined and we get the functions $\sqrt{\mathbb{1} + R_\delta^2} = (\cosh(K_\delta/2))^{-1}$, $R_\delta^{-1} = i \coth(K_\delta/2)$ and $R_\delta^{-1} \sqrt{\mathbb{1} + R_\delta^2} = i (\sinh(K_\delta/2))^{-1}$. Then, the results follow from the estimates of Theorem 3.1.2. $\square$

One possible extension of this discussion comes from analysing differences of more general functions of polarization operators, we refer to Appendix C for more general estimates regarding Lipschitz and Hölder continuous functions of operators.

Theorem 3.1.4. *Under the assumptions of Theorem 3.1.2, we have*

$$\|f(\Sigma_\delta) - f(\Sigma_0)\|_{\mathrm{HS}} \leq k \|\delta\|_{\mathrm{HS}}.$$

for any Lipschitz continuous function f on $[-1, 1]$ with Lipschitz constant k .

Proof. Because Σ_δ and Σ_0 are self-adjoint, it follows immediately from Corollary C.2.8 that

$$\|f(\Sigma_\delta) - f(\Sigma_0)\|_{\mathrm{HS}} \leq k \|\Sigma_\delta - \Sigma_0\|_{\mathrm{HS}}.$$

Lemma 3.1.1 for $p = 2$ then yields the result. $\square$

As discussed in Appendix C, results of the kind

$$\|f(\Sigma_\delta) - f(\Sigma_0)\|_p \leq C \|\Sigma_\delta - \Sigma_0\|_p,$$

with $C > 0$ finite, are known to exist for Lipschitz functions for $1 < p < \infty$ [PS11; Cas+14], and for α -Hölder functions with $0 < \alpha < 1$, one has that

$$\|f(\Sigma_\delta) - f(\Sigma_0)\|_p \leq C \|\Sigma_\delta - \Sigma_0\|_p^\alpha$$

for any $p > 0$ [AP10; HSZ22], with $C > 0$ finite. Comparing this to the functions of Theorem 3.1.2, this would allow to consider estimates at least for $f(x) = \sqrt{1 - x^2}$, which is not Lipschitz continuous but $\frac{1}{2}$ -Hölder continuous. Unfortunately, the constant C in these estimates is in general unknown and it may not equal the Lipschitz or Hölder constant of the function under consideration.

3.2 Applications to a real linear scalar field

In this section, we will specialise to a real linear scalar field φ in an ultrastatic spacetime $M = (\mathbb{R} \times \mathcal{C}, -dt^2 + h)$, where $(\mathcal{C}, h)$ is a complete Riemannian manifold. As discussed in Section 2.1.1, the Klein-Gordon equation $(-\square + m^2)\varphi = 0$ can be written in the form $(\partial_t^2 + A_m)\varphi = 0$, where $A_m = -\Delta + m^2$ is a t -independent differential operator on $\mathcal{C}$. For any open region $\mathcal{O} \subseteq \mathcal{C}$, the symplectic space $(D^{(\mathcal{O})}, \sigma)$ is given by the space of initial data

$$D^{(\mathcal{O})} = C_0^\infty(\mathcal{O}, \mathbb{R}) \oplus C_0^\infty(\mathcal{O}, \mathbb{R}), \quad (3.2.1)$$

with respect to the symplectic form

$$\sigma(f, g) = \int_{\mathcal{O}} (f_0 g_1 - f_1 g_0) dx, \quad (3.2.2)$$

where $f = (f_1, f_0), g = (g_1, g_0) \in D^{(\mathcal{O})}$. When $\mathcal{O} = \mathcal{C}$ we will write D instead of $D^{(\mathcal{O})}$.

A Gaussian state ω is determined by a two-point distribution λ_2 on M^2 , which can equivalently be characterised by its 2×2 -matrix of initial data on the Cauchy surface $x_0 = 0$, given by

$$\omega_2 = \begin{pmatrix} \omega_{2,00} & \omega_{2,01} \\ \omega_{2,10} & \omega_{2,11} \end{pmatrix} = \begin{pmatrix} \lambda_2(x, y)|_{x^0=y^0=0} & \partial_{y_0} \lambda_2(x, y)|_{x^0=y^0=0} \\ \partial_{x_0} \lambda_2(x, y)|_{x^0=y^0=0} & \partial_{x_0} \partial_{y_0} \lambda_2(x, y)|_{x^0=y^0=0} \end{pmatrix}.$$

The initial data are related to an inner product μ by Definition 1.3.1.

The classical stress tensor takes the form

$$T_{ab}[\varphi] = \partial_a \varphi \partial_b \varphi - \frac{1}{2} g_{ab} \left(\eta^{cd} \partial_c \varphi \partial_d \varphi + m^2 \varphi^2 \right),$$

and the energy density is the (00)-component,

$$T_{00}[\varphi] = \frac{1}{2} \left((\partial_0 \varphi)^2 + h^{ij} \partial_i \varphi \partial_j \varphi + m^2 \varphi^2 \right).$$

For two Gaussian states ω, ω' the difference between the energy densities can be defined by a point-splitting procedure, which leads to the expression

$$\begin{aligned} \varepsilon_{\omega', \omega}(x) = \frac{1}{2} \Big\{ & (\omega_{2,11}(x, y) - \omega'_{2,11}(x, y)) + \\ & + \left(\sum_{i,j=1}^n h^{ij}(x) \partial_{x_i} \partial_{y_j} + m^2 \right) (\omega_{2,00}(x, y) - \omega'_{2,00}(x, y)) \Big\} \Big|_{x=y}, \end{aligned} \quad (3.2.3)$$

when the expression in braces is a continuous function of x and y at all points on the diagonal $x = y$ of $\mathcal{C}$. (Here we use local coordinates $(0, x_i)$, with (x_i) local coordinates on $\mathcal{C}$.)

3.2.1 Perturbations of the Minkowski vacuum

We first consider the case where $(\mathcal{C}, h)$ is the n -dimensional Euclidean space $\mathbb{R}^n$ and $\mathcal{O} = \mathbb{R}^n$. (These results should generalize to vacuum states in general ultrastatic spacetimes. See also Sec. 3.2.2.)

The Minkowski vacuum is determined by $\kappa : D \rightarrow L^2(\mathbb{R}^n) : (f_1, f_0) \mapsto A_m^{-\frac{1}{4}} f_1 - i A_m^{\frac{1}{4}} f_0$, which yields

$$\mu_{\text{vac}}(f, g) := \left\langle f_1, A_m^{-\frac{1}{2}} g_1 \right\rangle_{L^2(\mathbb{R}^n, \mathbb{R})} + \left\langle f_0, A_m^{\frac{1}{2}} g_0 \right\rangle_{L^2(\mathbb{R}^n, \mathbb{R})} = \langle f, X^2 g \rangle_{L^2(\mathbb{R}^n, \mathbb{R})^{\oplus 2}} \quad (3.2.4)$$

with

$$X = \begin{pmatrix} A_m^{-\frac{1}{4}} & 0 \\ 0 & A_m^{\frac{1}{4}} \end{pmatrix}. \quad (3.2.5)$$

Comparing with the general notations of Section 1.3 there is an isometry $U_{\text{vac}} : \mathcal{K}_{\text{vac}, \mathbb{R}} \longrightarrow L^2(\mathbb{R}^n, \mathbb{R})^{\oplus 2}$ given by

$$U_{\text{vac}}(f) = Xf, \quad (3.2.6)$$

which extends to a unitary $U_{\text{vac}} : \mathcal{K}_{\text{vac}} \longrightarrow L^2(\mathbb{R}^n)^{\oplus 2}$ that we denote by the same symbol. Identifying $\mathcal{K}_{\text{vac}}$ with $L^2(\mathbb{R}^n)^{\oplus 2}$ in this way we see from (3.2.2) that the polarization operator is given by

$$R_{\text{vac}} = U_{\text{vac}}^* \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} U_{\text{vac}}. \quad (3.2.7)$$

Note that $R_{\text{vac}}^2 = -\mathbb{1}$. In particular, condition (1.3.11), used to define a modular operator, is not satisfied here.

We now consider a deformation of the vacuum state in the sense of Section 3.1. The operator δ on $\mathcal{K}_{\text{vac}, \mathbb{R}}$ is related to an operator $\delta_{L^2} = U_{\text{vac}} \delta U_{\text{vac}}^*$ on $L^2(\mathbb{R}^n, \mathbb{R})$, so that

$$\mu_{\delta}(f, g) = \langle f, X(\mathbb{1} + \delta_{L^2})Xg \rangle_{L^2(\mathbb{R}^n, \mathbb{R})^{\oplus 2}} \quad (3.2.8)$$

for all $f, g \in D$. The difference of the two-point functions of the perturbed state ω_{δ} and the vacuum ω_{vac} is then given by the initial data

$$\omega_{2, \delta}(f, g) - \omega_{2, \text{vac}}(f, g) = \frac{1}{2} \mu_{\delta}(f, g) - \frac{1}{2} \mu_{\text{vac}}(f, g) = \frac{1}{2} \langle f, X \delta_{L^2} Xg \rangle_{L^2}, \quad (3.2.9)$$

with $f, g \in D$. We can write δ_{L^2} as a 2×2 -matrix $\delta_{L^2} = \begin{pmatrix} \delta_{00} & \delta_{01} \\ \delta_{10} & \delta_{11} \end{pmatrix}$ acting on $L^2(\mathbb{R}^n, \mathbb{R})^{\oplus 2}$. For the difference in the energy densities we find the following result, where we only consider $m > 0$ for simplicity and we treat $A_m^{\frac{1}{4}}$ as a diagonal matrix, $\begin{pmatrix} A_m^{\frac{1}{4}} & 0 \\ 0 & A_m^{\frac{1}{4}} \end{pmatrix}$, on $L^2(\mathbb{R}^n, \mathbb{R})^{\oplus 2}$.

Proposition 3.2.1. *Assume that $m > 0$ and that δ_{L^2} is a bounded, positive operator on $L^2(\mathbb{R}^n, \mathbb{R})^{\oplus 2}$ such that $A_m^{\frac{1}{4}} \delta_{L^2} A_m^{\frac{1}{4}}$ is a trace-class operator. Then*

$$E_{\delta} := \frac{1}{4} \text{tr} \left(A_m^{\frac{1}{4}} \delta_{L^2} A_m^{\frac{1}{4}} \right) \geq \frac{m}{4} \text{tr} \delta_{L^2}.$$

If in addition the expression in braces in equation (3.2.3) for $\omega' = \omega_{\delta}$ and $\omega = \omega_{\text{vac}}$ is continuous in all points on the diagonal of $\mathcal{C}$, then

$$E_{\delta} = \int_{\mathbb{R}^n} \varepsilon_{\omega_{\delta}, \omega_{\text{vac}}} d^n x.$$

Proof. To obtain the inequality we estimate

$$\text{tr} \delta_{L^2} = \text{tr} \left(A_m^{-\frac{1}{4}} (A_m^{\frac{1}{4}} \delta_{L^2} A_m^{\frac{1}{4}}) A_m^{-\frac{1}{4}} \right) \leq \left\| A_m^{-\frac{1}{4}} \right\|^2 \text{tr} \left(A_m^{\frac{1}{4}} \delta_{L^2} A_m^{\frac{1}{4}} \right) = 4 \frac{E_{\delta}}{m}, \quad (3.2.10)$$

using the fact that $A_m \geq m^2 \mathbb{1} > 0$, which implies that A_m^{-s} is bounded when $s \geq 0$.

$A_m^{-\frac{1}{2}} \partial_i$ is bounded for each $i = 1, \dots, n$, so it follows from our assumptions that the operators

$$\begin{aligned} & A_m^{\frac{1}{4}} \delta_{11} A_m^{\frac{1}{4}} \\ & m^2 A_m^{-\frac{1}{4}} \delta_{00} A_m^{-\frac{1}{4}} = m^2 A_m^{-\frac{1}{2}} (A_m^{\frac{1}{4}} \delta_{00} A_m^{\frac{1}{4}}) A_m^{-\frac{1}{2}} \\ & -\partial_i A_m^{-\frac{1}{4}} \delta_{00} A_m^{-\frac{1}{4}} \partial_i = (-\partial_i A_m^{-\frac{1}{2}}) (A_m^{\frac{1}{4}} \delta_{00} A_m^{\frac{1}{4}}) (A_m^{-\frac{1}{2}} \partial_i) \end{aligned}$$

are all positive and trace-class, where we view the partial derivatives as operators. The sum

$$\frac{1}{2} \left(A_m^{\frac{1}{4}} \delta_{11} A_m^{\frac{1}{4}} + m^2 A_m^{-\frac{1}{4}} \delta_{00} A_m^{-\frac{1}{4}} + \sum_{i=1}^n (-\partial_i) A_m^{-\frac{1}{4}} \delta_{00} A_m^{-\frac{1}{4}} \partial_i \right) \quad (3.2.11)$$

is then again trace class and by (3.2.9) its integral kernel is the expression in braces in equation (3.2.3) for the energy density $\varepsilon_{\omega_\delta, \omega_{\text{vac}}}$. By our continuity assumption on this integral kernel and [Bri91, Corollary 3.2] we then find

$$\begin{aligned} \tilde{E}_\delta &:= \int_{\mathbb{R}^n} \varepsilon_{\omega_\delta, \omega_{\text{vac}}} d^n x \\ &= \frac{1}{4} \text{tr}_{L^2(\mathbb{R}^n, \mathbb{R})} \left(A_m^{\frac{1}{4}} \delta_{11} A_m^{\frac{1}{4}} + m^2 A_m^{-\frac{1}{4}} \delta_{00} A_m^{-\frac{1}{4}} + \sum_{i=1}^n (-\partial_i) A_m^{-\frac{1}{4}} \delta_{00} A_m^{-\frac{1}{4}} \partial_i \right), \end{aligned} \quad (3.2.12)$$

Indeed, the results of [Bri91] allow us to weaken the continuity assumption somewhat, at the cost of additional technical complications.

To show that $\tilde{E}_\delta = E_\delta$ we need to use the cyclicity of the trace, taking special care, because some of the operators involved are unbounded. We compute

$$\begin{aligned} \text{tr}_{L^2(\mathbb{R}^n, \mathbb{R})} \left(\sum_{i=1}^n (-\partial_i) A_m^{-\frac{1}{4}} \delta_{00} A_m^{-\frac{1}{4}} \partial_i \right) &= \sum_{i=1}^n \text{tr}_{L^2(\mathbb{R}^n, \mathbb{R})} \left((-\partial_i A_m^{-\frac{1}{2}}) (A_m^{\frac{1}{4}} \delta_{00} A_m^{\frac{1}{4}}) (A_m^{-\frac{1}{2}} \partial_i) \right) \\ &= \sum_{i=1}^n \text{tr}_{L^2(\mathbb{R}^n, \mathbb{R})} \left((A_m^{-\frac{1}{2}} (-\partial_i^2) A_m^{-\frac{1}{2}}) (A_m^{\frac{1}{4}} \delta_{00} A_m^{\frac{1}{4}}) \right) \\ &= \text{tr}_{L^2(\mathbb{R}^n, \mathbb{R})} \left((A_m^{-\frac{1}{2}} (A_m - m^2) A_m^{-\frac{1}{2}}) (A_m^{\frac{1}{4}} \delta_{00} A_m^{\frac{1}{4}}) \right) \\ &= \text{tr}_{L^2(\mathbb{R}^n, \mathbb{R})} \left(A_m^{\frac{1}{4}} \delta_{00} A_m^{\frac{1}{4}} - m^2 A_m^{-\frac{1}{4}} \delta_{00} A_m^{-\frac{1}{4}} \right). \end{aligned}$$

Combining this identity with (3.2.12) yields $\tilde{E}_\delta = \frac{1}{4} \text{tr}_{L^2(\mathbb{R}^n, \mathbb{R})} \left(A_m^{\frac{1}{4}} \delta_{11} A_m^{\frac{1}{4}} + A_m^{\frac{1}{4}} \delta_{00} A_m^{\frac{1}{4}} \right) = E_\delta$. $\square$

Combining Proposition 3.2.1 with the results of Section 3.1 we find

Theorem 3.2.2. *If $m > 0$ and δ_{L^2} is a bounded, strictly positive operator on $L^2(\mathbb{R}^n, \mathbb{R})^{\oplus 2}$ such that $E_\delta = \frac{1}{4} \text{tr} \left(A_m^{\frac{1}{4}} \delta_{L^2} A_m^{\frac{1}{4}} \right) < \infty$, then the Gaussian state ω_δ determined by μ_δ is quasi-equivalent*

to the Minkowski vacuum ω_{vac} and we have

$$\text{tr} \left| i \coth \left(\frac{K_\delta}{2} \right) - R_{\text{vac}}^{-1} \right| \leq 4 \frac{E_\delta}{m}, \quad (3.2.13)$$

$$\left\| \frac{1}{\cosh \left(\frac{K_\delta}{2} \right)} \right\|_{\text{HS}}^2 \leq 8 \frac{E_\delta}{m}, \quad (3.2.14)$$

$$\left\| \frac{1}{\sinh \left(\frac{K_\delta}{2} \right)} \right\|_{\text{HS}}^2 \leq 16 \frac{E_\delta}{m} \left(1 + 2 \frac{E_\delta}{m} \right), \quad (3.2.15)$$

Proof. Note that K_δ is well-defined, as δ_{L^2} is strictly positive and trace-class. The proof then follows immediately from Corollary 3.1.3 and Proposition 3.2.1 together with the fact that $R_{\text{vac}}^{-1} = -R_{\text{vac}}$, which implies $\|R_{\text{vac}}^{-1}\| = 1$ and $\sqrt{\mathbb{1} + R_{\text{vac}}^2} = 0$. $\square$

Note that a different approach to obtain inequalities involving modular operators and energies has been pursued in [MPV22].

3.2.2 Thermal states

As a further example, we consider thermal (KMS) states at inverse temperature $\beta > 0$ for a scalar field with mass $m > 0$. We refer to Section A.2 for general properties of thermal states. We will assume that $\mathcal{C}$ is compact, to ensure that all thermal states are quasi-equivalent [Ver94]. Note that A_m has a pure point spectrum under this assumption (see e.g. [Jos17; MS67]).

Gaussian thermal states are given by the inner product

$$\mu_\beta(f, g) = \left\langle f, X \coth \left(\frac{\beta}{2} A_m^{\frac{1}{2}} \right) X g \right\rangle_{L^2(\mathcal{C}, \mathbb{R})^{\oplus 2}} \quad (3.2.16)$$

with X as in equation (3.2.5). Using the identity $\coth \left(\frac{\beta}{2} x \right) = 1 + \frac{2}{e^{\beta x} - 1}$ for all $x \neq 0$ we can view thermal states as perturbations of the vacuum in the context of Section 3.1 with the operator $\delta_{L^2} = \delta_\beta$ given by

$$\delta_\beta = \frac{2}{e^{\beta A_m^{\frac{1}{2}}} - \mathbb{1}} \quad (3.2.17)$$

as a diagonal 2×2 -matrix. Notice that $\delta_\beta > 0$ is strictly positive (because A_m is) and trace-class, due to Weyl's asymptotic formula, cf. [Jos17; MS67]. For similar reasons, $A_m^{\frac{1}{4}} \delta_\beta A_m^{\frac{1}{4}} = \frac{2A_m^{\frac{1}{2}}}{e^{\beta A_m^{\frac{1}{2}}} - \mathbb{1}}$ is also trace-class. We have

$$\begin{aligned} \Sigma_\beta &:= V_{\delta_\beta} \Sigma_{\delta_\beta} V_{\delta_\beta}^* \\ &= (\mathbb{1} + \delta_\beta)^{-\frac{1}{2}} \Sigma_{\text{vac}} (\mathbb{1} + \delta_\beta)^{-\frac{1}{2}} \\ &= \tanh \left(\frac{\beta}{2} A_m^{\frac{1}{2}} \right) \Sigma_{\text{vac}} \end{aligned} \quad (3.2.18)$$

with $\Sigma_{\text{vac}} = \begin{pmatrix} 0 & -i\mathbb{1} \\ i\mathbb{1} & 0 \end{pmatrix}$. We will also write $R_\beta = -i\Sigma_\beta$ and for the modular Hamiltonian we find

$$K_\beta := V_{\delta_\beta} K_{\delta_\beta} V_{\delta_\beta}^* = 2 \operatorname{artanh}(\Sigma_\beta) = \beta A_m^{\frac{1}{2}} \Sigma_{\text{vac}} \quad (3.2.19)$$

using (1.3.12) and diagonalising the 2×2 -matrix Σ_{vac} using the unitary $\frac{1}{\sqrt{2}} \begin{pmatrix} -i\mathbb{1} & i\mathbb{1} \\ \mathbb{1} & \mathbb{1} \end{pmatrix}$.

We now examine the estimates of Theorem 3.1.2 in this specific setting, where more explicit computations are possible. For example, from equation (3.2.18) we see that

$$R_\beta^{-1} - R_{\text{vac}}^{-1} = i \left(\mathbb{1} - \coth \left(\frac{\beta}{2} A_m^{\frac{1}{2}} \right) \right) \Sigma_{\text{vac}}$$

and it follows that

$$\begin{aligned} \text{tr} \left| R_\beta^{-1} - R_{\text{vac}}^{-1} \right| &= \text{tr} \left| i \left(\mathbb{1} - \coth \left(\frac{\beta}{2} A_m^{\frac{1}{2}} \right) \right) \Sigma_{\text{vac}} \right| \\ &= \text{tr} \left(\coth \left(\frac{\beta}{2} A_m^{\frac{1}{2}} \right) - \mathbb{1} \right) \\ &= \text{tr} \delta_\beta, \end{aligned}$$

where we recall that the trace is over $L^2(\mathcal{C}, \mathbb{C})$. Similarly, for estimate (3.1.10),

$$\begin{aligned} \left\| \sqrt{\mathbb{1} + R_\beta^2} - \sqrt{\mathbb{1} + R_{\text{vac}}^2} \right\|_{\text{HS}}^2 &= \left\| \sqrt{\mathbb{1} + R_\beta^2} \right\|_{\text{HS}}^2 \\ &= \text{tr} \left| \mathbb{1} + R_\beta^2 \right| \\ &= \text{tr} \left(\tanh \left(\frac{\beta}{2} A_m^{\frac{1}{2}} \right) \left(\mathbb{1} + \tanh \left(\frac{\beta}{2} A_m^{\frac{1}{2}} \right) \right) \delta_\beta \right) \\ &< 2 \text{tr} \delta_\beta \end{aligned}$$

where we used $\delta_\beta = \coth \left(\frac{\beta}{2} A_m^{\frac{1}{2}} \right) - \mathbb{1}$ and $\left\| \tanh \left(\frac{\beta}{2} A_m^{\frac{1}{2}} \right) \right\| \leq 1$. Here the inequality is strict, since $1 - \tanh^2 \left(\frac{x}{2} \right) < 2 \frac{2}{e^x - 1}$, for all $x > 0$. However, as $\beta \rightarrow \infty$ the left-hand side converges to $2 \text{tr} \delta_\beta$. Finally, regarding estimate (3.1.12),

$$\begin{aligned} \left\| R_\beta^{-1} \sqrt{\mathbb{1} + R_\beta^2} - R_{\text{vac}}^{-1} \sqrt{\mathbb{1} + R_{\text{vac}}^2} \right\|_{\text{HS}}^2 &= \left\| R_\beta^{-1} \sqrt{\mathbb{1} + R_\beta^2} \right\|_{\text{HS}}^2 \\ &= \text{tr} \left(-R_\beta^{-2} - \mathbb{1} \right) \\ &= \text{tr} \left(\coth^2 \left(\frac{\beta}{2} A_m^{\frac{1}{2}} \right) - \mathbb{1} \right) \\ &= \text{tr} \delta_\beta (\delta_\beta + 2) \\ &\leq 2 \text{tr} \delta_\beta + (\text{tr} \delta_\beta)^2 \end{aligned}$$

where we used $\text{tr}(A^2) \leq \|A\| \text{tr}(A) \leq (\text{tr}(A))^2$ for $A \geq 0$. This should be compared with the more general estimate (3.1.12), which has an additional overall factor 2 on the right-hand side.

3.2.3 Local perturbations of the vacuum

To conclude this chapter, we will briefly comment on states on a bounded open region $\mathcal{O} \subset \mathbb{R}^n$ in an inertial time slice of Minkowski space. Here, two issues arise that make the situation noticeably more complicated than in Sections 3.2.1 and 3.2.2.

Due to the Reeh-Schlieder Theorem 2.2.1, the one-particle Hilbert space $\mathcal{H}_0$ of the Minkowski vacuum remains the same, even if we restrict the theory to the bounded open region $\mathcal{O}$. The same is not true, however, for the spaces $\mathcal{K}_{0,\mathbb{R}}$ and $\mathcal{K}_0$. In general, we find for the region $\mathcal{O}$ a subspace

$\mathcal{K}_{0,\mathbb{R}}^{(\mathcal{O})} \subset \mathcal{K}_{0,\mathbb{R}}$, where the inner product on the symplectic space $D^{(\mathcal{O})}$ is given by the fractional operators $A_m^{\pm\frac{1}{2}}|_{\mathcal{O}}$, which are defined as quadratic forms on $L^2(\mathcal{O})$ essentially by restricting the integral kernels of these operators to $\mathcal{O} \times \mathcal{O}$. It is important to note that the operators $A_m^{\pm\frac{1}{2}}|_{\mathcal{O}}$ are not each other's inverses.

The change in the inner product also leads to a change in the polarization operator R_0 . Because R_0 does not preserve the subspace $\mathcal{K}_{0,\mathbb{R}}^{(\mathcal{O})}$, the desired polarization operator $R_0^{(\mathcal{O})}$ is not the restriction of R_0 to this subspace. Instead, we find a more complicated expression and, more importantly, we no longer expect to have $R_0^2 = -\mathbb{1}$, because the vacuum restricted to a bounded region is no longer a pure state. Indeed, we generally cannot expect that $\|(R_0^{(\mathcal{O})})^{-1}\| < \infty$, so some of our general estimates from Section 3.1 no longer apply. E.g., it is well-known that a massless free scalar field on the open unit ball can be conformally mapped to a wedge region, where the Bisognano-Wichmann Theorem tells us that the modular flow is given by Lorentz boosts [HL82; BW76]. The generator of this flow has spectrum $\mathbb{R}$, which means that the same is true for the modular Hamiltonian of the ball [LM23]. Hence, the spectrum of $R_0^{(\mathcal{O})}$ is $[-1, 1]$ (with 1 and -1 not in the point spectrum) and its inverse is unbounded.

This issue can be avoided if we only consider estimates that do not involve $\|(R_0^{(\mathcal{O})})^{-1}\|$. However, even in that case there are still difficulties expressing the upper bounds of our estimates in terms of the energy of a state. Indeed, the change in the inner product also renders our proof of Proposition 3.2.1 invalid. The extension of our estimates of Theorem 3.2.2 to bounded regions will therefore require further investigation.

Chapter 4

Bounds on relative modular Hamiltonians

In this chapter, following the results in [CMS26], we will present a scheme for general AQFTs that allows us to estimate relative modular Hamiltonians, and hence also relative entropies, between suitable pairs of states from above, resp. below, in terms of modular Hamiltonians of a reference state on a larger, resp. smaller, region, and we will discuss the relation between the applicability of this scheme and the possibility of superluminal signalling in the context of Sorkin's impossible measurements. To investigate the strength of our estimates, we also consider coherent states for CCR systems, focussing particularly on free scalar fields.

4.1 General estimates for relative modular theory

We shall start by briefly recalling some of the concepts we introduced in Sections 1.1.4 and 1.2. Given a C^* -algebra $\mathcal{A}$ with unit $\mathbf{1}$ and a state ω (i.e. a normalised positive linear functional $\omega : \mathcal{A} \rightarrow \mathbb{C}$), its GNS-representation is characterised by the GNS-triple $(\pi_\omega, \mathcal{H}_\omega, \Omega_\omega)$ and we define the von Neumann algebra $\mathcal{R}_\omega := \pi_\omega(\mathcal{A})''$. We call Ω_ω a standard vector for $\mathcal{R}_\omega$ iff it is both separating and cyclic, i.e., $\mathcal{R}_\omega \ni a \mapsto a\Omega_\omega \subset \mathcal{H}_\omega$ is injective and has a dense range, cf. Section 1.1.4. (Note that we will now denote generic C^* -algebras as $\mathcal{A}$ and von Neumann algebras as $\mathcal{R}$, as to highlight the distinction.)

Now, let $\tilde{\omega}$ be another state on $\mathcal{A}$ with GNS-triple $(\pi_{\tilde{\omega}}, \mathcal{H}_{\tilde{\omega}}, \Omega_{\tilde{\omega}})$. The states ω and $\tilde{\omega}$ are called quasi-equivalent iff the von Neumann algebras $\mathcal{R}_\omega$ and $\mathcal{R}_{\tilde{\omega}}$ are isomorphic and the isomorphism $\Phi : \mathcal{R}_\omega \rightarrow \mathcal{R}_{\tilde{\omega}}$ must satisfy $\Phi(\pi_\omega(A)) = \pi_{\tilde{\omega}}(A)$ for all $A \in \mathcal{A}$, i.e. it must intertwine their GNS-representations. If in addition both Ω_ω and $\Omega_{\tilde{\omega}}$ are standard vectors, then the Unitary Implementation Theorem 1.1.6 states that we can identify $\mathcal{H} := \mathcal{H}_{\tilde{\omega}} = \mathcal{H}_\omega$ and $\pi_{\tilde{\omega}} = \pi_\omega$, so the vectors Ω_ω and $\Omega_{\tilde{\omega}}$ lie in the same Hilbert space. This is the situation that we will now consider and for simplicity we will denote the vectors by Ω and $\tilde{\Omega}$ and drop the subscripts ω and $\tilde{\omega}$.

Given two standard unit vectors $\Omega, \tilde{\Omega} \in \mathcal{H}$ for the von Neumann algebra $\mathcal{R}$ one defines the relative Tomita operator $S_{\tilde{\Omega}, \Omega}$ by $S_{\tilde{\Omega}, \Omega} a \Omega := a^* \tilde{\Omega}$ for all $a \in \mathcal{R}$. This operator is densely defined and closable and we will denote the closure by the same symbol, cf. Section 1.2. Its polar decomposition $S_{\tilde{\Omega}, \Omega} = J_{\tilde{\Omega}, \Omega} \Delta_{\tilde{\Omega}, \Omega}^{1/2}$ uniquely defines the relative modular operator $\Delta_{\tilde{\Omega}, \Omega}$, which is strictly positive, and the relative modular conjugation $J_{\tilde{\Omega}, \Omega}$, which is anti-unitary, $J_{\tilde{\Omega}, \Omega}^* = J_{\tilde{\Omega}, \Omega}^{-1}$. The relative modular Hamiltonian is the self-adjoint operator

$$K_{\tilde{\Omega}, \Omega} := -\log \left(\Delta_{\tilde{\Omega}, \Omega} \right). \quad (4.1.1)$$

These operators will satisfy $J_{\Omega, \tilde{\Omega}} = J_{\tilde{\Omega}, \Omega}^*$, $\Delta_{\Omega, \tilde{\Omega}}^{\frac{1}{2}} = J_{\tilde{\Omega}, \Omega} \Delta_{\tilde{\Omega}, \Omega}^{-\frac{1}{2}} J_{\tilde{\Omega}, \Omega}^*$ and $K_{\Omega, \tilde{\Omega}} = -J_{\tilde{\Omega}, \Omega} K_{\tilde{\Omega}, \Omega} J_{\tilde{\Omega}, \Omega}^*$.

We will now supplement the general theory of Section 1.2 with some additional estimates regarding relative modular operators, relative modular conjugations and relative modular Hamiltonians, starting with the following lemma, cf. [CGP19, Lemma 5.1].

Lemma 4.1.1. *If a unitary u acting on $\mathcal{H}$ satisfies $u\mathcal{R}u^* = \mathcal{R}$, then $u\Omega$ and $u\tilde{\Omega}$ are also standard and we have*

$$\begin{aligned} J_{u\tilde{\Omega}, u\Omega} &= uJ_{\tilde{\Omega}, \Omega}u^* \\ K_{u\tilde{\Omega}, u\Omega} &= uK_{\tilde{\Omega}, \Omega}u^*. \end{aligned}$$

By functional calculus it then follows that $\Delta_{u\tilde{\Omega}, u\Omega} = u\Delta_{\tilde{\Omega}, \Omega}u^*$ and $S_{u\tilde{\Omega}, u\Omega} = uS_{\tilde{\Omega}, \Omega}u^*$.

Proof. As $\mathcal{R}u\Omega = u\mathcal{R}\Omega$, $u\Omega$ is cyclic for $\mathcal{R}$. Using $u\mathcal{R}'u^* = \mathcal{R}'$ we see from the same argument that $u\Omega$ is also cyclic for $\mathcal{R}'$ and hence separating and standard for $\mathcal{R}$. The same applies to $u\tilde{\Omega}$. Now $\mathcal{R}u\Omega = u\mathcal{R}\Omega$ is a core for both $S_{u\tilde{\Omega}, u\Omega}$ and $uS_{\tilde{\Omega}, \Omega}u^*$ and for all $a \in \mathcal{R}$ we have

$$uS_{\tilde{\Omega}, \Omega}u^*au\Omega = u(u^*au)^*\tilde{\Omega} = a^*u\tilde{\Omega} = S_{u\tilde{\Omega}, u\Omega}au\Omega,$$

so $S_{u\tilde{\Omega}, u\Omega} = uS_{\tilde{\Omega}, \Omega}u^* = (uJ_{\tilde{\Omega}, \Omega}u^*)(u\Delta_{\tilde{\Omega}, \Omega}^{\frac{1}{2}}u^*)$, from which we infer all the desired relations using the uniqueness of the polar decomposition. $\square$

As explained in Section 1.2, when $\tilde{\Omega} = \Omega$ we drop the adjective ‘relative’ and we use the single subscript Ω .

Following [Ara75; Ara77], the relative entropy between the states Ω and $\tilde{\Omega}$ for the algebra $\mathcal{R}$ is defined by

$$H(\Omega, \tilde{\Omega}) := \langle \Omega, K_{\tilde{\Omega}, \Omega} \Omega \rangle = -\langle \Omega, \log(\Delta_{\tilde{\Omega}, \Omega}) \Omega \rangle. \quad (4.1.2)$$

Now suppose that $\hat{\Omega}$ is another standard unit vector for $\mathcal{R}$ which gives the same expectation values as Ω . Then there is a unitary $u' \in \mathcal{R}'$ given by

$$u'a\Omega := a\hat{\Omega} \quad (4.1.3)$$

for all $a \in \mathcal{R}$. Because both vectors define the same state on $\mathcal{R}$, one expects that $H(\hat{\Omega}, \tilde{\Omega}) = H(\Omega, \tilde{\Omega})$ and $H(\tilde{\Omega}, \hat{\Omega}) = H(\tilde{\Omega}, \Omega)$. We will now explain why this does indeed work out, taking a slightly more general perspective.

Lemma 4.1.2. *Suppose that $u, v \in \mathcal{R}$ and $u', v' \in \mathcal{R}'$ are unitaries. Then*

$$\begin{aligned} J_{uu'\tilde{\Omega}, vv'\Omega} &= u'vJ_{\tilde{\Omega}, \Omega}u^*v'^* \\ K_{uu'\tilde{\Omega}, vv'\Omega} &= v'uK_{\tilde{\Omega}, \Omega}u^*v'^* \end{aligned} \quad (4.1.4a)$$

$$H(vv'\Omega, uu'\tilde{\Omega}) = \langle u^*v\Omega, K_{\tilde{\Omega}, \Omega}u^*v\Omega \rangle. \quad (4.1.4b)$$

Proof. We will first prove the first two identities when $v = v' = \mathbb{1}$. Because $uu'\mathcal{R}(uu')^* = u\mathcal{R}u^* = \mathcal{R}$ we see from Lemma 4.1.1 that $uu'\tilde{\Omega}$ is again standard for $\mathcal{R}$. For all $a \in \mathcal{R}$ we have

$$\begin{aligned} S_{uu'\tilde{\Omega}, \Omega}a\Omega &= a^*uu'\tilde{\Omega} \\ &= u'(u^*a)^*\tilde{\Omega} \\ &= u'S_{\tilde{\Omega}, \Omega}u^*a\Omega. \end{aligned}$$

As $\mathcal{R}\Omega$ is a core for both $S_{uu'\tilde{\Omega},\Omega}$ and $u'S_{\tilde{\Omega},\Omega}u^*$ we find $S_{uu'\tilde{\Omega},\Omega} = u'S_{\tilde{\Omega},\Omega}u^*$. Using $\Delta_{\tilde{\Omega},\Omega} = S_{\tilde{\Omega},\Omega}^* S_{\tilde{\Omega},\Omega}$, $J_{\tilde{\Omega},\Omega} = S_{\tilde{\Omega},\Omega} \Delta_{\tilde{\Omega},\Omega}^{-\frac{1}{2}}$, and the functional calculus, this yields the first two identities when $v = v' = \mathbf{1}$. The general case then follows from Lemma 4.1.1 for the unitary vv' and a change of notation. For the final identity we compute

$$\begin{aligned} H(vv'\Omega, uu'\tilde{\Omega}) &= \left\langle vv'\Omega, v'uK_{\tilde{\Omega},\Omega}u^*v'^*vv'\Omega \right\rangle \\ &= \left\langle u^*v\Omega, K_{\tilde{\Omega},\Omega}u^*v\Omega \right\rangle. \end{aligned}$$

□

Note that u', v' cancel out in (4.1.4b) as anticipated above, so in particular $H(v'\Omega, u'\tilde{\Omega}) = H(\Omega, \tilde{\Omega})$. If $\mathcal{R}$ is a type III₁ von Neumann factor, a theorem of Connes and Størmer tells us that the set of states $\{\tilde{\Omega} = u'u\hat{\Omega} \mid u \in \mathcal{R}, u' \in \mathcal{R}'\}$ is dense in the unit sphere of $\mathcal{H}$ when $\hat{\Omega}$ is standard for $\mathcal{R}$, cf. [CS78, Cor. 6]. In the case where $\tilde{\Omega} = \Omega$ we find for the relative entropy

$$H(vv'\Omega, uu'\Omega) = \langle u^*v\Omega, K_{\Omega}u^*v\Omega \rangle. \quad (4.1.5)$$

Remark. In our applications to QFT, we may start with algebraic states $\omega, \tilde{\omega}$ on a C^* -algebra $\mathcal{A}$ and write $H(\tilde{\omega}, \omega)$ instead of $H(\tilde{\Omega}, \Omega)$, where we assume that both states can be represented by standard vectors Ω , resp. $\tilde{\Omega}$, in the GNS-representation space of ω and we take $\mathcal{R} = \pi_{\omega}(\mathcal{A})''$. We can see from (4.1.4b) that the choice of the representing vectors is irrelevant for the computation of the relative entropy, because the unitary $u' \in \mathcal{R}'$ defined as in (4.1.3) cancels out.

In the following lemma we consider two von Neumann algebras, $\mathcal{R}_1$ and $\mathcal{R}_2$, and we distinguish the corresponding modular data by the same label.

Lemma 4.1.3. *Let $\mathcal{R}_1 \subset \mathcal{R}_2$ be an inclusion of von Neumann algebras acting on $\mathcal{H}$ and $\Omega, \tilde{\Omega}$ standard vectors for both $\mathcal{R}_i$. Then*

$$K_{\tilde{\Omega},\Omega}^{(1)} \leq K_{\tilde{\Omega},\Omega}^{(2)} \quad (4.1.6a)$$

$$H^{(1)}(\Omega, \tilde{\Omega}) \leq H^{(2)}(\Omega, \tilde{\Omega}). \quad (4.1.6b)$$

Proof. The Tomita operator $S_{\tilde{\Omega},\Omega}^{(2)}$ for $\mathcal{R}_2$ extends the Tomita operator $S_{\tilde{\Omega},\Omega}^{(1)}$ for $\mathcal{R}_1$, so for any $a \in \mathcal{R}_1$ we have

$$\left\| \left(\Delta_{\tilde{\Omega},\Omega}^{(2)} \right)^{\frac{1}{2}} a\Omega \right\| = \left\| S_{\tilde{\Omega},\Omega}^{(2)} a\Omega \right\| = \|a^*\tilde{\Omega}\| = \left\| \left(\Delta_{\tilde{\Omega},\Omega}^{(1)} \right)^{\frac{1}{2}} a\Omega \right\|.$$

Now, $(\Delta_{\tilde{\Omega},\Omega}^{(1)})^{1/2}$ has a dense range on the core $\mathcal{R}_1\Omega$, so on this range we may define the operator

$$C := \left(\Delta_{\tilde{\Omega},\Omega}^{(2)} \right)^{\frac{1}{2}} \left(\Delta_{\tilde{\Omega},\Omega}^{(1)} \right)^{-\frac{1}{2}},$$

which is an isometry by the above computation, $C^*C = \mathbf{1}$. In particular, $\|C^*\| = \|C\| = 1$, so we find $CC^* \leq \mathbf{1}$, where $C^*a\Omega = (\Delta_{\tilde{\Omega},\Omega}^{(1)})^{-1/2}(\Delta_{\tilde{\Omega},\Omega}^{(2)})^{1/2}a\Omega$ for all $a \in \mathcal{R}_2$. This entails

$$0 < \left(\Delta_{\tilde{\Omega},\Omega}^{(1)} \right)^{-1} \leq \left(\Delta_{\tilde{\Omega},\Omega}^{(2)} \right)^{-1}$$

on the domain of $(\Delta_{\tilde{\Omega},\Omega}^{(2)})^{-1/2}$. Since the log function is operator monotone, cf. Section B.1, the result follows from the definitions (4.1.1) and (4.1.2). □

We will use the inequalities (4.1.6a) and (4.1.6b) in combination with (4.1.4a), (4.1.4b) and (4.1.5) by means of the following basic estimates.

Theorem 4.1.4. *Let $\mathcal{R}_1 \subset \mathcal{R}_2$ be an inclusion of von Neumann algebras acting on a Hilbert space $\mathcal{H}$ and let $u, v \in \mathcal{R}_2$ and $u', v' \in \mathcal{R}_1'$ be unitaries.*

i. If both vectors $u\Omega$ and $v\Omega$ are standard for both $\mathcal{R}_i$, then

$$K_{u'u\Omega, v'v\Omega}^{(1)} \leq v'uK_{\Omega}^{(2)}u^*v'^* \quad (4.1.7a)$$

$$H^{(1)}(v'v\Omega, u'u\Omega) \leq \left\langle u^*v\Omega, K_{\Omega}^{(2)}u^*v\Omega \right\rangle. \quad (4.1.7b)$$

ii. If both vectors $u'\Omega$ and $v'\Omega$ are standard for both $\mathcal{R}_i$, then

$$K_{uu'\Omega, vv'\Omega}^{(2)} \geq uv'K_{\Omega}^{(1)}v'^*u^* \quad (4.1.8a)$$

$$H^{(2)}(vv'\Omega, uu'\Omega) \geq \left\langle v'^*u^*vv'\Omega, K_{\Omega}^{(1)}v'^*u^*vv'\Omega \right\rangle. \quad (4.1.8b)$$

Beware of the different ordering of u and u' , resp. v and v' , in the two statements of this theorem.

Proof. Even if u and v are not in $\mathcal{R}_1$ and if they do not commute with u', v' , we can estimate

$$\begin{aligned} K_{u'u\Omega, v'v\Omega}^{(1)} &= v'K_{u\Omega, v\Omega}^{(1)}v'^* \\ &\leq v'K_{u\Omega, v\Omega}^{(2)}v'^* \\ &= v'uK_{\Omega}^{(2)}u^*v'^*, \end{aligned}$$

where we used (4.1.4a) for u', v' in the first line and for u, v in the last line, and (4.1.6a) for the inequality. Analogously,

$$\begin{aligned} H^{(1)}(v'v\Omega, u'u\Omega) &= H^{(1)}(v\Omega, u\Omega) \\ &\leq H^{(2)}(v\Omega, u\Omega) \\ &= \left\langle u^*v\Omega, K_{\Omega}^{(2)}u^*v\Omega \right\rangle, \end{aligned}$$

where we first used the identity (4.1.4b) to discard u', v' , then applied the estimate (4.1.6b) and finally used the identity (4.1.5), but now for the larger algebra $\mathcal{R}_2$, which does contain u and v . Similarly we can estimate

$$\begin{aligned} K_{uu'\Omega, vv'\Omega}^{(2)} &= uK_{u'\Omega, v'\Omega}^{(2)}u^* \\ &\geq uK_{u'\Omega, v'\Omega}^{(1)}u^* \\ &= uv'K_{\Omega}^{(1)}v'^*u^* \end{aligned}$$

and

$$\begin{aligned} H^{(2)}(vv'\Omega, uu'\Omega) &= \left\langle u^*vv'\Omega, K_{u'\Omega, v'\Omega}^{(2)}u^*vv'\Omega \right\rangle \\ &\geq \left\langle u^*vv'\Omega, K_{u'\Omega, v'\Omega}^{(1)}u^*vv'\Omega \right\rangle \\ &= \left\langle v'^*u^*vv'\Omega, K_{\Omega}^{(1)}v'^*u^*vv'\Omega \right\rangle. \end{aligned}$$

□

Remark. By similar arguments, using an exponentiated version of (4.1.4a) in Lemma 4.1.2 and $\Delta_{\tilde{\Omega},\Omega}^{(1)} \geq \Delta_{\tilde{\Omega},\Omega}^{(2)}$ instead of Lemma 4.1.3 one can also show that under the assumptions of Theorem 4.1.4 we have (i) $\Delta_{u'u\Omega, v'v\Omega}^{(1)} \geq v'u\Delta_{\Omega}^{(2)} u^* v'^*$ and (ii) $\Delta_{uu'\Omega, vv'\Omega}^{(2)} \leq uv'\Delta_{\Omega}^{(1)} v'^* u^*$.

Note that the assumptions of Theorem 4.1.4 only depend on the states on the algebra $\mathcal{R}_2$, not on the choice of vectors that implement these states. Indeed, if $\tilde{\Omega}$ defines the same state as $v'v\Omega$ on $\mathcal{R}_2$, then $\tilde{\Omega} = w'v'v\Omega$ for some unitary $w' \in \mathcal{R}'_2$ by (4.1.3), so the assumption of item (i) still holds with $w'v'$ instead of v' . A similar argument holds for the vectors $u'u\Omega$, $vv'\Omega$ and $uu'\Omega$. In the estimates for the relative entropies, the unitaries from $\mathcal{R}'_2$ cancel out.

4.1.1 Estimates on relative modular Hamiltonians in quantum field theory

Let $M = (\mathcal{M}, g)$ be a smooth globally hyperbolic Lorentzian manifold. To describe a QFT in M we assign to each causally convex open subset $V \subset M$ a C^* -algebra $\mathcal{A}_V$, which we think of as being generated by smearing any quantum fields of the theory with smooth test functions (or tensors) compactly supported in V . We will make the following standard assumption:

$$V_1 \subset V_2 \quad \Rightarrow \quad \mathcal{A}_{V_1} \subset \mathcal{A}_{V_2}. \quad (\text{isotony})$$

Any algebraic state ω on $\mathcal{A}_M$ restricts to a state on $\mathcal{A}_V$ for any causally convex open region $V \subset M$ and we denote by $\mathcal{R}_{\omega}^{(V)}$ the von Neumann algebra $\pi_{\omega}(\mathcal{A}_V)''$ generated from $\mathcal{A}_V$ in the GNS-representation of $\omega|_{\mathcal{A}_V}$.

If V is bounded, physically reasonable states on $\mathcal{A}_M$ are expected to have quasi-equivalent restrictions to $\mathcal{A}_V$. This means that every such state can be expressed by a density matrix in the GNS-representation of any other such state. This explains why the choice of Hilbert space representation is irrelevant for the description of local phenomena in QFT, cf. [Wit22; Haa12].

In many cases the GNS-vector Ω_{ω} is a standard vector for $\mathcal{R}_{\omega}^{(V)}$. This occurs e.g. when ω is a vacuum vector in Minkowski space and V is a bounded open region [RS61]. For more details on this property we refer to Section II of the nice review by Witten [Wit18].

Given any two quasi-equivalent states $\omega, \tilde{\omega}$ on $\mathcal{A}_V$ whose GNS-vectors are both standard, the Unitary Implementation Theorem applies, so we can represent both states by unit vectors Ω and $\tilde{\Omega}$ in a single (GNS-)Hilbert space representation. Moreover, we can introduce the relative modular theory of Section 1.2. Let us fix a standard unit vector $\hat{\Omega}$ for $\mathcal{R} = \mathcal{R}_{\omega}^{(V)}$ for reference purposes. If we can write $\Omega = vv'\hat{\Omega}$ and $\tilde{\Omega} = uu'\hat{\Omega}$ for some unitaries $u, v \in \mathcal{R}$ and $u', v' \in \mathcal{R}'$, then we can obtain results about the relative modular Hamiltonian and the relative entropy directly from Lemma 4.1.2. This case already covers a lot of states, due to the Connes-Størmer Theorem [CS78].

More generally, if we have three causally convex regions $V_1 \subset V_2 \subset V_3$ in M and if $\hat{\Omega}$ is a reference state that is standard for all three algebras $\mathcal{R}_i := \pi_{\hat{\omega}}(\mathcal{A}_{V_i})''$, $i = 1, 2, 3$, then we may try to apply the results of Theorem 4.1.4 to estimate the relative modular Hamiltonian $K_{\tilde{\Omega},\Omega}^{(2)}$ and the relative entropy $H^{(2)}(\Omega, \tilde{\Omega})$ from below, in terms of $K_{\hat{\Omega}}^{(1)}$, and from above, in terms of $K_{\hat{\Omega}}^{(3)}$. To apply the theorem, however, we need to be able to express the states $\tilde{\Omega}$ and Ω in terms of the reference state $\hat{\Omega}$ and suitably localised unitaries. To examine what this implies, let us analyse item (i) of Theorem 4.1.4, considering only the two regions $V_2 \subset V_3$ (with appropriate relabelling), cf. Figure 4.1a. (A similar argument could be made for item (ii) with regions $V_1 \subset V_2$.)

Item (i) of the Theorem 4.1.4 requires $\Omega = v'v\hat{\Omega}$, with $v' \in \mathcal{R}'_2$, $v \in \mathcal{R}_3$ and similarly for $\tilde{\Omega}$. Note that these conditions are independent of the choice of vectors, as long as they define the same state

on $\mathcal{R}_3$. Indeed, if Ω' , resp. $\hat{\Omega}'$, define the same states on $\mathcal{R}_3$ as Ω , resp. $\hat{\Omega}$, then we must have $\Omega' = w\Omega$, $\hat{\Omega}' = \hat{w}\hat{\Omega}$ for some unitaries $w, \hat{w} \in \mathcal{R}'_3$. The assumption of item (i) is then still verified with $wv'\hat{w}^*$ instead of v' .

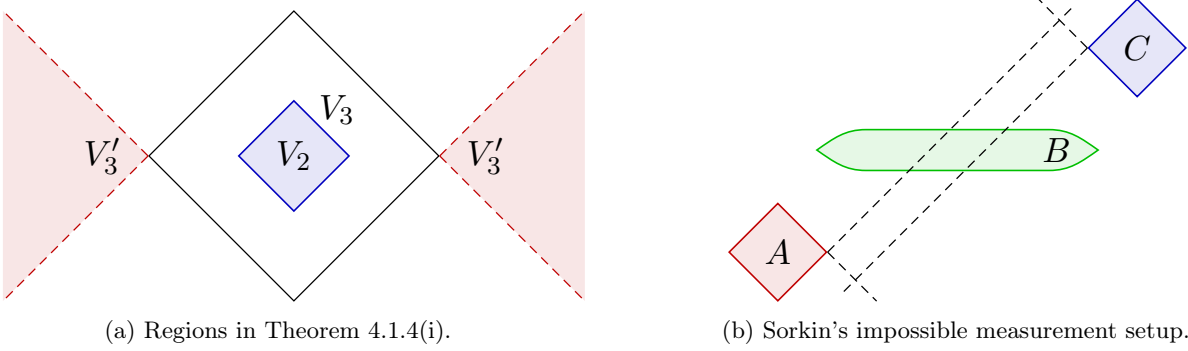


Figure 4.1: A comparison of the setup described in [Sor93] and Theorem 4.1.4(i).

To simplify the discussion, take the case where $\Omega = \hat{\Omega}$, i.e. one of the two states is our reference state. Then, in this setting, the theorem requires $\hat{\Omega} = u'u\Omega$, with $u' \in \mathcal{R}'_2$, $u \in \mathcal{R}_3$. It is then interesting to note that the applicability of Theorem 4.1.4 is related to Sorkin's paradox. In [Sor93], Sorkin points out that it is possible to construct examples of superluminal signalling, so-called 'impossible measurements'. More recently, [BJK21] and [Jub22] have formulated this discussion in terms of conditions on unitary operations to be non-signalling. The typical setting of these impossible measurements considers three observers, Alice, Bob and Charlie, located in corresponding regions A, B, C , such that A and C are spacelike separated, so Alice's actions cannot influence Charlie. However, B may lie partially in the future of A and partially in the past of C , so Alice's actions can influence Bob and Bob's actions can influence Charlie, cf. Figure 4.1b. An impossible measurement is a unitary operation performed by Bob in B that allows Charlie to determine whether Alice has performed some unitary operation on the shared quantum system or not. The existence of such impossible measurements is paradoxical, because it apparently violates the causality between A and C .

In the context of QFT, we may formalise this situation in the following way. Let $\mathcal{R}_A$ and $\mathcal{R}_C$ be the local algebras relative to regions A and C acting on a Hilbert space $\mathcal{H}$, so $[\mathcal{R}_A, \mathcal{R}_C] = 0$. Then, Bob's measurement in B is given by the adjoint action of some unitary w on $\mathcal{H}$ and

$$\begin{aligned} w \text{ does not allow signalling from } A \text{ to } C &\text{ iff } w\mathcal{R}_Aw^* \subset \mathcal{R}'_C, \\ w \text{ does not allow signalling from } C \text{ to } A &\text{ iff } w\mathcal{R}_Cw^* \subset \mathcal{R}'_A, \end{aligned}$$

cf. [BJK21, Sec. III].

As an example we consider unitaries of the simple product form $w = u'u$, with $u' \in \mathcal{R}'_C$, $u \in \mathcal{R}'_A$. Such operators are clearly non-signalling, as

$$w\mathcal{R}_Aw^* = u'u\mathcal{R}_Au^*u'^* = u'\mathcal{R}_Au'^* \subset \mathcal{R}'_C.$$

We may now relate the discussion back to the unitaries of Theorem 4.1.4, considering the regions $V_2 \subset V_3$ and identifying $A = V'_3$ and $C = V_2$ as shown in Figure 4.1, so $u \in \mathcal{R}'_A = \mathcal{R}_3$ and $u' \in \mathcal{R}'_C = \mathcal{R}'_2$. In this way, we are comparing signalling in the direction A to C with Theorem 4.1.4(i) (similarly, (ii) could be compared with signalling from C to A considering regions $V_1 \subset V_2$).

Now, one may ask how many pairs of states can be covered by our scheme. As mentioned before, Connes and Størmer [CS78] tell us that if $\mathcal{R}_2$ is a type III₁ von Neumann factor, the set of states $\{\tilde{\Omega} = u'u\hat{\Omega} \mid u \in \mathcal{R}_2, u' \in \mathcal{R}'_2\}$ is dense in the unit ball of $\mathcal{H}$. Because $u'u\hat{\Omega} = uu'\hat{\Omega}$ we see that this set of states satisfies the assumptions of part (i) of Theorem 4.1.4 w.r.t. $\mathcal{R}_2$ and $\mathcal{R}_3$ and of part (ii) w.r.t. $\mathcal{R}_1$ and $\mathcal{R}_2$. We can therefore certainly use any $\Omega, \tilde{\Omega}$ from this dense set.

On the other hand, it follows from the previous paragraphs that for $\Omega = \hat{\Omega}$ our upper estimate only applies if there is a unitary w such that $\tilde{\Omega} = w\Omega$ and w does not allow signalling from V'_3 to V_2 . (If we allow general unitaries on $\mathcal{H}$, this may not preclude the existence of another unitary w' such that $\tilde{\Omega} = w'\Omega$ and w' does allow signalling.) One may now ask whether the existence of such a non-signalling unitary w satisfying $\tilde{\Omega} = w\Omega$ is also sufficient to ensure that our upper estimate applies. In complete analogy, for our lower bound to apply it is necessary that there exists a unitary w such that $\tilde{\Omega} = w\Omega$ and w does not allow signalling from V_1 to V'_2 and one may wonder whether the existence of such a w is also sufficient for the lower bound to apply.

For type I_∞ factors the following (counter-)example shows that this is not the case.

Example 4.1.5 (Type I_∞ factors). *Let $\mathcal{H}$ be an infinite dimensional Hilbert space, $n \in \mathbb{N}$ and $\{u_i\}_{i=1}^n$ operators on $\mathcal{H}$ satisfying*

$$u_i u_j^* = \delta_{ij} \mathbb{1}, \quad \sum_i u_i^* u_i = \mathbb{1}. \quad (4.1.9)$$

Then, the operators u_i generate a Cuntz algebra. We note that a von Neumann algebra $\mathcal{R}$ acting on $\mathcal{H}$ contains operators $u_i \in \mathcal{R}$ with these properties if it is a von Neumann factor of type I_∞ or of type III, cf. [KR97b, Def. 6.5.1 and Lemma 6.3.3]. (See also the discussion in Section 1.1.3.)

Now consider the type I_∞ von Neumann factors $\mathcal{R}_2 = \mathcal{R}_3 = \mathbb{C}\mathbb{1} \otimes \mathcal{B}(\mathcal{H})$ on $\mathcal{H} \otimes \mathcal{H}$ and operators $u_i \in \mathcal{R}_3$ and $u'_i \in \mathcal{R}'_2 = \mathcal{B}(\mathcal{H}) \otimes \mathbb{C}\mathbb{1}$ such that u_i and $(u'_i)^*$ satisfy the relations (4.1.9). Then $w := \sum_{i=1}^n u'_i u_i$ is a unitary which is non-signalling between $\mathcal{R}'_3$ and $\mathcal{R}_2$, because

$$w \mathcal{R}'_3 w^* = \sum_{i,j=1}^n u'_i u_i \mathcal{R}'_3 u_j^* u_j^* = \sum_{i,j=1}^n u'_i u_i u_j^* \mathcal{R}'_3 u_j^* = \sum_{i=1}^n u'_i \mathcal{R}'_3 u_i^* \subset \mathcal{R}'_2. \quad (4.1.10)$$

We may write $u_i = \mathbb{1} \otimes v_i$ and $u'_i = v'_i \otimes \mathbb{1}$, where v_i and $(v'_i)^*$ also satisfy the relations (4.1.9). Let the subspaces $\mathcal{H}'_i$ be the ranges of the projections $v'_i v_i^*$, so $\mathcal{H} = \bigoplus_{i=1}^n \mathcal{H}'_i$ and similarly for $\mathcal{H}_i$ with $v_i^* v_i$. For $n > 1$, we will choose a suitable standard vector $\hat{\Omega}$ for $\mathcal{R}_2 = \mathcal{R}_3$ as follows. We fix two orthonormal vectors $\chi_1, \chi_2 \in \mathcal{H}$ and we define the unit vector $\psi_1 := \frac{1}{\sqrt{2}}(v_1^* \chi_1 + v_2^* \chi_2)$. We extend the vector ψ_1 to an orthonormal basis $\{\psi_i\}$ of $\mathcal{H}$ and we choose another orthonormal basis $\{\psi'_i\}$. For any $\varepsilon \in (0, 1)$ we then choose a sequence of positive numbers $\{c_i\}$ with $c_1 = 1 - \varepsilon$ and we set $\hat{\Omega} := \sum_{i=1}^{\infty} c_i \psi'_i \otimes \psi_i$. This is indeed a standard vector, because $c_i > 0$ for all i . Now suppose that there exist two unitaries u, u' on $\mathcal{H}$ such that $w\hat{\Omega} = u' \otimes u\hat{\Omega}$. We will derive a contradiction, showing that no such u, u' exist.

Note that $\|\hat{\Omega} - c_1 \psi'_1 \otimes \psi_1\|^2 = 1 - c_1^2 = 2\varepsilon - \varepsilon^2$, so $\|\hat{\Omega} - c_1 \psi'_1 \otimes \psi_1\| \leq \sqrt{2\varepsilon}$. Because w and $u' \otimes u$ are unitaries, we similarly have $\|w(\hat{\Omega} - c_1 \psi'_1 \otimes \psi_1)\| \leq \sqrt{2\varepsilon}$ and $\|u' \otimes u(\hat{\Omega} - c_1 \psi'_1 \otimes \psi_1)\| \leq \sqrt{2\varepsilon}$ and hence

$$\|(u' \otimes u)\hat{\Omega} - w\hat{\Omega}\| \geq (1 - \varepsilon)\|u' \psi'_1 \otimes u\psi_1 - w\psi'_1 \otimes \psi_1\| - 2\sqrt{2\varepsilon},$$

where we used $c_1 = 1 - \varepsilon$. Now, $w = \sum_{i=1}^n v'_i \otimes v_i$ and $v_i \psi_1 = \frac{1}{\sqrt{2}} \chi_i$ with $\chi_i = 0$ for $i > 2$ imply

$$w\psi'_1 \otimes \psi_1 = \sum_{i=1}^n v'_i \psi'_1 \otimes v_i \psi_1 = \frac{1}{\sqrt{2}} \sum_{i=1}^2 v'_i \psi'_1 \otimes \chi_i.$$

With this and the Cauchy-Schwarz inequality we estimate

$$\begin{aligned}
\|u'\psi'_1 \otimes u\psi_1 - w\psi'_1 \otimes \psi_1\|^2 &= 2 - \sqrt{2} \sum_{i=1}^2 \operatorname{Re} \langle u'\psi'_1, v'_i\psi'_1 \rangle \langle u\psi_1, \chi_i \rangle \\
&\geq 2 - \sqrt{2} \sum_{i=1}^2 |\langle u'\psi'_1, v'_i\psi'_1 \rangle| |\langle u\psi_1, \chi_i \rangle| \\
&\geq 2 - \sqrt{2} \sqrt{\sum_{i=1}^2 |\langle u'\psi'_1, v'_i\psi'_1 \rangle|^2} \sqrt{\sum_{i=1}^2 |\langle u\psi_1, \chi_i \rangle|^2} \\
&\geq 2 - \sqrt{2} \sqrt{\|u'\psi'_1\|^2} \sqrt{\|u\psi_1\|^2} \\
&= 2 - \sqrt{2},
\end{aligned}$$

where we used the fact that the vectors $v'_i\psi'_1$ are orthonormal. It then follows that

$$\|(u' \otimes u)\hat{\Omega} - w\hat{\Omega}\| \geq (1 - \varepsilon) \sqrt{2 - \sqrt{2}} - 2\sqrt{2}\varepsilon$$

which is strictly positive when ε is sufficiently small.

Note that the unitaries w described in this example are thus non-signalling but not of the simple product form $w = u'u$ of Theorem 4.1.4 when $n > 1$, for otherwise $w\psi'_1 \otimes \psi_1$ would also be a simple tensor product, which is not the case. In the QFT case, however, if $\mathcal{R}'_2 \cap \mathcal{R}_3$ is a type III₁ factor, then $w = u'u$. To see this, we note that we can choose operators $c_1, \dots, c_n \in \mathcal{R}'_2 \cap \mathcal{R}_3$ generating a Cuntz algebra, so $c_i^*c_j = \delta_{ij}\mathbb{1}$ and $\sum_i c_i c_i^* = \mathbb{1}$. Then we can define $u' := \sum_i u'_i c_i^*$ and $u := \sum_i c_i u_i$, which will be unitary by the relations (4.1.9), and we get that

$$u'u = \sum_{i,j=1}^n u'_i c_i^* c_j u_j = w.$$

The reason why this argument breaks down in the example is that there we had $\mathcal{R}'_2 \cap \mathcal{R}_3 = \mathbb{C}\mathbb{1} \otimes \mathbb{1}$, which does not contain operators c_i satisfying (4.1.9).

Remark. The construction described in this section may also be formulated through the split property we defined in Section 2.2, cf. Proposition 2.2.2. Indeed, consider algebras $\mathcal{R}_A, \mathcal{R}_C$ corresponding to strictly spacelike separated regions A and C , as in Figure 4.1b. For convenience, we may consider $B = (A \cup C)''$, so Bob's measurement in B is given by the adjoint action of a unitary $u \in \mathcal{R}_B$. Then, if we assume that the incoming (reference) state for the experiment, $\hat{\Omega}$, is standard for $\mathcal{R}'_A \wedge \mathcal{R}'_C$, we have that $\mathcal{R}_A \subset \mathcal{R}'_C$ is a standard¹ split inclusion w.r.t. $\hat{\Omega}$, so we get an isomorphism $\mathcal{R}_B = \mathcal{R}_A \vee \mathcal{R}_C \cong \mathcal{R}_A \otimes \mathcal{R}_C$ acting on $\mathcal{H} \otimes \mathcal{H}$ and we can consider Bob's unitary to be acting on this tensor product of algebras, as for Proposition 2.2.2. In Example 4.1.5, this logic was already applied in the case of type I_∞ factors. If we try to extend the discussion to type III factors, as we have that $\mathcal{R}_A \otimes \mathbb{1} \subset \mathcal{B}(\mathcal{H}) \otimes \mathbb{1}$ and $\mathbb{1} \otimes \mathcal{R}_C \subset \mathbb{1} \otimes \mathcal{B}(\mathcal{H})$, where the inclusions are strict, and $(\mathcal{R}_A \otimes \mathbb{1})' = \mathcal{R}'_A \otimes \mathcal{B}(\mathcal{H})$ and $(\mathbb{1} \otimes \mathcal{R}_C)' = \mathcal{B}(\mathcal{H}) \otimes \mathcal{R}'_C$, we may write the non-signalling condition from A to C as $w(\mathcal{R}_A \otimes \mathbb{1})w^* \subset (\mathbb{1} \otimes \mathcal{R}_C)' = \mathcal{B}(\mathcal{H}) \otimes \mathcal{R}'_C$. This does not however seem to be of help to generalize the class of non-signalling unitaries beyond simple products in the case of type III factors.

¹In the language of [DL84], it is a *semi-standard* split inclusion, cf. Section 2.2.

As a last point, we will note that the class of unitaries susceptible to our scheme in QFT, i.e. the simple products $w = u'u$, with $u' \in \mathcal{R}'_2$, $u \in \mathcal{R}_3$, contains the unitaries generating the dynamical algebra $\mathcal{A}_M^{(\mathcal{L})}$ in the Buchholz-Fredenhagen approach to Lagrangian QFTs presented in Section 2.1.3, w.r.t. a spacetime $M = (\mathcal{M}, g)$ and a Lagrangian $\mathcal{L}$ describing a scalar field. This is a direct consequence of causal factorization, point *iv.* of Definition 2.1.10.

Proposition 4.1.6. *Let $M = (\mathcal{M}, g)$ be a globally hyperbolic spacetime and $\mathcal{A}_M^{(\mathcal{L})}$ the dynamical algebra associated with a scalar field Lagrangian $\mathcal{L}$, satisfying the time-slice axiom. Let $V_2 \subset V_3$ be causally convex open regions in M , and let $\mathcal{R}_i = \pi(\mathcal{A}(V_i))''$ ($i = 2, 3$) be the associated local von Neumann algebras in a given representation π . Let $U(F)$ be a unitary generator of $\mathcal{A}_M^{(\mathcal{L})}$ associated with an admissible functional $F \in \mathcal{F}(M, \mathcal{L})$. (By the time-slice axiom, assume w.l.o.g. that F is supported within a Cauchy slice intersecting both V_2 and V_3 .) Then, given a smooth partition of unity decomposing $F = F_1 + F_2 + F_3$ such that*

- i.* $\text{supp}(F_1) \subset V'_2$, $\text{supp}(F_2) \subset V_3$, and $\text{supp}(F_3) \subset V'_2 \cap V_3$;
- ii.* the functionals $F_1 + F_3$, $F_2 + F_3$, and F_3 belong to $\mathcal{F}(M, \mathcal{L})$;
- iii.* $\text{supp}(F_1) \cap J_{(M, g_{F_3})}^-(\text{supp}(F_2)) = \emptyset$;

we have that $U(F)$ factorizes as $U(F) = u'u$, where $u' \in \mathcal{R}'_2$ and $u \in \mathcal{R}_3$.

Proof. As $F = F_1 + F_2 + F_3$ and conditions *ii.* and *iii.* hold, we may directly apply the causal factorization property of the dynamical algebra, point *iv.* of Definition 2.1.10. This yields

$$U(F) = U(F_1 + F_3 + F_2) = U(F_1 + F_3)U(F_3)^*U(F_3 + F_2).$$

Since both F_1 and F_3 are supported in V'_2 , $U(F_1 + F_3) \in \mathcal{R}'_2$. Similarly, since both F_2 and F_3 are supported in V_3 , we have $U(F_3 + F_2) \in \mathcal{R}_3$. Because $\text{supp}(F_3) \subset V'_2 \cap V_3$, we also have that $U(F_3)$ and $U(F_3)^*$ belong to both algebras. We can then define $u := U(F_3)^*U(F_3 + F_2) \in \mathcal{R}_3$, and set $u' := U(F_1 + F_3) \in \mathcal{R}'_2$. By identifying u' and u in this manner, $U(F)$ factorizes as $w = u'u$. $\square$

In particular, we can always obtain a functional of the kind prescribed by Proposition 4.1.6 in our setting, provided the perturbations of the metric are sufficiently small. As the regions V'_2 and V_3 overlap and lack a strict global time ordering, we need to consider suitably supported functionals to be able to apply causal factorization. Note that partitioning an arbitrary functional F spatially and temporally may fail if F is supported infinitely far in the past outside of V_3 . However, this reasoning retains generality thanks to the time-slice axiom, which allows the entire dynamical algebra to be generated by functionals supported in an arbitrarily thin Cauchy slice, which we may assume to intersect both V_2 and V_3 . Within this bounded region, we may use a smooth partition of unity to write $F = F_1 + F_3 + F_2$. Because M is globally hyperbolic, its causal structure admits a foliation by Cauchy surfaces, allowing us to choose cutoff functions such that no part of F_1 lies in the causal past of F_2 . This separation must hold w.r.t. the deformed metric g_{F_3} , ensuring $\text{supp}(F_1) \cap J_{(M, g_{F_3})}^-(\text{supp}(F_2)) = \emptyset$. At the same time, because $V_2 \subset V_3$, we can choose the spatial boundaries of these cutoffs such that $\text{supp}(F_1) \subset V'_2$, $\text{supp}(F_2) \subset V_3$, and $\text{supp}(F_3) \subset V'_2 \cap V_3$, so F_3 is supported at spacelike separation to both V_2 and V'_3 . Then, to guarantee that the partitioned functionals satisfy condition *ii.*, we can restrict our generating unitaries to sufficiently small perturbations γ^{ab} such that truncating them via the smooth partition of unity does not destroy the global hyperbolicity of the underlying spacetime. With these geometric and causal conditions satisfied, we are then able to apply Proposition 4.1.6, so the dynamical algebra generators belong to the class of simple products to which our scheme applies.

(A similar argument can be also made in the case of regions $V_1 \subset V_2$, corresponding to point *ii.* of Theorem 4.1.4.)

4.2 Generalities on coherent states

In this section, we consider coherent states in general, bosonic CCR systems. Before we apply our general estimates to these states, we first review the fact that one can often compute relative modular Hamiltonians explicitly due to some remarkable simplifications. Moreover, the relative entropy can always be determined, but it might be infinite. Let us begin by recalling some general concepts and fixing our notations following Section A.1, to which we refer for more technical details.

Let $\mathcal{H}$ be a complex Hilbert space and $\mathcal{F}_+(\mathcal{H}) = \bigoplus_{n=0}^{\infty} \mathcal{H}^{\otimes n}$ its bosonic Fock space with Fock vector $\Omega_F \in \mathcal{H}^{\otimes 0} = \mathbb{C}$. For any unitary u on $\mathcal{H}$ we denote the second quantised unitary on $\mathcal{F}_+(\mathcal{H})$ by $\Gamma(u)$, so that $\Gamma(u)^* = \Gamma(u^*)$. For a self-adjoint operator h on $\mathcal{H}$ we define $d\Gamma(h)$ implicitly by $e^{itd\Gamma(h)} = \Gamma(e^{ith})$ for all $t \in \mathbb{R}$. For any $\chi \in \mathcal{H}$ we let $a^*(\chi)$ and $a(\chi)$ denote the usual creation and annihilation operators, satisfying $a(\chi)\Omega_F = 0$ and the canonical commutation relations (CCR)

$$\begin{aligned} [a(\chi), a^*(\xi)] &= \langle \chi, \xi \rangle \mathbb{1} \\ [a(\chi), a(\xi)] &= 0 \end{aligned}$$

for all $\chi, \xi \in \mathcal{H}$. Note that the operators $a^*(\chi)$ and $a(\chi)$ are closed, unbounded if $\chi \neq 0$ and each other's adjoints. We define the Segal field operator by

$$\varphi_S(\chi) := \frac{1}{\sqrt{2}}(a^*(\chi) + a(\chi))$$

for any $\chi \in \mathcal{H}$. This operator is self-adjoint and unbounded if $\chi \neq 0$. Weyl operators are unitaries defined by $W(\chi) := e^{i\varphi_S(\chi)}$ for $\chi \in \mathcal{H}$ and they satisfy the Weyl relations

$$W(\chi)W(\xi) = e^{-\frac{i}{2}\text{Im}\langle \chi, \xi \rangle} W(\chi + \xi) \quad (4.2.1)$$

for all $\chi, \xi \in \mathcal{H}$. For any closed real linear subspace $H \subset \mathcal{H}$ we consider the von Neumann algebra $\mathcal{R}(H) := \{W(\chi) \mid \chi \in H\}''$ generated by the Weyl operators with $\chi \in H$. It is known that Ω_F is a cyclic, resp. separating, vector for $\mathcal{R}(H)$ iff $\overline{H + iH} = \mathcal{H}$, resp. $H \cap iH = \{0\}$, cf. [AY82, Thm. 3.12]. To have a standard vector we therefore need to assume both these properties and in that case H is called a standard subspace. If $H \subset \mathcal{H}$ is standard, then it is known that the modular Hamiltonian of $\mathcal{R}(H)$ for Ω_F is of second quantised form,

$$K_{\Omega_F} = d\Gamma(K_H),$$

where K_H is a self-adjoint operator on $\mathcal{H}$. Indeed, modular theory can be developed for standard subspaces [Lon08], where we have $K_H = -\log(\Delta_H)$ and Δ_H appears in the polar decomposition $S_H = J_H \sqrt{\Delta_H}$ of the closed antilinear operator $S_H : H + iH \rightarrow H + iH$ defined by $S_H(\chi + i\xi) = \chi - i\xi$ for all $\chi, \xi \in H$.

For later convenience we mention here the following technical lemma.

Lemma 4.2.1. *Let $I \subset \mathbb{R}$ be an open interval containing 0 and $h : I \rightarrow \mathcal{H}$ a continuous $\mathcal{H}$ -valued function with $h(0) = 0$. If $h'(0)$ exists and $\psi \in \mathcal{F}_+(\mathcal{H})$ is a finite particle vector, then*

$$\left. \frac{d}{dt} W(h(t))\psi \right|_{t=0} = i\varphi_S(h'(0))\psi.$$

Proof. The proof uses standard particle number estimates. Suppose $\psi \in \bigoplus_{n=0}^N \mathcal{H}^{\otimes n}$ has at most N particles for some $N \in \mathbb{Z}_{\geq 0}$. For any $\chi \in \mathcal{H}$ we then have $\|a^*(\chi)\psi\| \leq \sqrt{N+1}\|\chi\| \cdot \|\psi\|$ and $\|a(\chi)\psi\| \leq \sqrt{N}\|\chi\| \cdot \|\psi\|$ and therefore also $\|\varphi_S(\chi)\psi\| \leq \sqrt{2(N+1)}\|\chi\| \cdot \|\psi\|$. Iterating this estimate

n times we find $\|\varphi_S(\chi)^n \psi\| \leq 2^{\frac{n}{2}} \sqrt{\frac{(N+n)!}{N!}} \|\chi\|^n \|\psi\|$ for any $n \in \mathbb{N}$. Using $\sqrt{\frac{(N+n)!}{N!}} \leq (N+1)^{\frac{n}{2}} \sqrt{n!}$ this estimate can be brought into the more convenient form

$$\|\varphi_S(\chi)^n \psi\| \leq (2(N+1))^{\frac{n}{2}} \|\chi\|^n \sqrt{n!} \|\psi\|. \quad (4.2.2)$$

It follows that the power series expansion for $W(\chi)\psi$ converges absolutely, because

$$\left\| \sum_{n=0}^{\infty} \frac{i^n}{n!} \varphi_S(\chi)^n \psi \right\| \leq \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} (2(N+1))^{\frac{n}{2}} \|\chi\|^n \|\psi\| < \infty.$$

Similarly, for $t \neq 0$ the series

$$\frac{1}{t} \left[W(h(t))\psi - \psi \right] - i\varphi_S(h'(0))\psi = i\varphi_S \left(\frac{1}{t}h(t) - h'(0) \right) \psi + \sum_{n=2}^{\infty} \frac{i^n}{n!} \frac{1}{t} \varphi_S(h(t))^n \psi$$

converges absolutely. To estimate the terms in the series we use the assumptions on $h(t)$. For any $\varepsilon \in (0, 1]$ there is a $\delta > 0$ such that $|t| < \delta$ implies $\left\| \frac{1}{t}h(t) - h'(0) \right\| < \varepsilon \leq 1$ and hence $\|h(t)\| < c|t|$ with $c := 1 + \|h'(0)\|$. Using (4.2.2) we then find

$$\left\| \frac{1}{t} \left[W(h(t))\psi - \psi \right] - i\varphi_S(h'(0))\psi \right\| \leq \sqrt{2(N+1)\varepsilon} \|\psi\| + \sum_{n=2}^{\infty} \frac{1}{\sqrt{n!}} (2(N+1)c^2)^{\frac{n}{2}} |t|^{n-1} \|\psi\|$$

if $|t| < \delta$. The series converges for any $t \in \mathbb{R}$ and we can make it arbitrarily small by choosing $|t|$ sufficiently small. Because $\varepsilon > 0$ was arbitrary we find

$$\lim_{t \rightarrow 0} \frac{1}{t} \left[W(h(t))\psi - \psi \right] - i\varphi_S(h'(0))\psi = 0.$$

The result then follows from the observation that $W(h(0))\psi = W(0)\psi = \psi$. □

4.2.1 Relative modular Hamiltonians for coherent states

A coherent state, or rather a coherent excitation of Ω_F , is a unit vector of the form $W(\chi)\Omega_F$ for some $\chi \in \mathcal{H}$. Note that the unitary $W(\chi)$ preserves any von Neumann algebra of the form $\mathcal{R}(H)$ with $H \subset \mathcal{H}$ closed, because the Weyl relations imply

$$W(-\chi)W(\xi)W(\chi) = e^{i\text{Im}\langle \chi, \xi \rangle} W(\xi) \quad (4.2.3)$$

for any $\xi \in H$. This means that relative modular Hamiltonians exist for any pair of coherent states and also the relative entropy can always be defined, although it may sometimes be infinite.

For many pairs of coherent states the relative modular Hamiltonian can be computed exactly. The following result concerns a slightly more general class of states, but uses the same methods as [CLR20; Lon19].

Proposition 4.2.2. *Let $H \subset \mathcal{H}$ be a standard subspace, $\hat{\Omega} \in \mathcal{F}_+(\mathcal{H})$ a standard vector for $\mathcal{R}(H)$ and $\Omega := W(\chi)\hat{\Omega}$, $\tilde{\Omega} := W(\tilde{\chi})\hat{\Omega}$ for some $\chi, \tilde{\chi} \in \mathcal{H}$. If there are $h \in H$ and $h' \in H'$ such that $\chi - \tilde{\chi} = h + h'$, then $W(\chi)\mathcal{R}(H)W(-\chi) = \mathcal{R}(H)$ and*

$$\begin{aligned} J_{\tilde{\Omega}, \Omega} &= W(\tilde{\chi} + h) J_{\hat{\Omega}} W(-\chi + h) \\ K_{\tilde{\Omega}, \Omega} &= W(\chi - h) K_{\hat{\Omega}} W(-\chi + h). \end{aligned}$$

Proof. It follows from (4.2.3) that the adjoint action of $W(\chi)$ preserves a strongly dense sub-algebra of $\mathcal{R}(H)$ and therefore it preserves $\mathcal{R}(H)$, $W(\chi)\mathcal{R}(H)W(-\chi) = \mathcal{R}(H)$. The same applies to $W(\tilde{\chi})$ and using Lemma 4.1.1 with $u = W(\tilde{\chi})$, the identity $W(-\tilde{\chi})W(\chi) = e^{\frac{i}{2}\text{Im}\langle\tilde{\chi},\chi\rangle}W(h)W(h')$, and Lemma 4.1.2 we find

$$\begin{aligned} S_{\tilde{\Omega},\Omega} &= W(\tilde{\chi})S_{\hat{\Omega},W(-\tilde{\chi})W(\chi)\hat{\Omega}}W(-\tilde{\chi}) \\ &= e^{\frac{i}{2}\text{Im}\langle\tilde{\chi},\chi\rangle}W(\tilde{\chi})W(h)S_{\hat{\Omega}}W(-h')W(-\tilde{\chi}) \\ &= e^{\frac{i}{2}\text{Im}\langle\tilde{\chi},\chi-h\rangle}W(\tilde{\chi}+h)S_{\hat{\Omega}}e^{\frac{i}{2}\text{Im}\langle\tilde{\chi},h'\rangle}W(-\tilde{\chi}-h') \\ &= W(\tilde{\chi}+h)S_{\hat{\Omega}}W(-\chi+h), \end{aligned}$$

where we recall that $\chi - \tilde{\chi} = h + h'$ and $S_{\hat{\Omega}}$ is antilinear. Using the polar decomposition of $S_{\tilde{\Omega},\Omega}$ and the spectral calculus the results now follow. $\square$

If $\hat{\Omega} = \Omega_F$ is the Fock vector, then the states $\Omega, \tilde{\Omega}$ are coherent. In that case, we can use the Fock space structure to further simplify the formula for the relative modular Hamiltonian in Proposition 4.2.2, cf. the results of Section A.4.1.

Corollary 4.2.3. *Under the assumptions of Proposition 4.2.2, if $\hat{\Omega} = \Omega_F$ and $\chi - h$ is in the domain of K_H , then*

$$K_{\tilde{\Omega},\Omega} = K_{\Omega_F} + \frac{1}{2}\langle\chi - h, K_H(\chi - h)\rangle\mathbb{1} - \varphi_S(iK_H(\chi - h)),$$

when acting on finite particle vectors in the domain of K_{Ω_F} .

Proof. For any unitary u on $\mathcal{H}$ and any $\xi \in \mathcal{H}$, we have $\Gamma(u)a^*(\xi)\Gamma(u)^* = a^*(u\xi)$. Using this identity and its adjoint we find $\Gamma(u)\varphi_S(\xi)\Gamma(u)^* = \varphi_S(u\xi)$ and hence

$$\Gamma(u)W(\xi)\Gamma(u)^* = W(u\xi). \quad (4.2.4)$$

By the Weyl relations this yields

$$W(-\xi)\Gamma(u)W(\xi)\Gamma(u)^* = W(-\xi)W(u\xi) = e^{\frac{i}{2}\text{Im}\langle\xi,u\xi\rangle}W((u-1)\xi).$$

Taking $u = e^{itK}$ for a self-adjoint operator K whose domain contains ξ , we may use Lemma 4.2.1 for $h(t) = (e^{itK} - 1)\xi$ to differentiate w.r.t. t at $t = 0$, which yields

$$W(-\xi)d\Gamma(K)W(\xi) - d\Gamma(K) = \frac{1}{2}\langle\xi, K\xi\rangle\mathbb{1} + \varphi_S(iK\xi) \quad (4.2.5)$$

when acting on any finite particle vector in the domain of $d\Gamma(K)$. Taking $K = K_H$ and $\xi = h - \chi$ then yields the result. $\square$

Using similar arguments one may compute the relative entropy.

Corollary 4.2.4. *Under the assumptions of Proposition 4.2.2, if $\hat{\Omega} = \Omega_F$ and h is in the domain of K_H , then*

$$H(\Omega, \tilde{\Omega}) = \frac{1}{2}\langle h, K_H h \rangle.$$

Proof. From Proposition 4.2.2 and the Weyl relations (1.3.1), we find

$$H(\Omega, \tilde{\Omega}) = \langle W(h - \chi)\Omega, K_{\Omega_F} W(h - \chi)\Omega \rangle = \langle \Omega_F, W(-h)K_{\Omega_F} W(h)\Omega_F \rangle.$$

Because h is in the domain of K_H and $K_{\Omega_F}\Omega_F = 0$, we may apply the identity (4.2.5) to find the result. (The fact that $H(\Omega, \tilde{\Omega}) \geq 0$ is not clear from this formula, but follows from passivity [LM23; PW78].) $\square$

More generally, [CLR20, Thm. 4.5] determines the relative entropy of any two standard coherent states by approximating them by states to which Proposition 4.2.2 applies and by using the lower semi-continuity of the relative entropy [Ara75; Kos86]. The result is then well-defined, but may be infinite. A further generalization to relative entropies for non-standard states can be found in [BCD22]. Note that the approximation argument may not apply to the relative modular Hamiltonian as an operator. In such cases it may be useful to consider estimates.

4.2.2 Estimates for coherent states

In order to apply our estimates to coherent states, we fix two standard subspaces $H_i \subset \mathcal{H}$ with $H_1 \subset H_2$, the reference state $\hat{\Omega} = \Omega_F$, which is standard for both $\mathcal{R}(H_i)$, and two coherent states, $\Omega = W(\chi)\Omega_F$ and $\tilde{\Omega} = W(\tilde{\chi})\Omega_F$ with $\chi, \tilde{\chi} \in \mathcal{H}$. Furthermore, we assume that $\chi = \chi_1 + \chi_2$ and $\tilde{\chi} = \tilde{\chi}_1 + \tilde{\chi}_2$ with $\chi_2, \tilde{\chi}_2 \in H_2$ and $\chi_1, \tilde{\chi}_1 \in H'_1 = (iH_1)^{\perp r}$, the symplectic adjoint of H_1 . Then we can decompose the Weyl operator

$$\begin{aligned} W(\chi) &= e^{\frac{i}{2} \text{Im}\langle \chi_1, \chi_2 \rangle} W(\chi_1) W(\chi_2) \\ &= e^{-\frac{i}{2} \text{Im}\langle \chi_1, \chi_2 \rangle} W(\chi_2) W(\chi_1) \end{aligned} \quad (4.2.6)$$

and similarly for $W(\tilde{\chi})$. The Weyl operators $W(\chi_i)$ are unitaries in $\mathcal{R}(H_i)$, so we can combine Theorem 4.1.4 with Equation (4.2.5) to find

$$\begin{aligned} K_{\tilde{\Omega}, \Omega}^{(1)} &\leq W(\chi_1 + \tilde{\chi}_2) K_{\Omega_F}^{(2)} W(-\chi_1 - \tilde{\chi}_2) \\ &= K_{\Omega_F}^{(2)} + \frac{1}{2} \langle \chi_1 + \tilde{\chi}_2, K_{H_2}(\chi_1 + \tilde{\chi}_2) \rangle - \varphi_S(iK_{H_2}(\chi_1 + \tilde{\chi}_2)) \\ K_{\tilde{\Omega}, \Omega}^{(2)} &\geq W(\chi_1 + \tilde{\chi}_2) K_{\Omega_F}^{(1)} W(-\chi_1 - \tilde{\chi}_2) \\ &= K_{\Omega_F}^{(1)} + \frac{1}{2} \langle \chi_1 + \tilde{\chi}_2, K_{H_1}(\chi_1 + \tilde{\chi}_2) \rangle - \varphi_S(iK_{H_1}(\chi_1 + \tilde{\chi}_2)), \end{aligned}$$

where the second, resp. fourth, line holds if $\chi_1 + \tilde{\chi}_2$ is in the domain of K_{H_2} , resp. K_{H_1} , and the expression acts on a finite particle vector in the domain of $K_{\Omega_F}^{(2)}$, resp. $K_{\Omega_F}^{(1)}$. If $\chi_1 - \tilde{\chi}_1 \in H'_2$, then we may apply Corollary 4.2.3 to see that the right-hand side of the first estimate is $K_{\tilde{\Omega}, \Omega}^{(2)}$. Similarly, if $\chi_2 - \tilde{\chi}_2 \in H_1$, then the right-hand side of the second estimate is $K_{\tilde{\Omega}, \Omega}^{(1)}$.

For the relative entropy we find in a similar way

$$\begin{aligned} H^{(1)}(\Omega, \tilde{\Omega}) &\leq \frac{1}{2} \langle \chi_2 - \tilde{\chi}_2, K_{H_2}(\chi_2 - \tilde{\chi}_2) \rangle \\ H^{(2)}(\Omega, \tilde{\Omega}) &\geq \frac{1}{2} \langle \chi_2 - \tilde{\chi}_2, K_{H_1}(\chi_2 - \tilde{\chi}_2) \rangle \end{aligned}$$

if $\chi_2 - \tilde{\chi}_2$ is in the domain of K_{H_2} (for the upper bound), resp. K_{H_1} (for the lower bound). If $\chi_1 - \tilde{\chi}_1 \in H'_2$, resp. $\chi_2 - \tilde{\chi}_2 \in H_1$, then we may apply Corollary 4.2.4 to see that the right-hand side of the first, resp. second, estimate is $H^{(2)}(\Omega, \tilde{\Omega})$, resp. $H^{(1)}(\Omega, \tilde{\Omega})$.

4.3 Coherent excitations in free scalar QFT

To investigate the quality of our estimates we will now consider the simplest toy model, the free scalar field in the Minkowski vacuum representation.

In $(d+1)$ -dimensional Minkowski spacetime with signature $(-, +, \dots, +)$ we choose the inertial time 0 surface $\mathbb{R}^d$ as a Cauchy surface. To the Klein-Gordon equation $(-\square + m^2)\varphi = 0$ of mass $m \geq 0$ we associate the self-adjoint operator $A := -\Delta + m^2$ on $L^2(\mathbb{R}^d)$, where Δ is the Laplacian. If $m > 0$ or $d > 1$ we define the real Sobolev spaces $H^{(\pm 1/2)}(\mathbb{R}^d, \mathbb{R})$ as the completions of $C_0^\infty(\mathbb{R}^d, \mathbb{R})$ with the inner product given by $\frac{1}{2}\langle f, A^{\pm 1/2}g \rangle$. We take the one-particle Hilbert space to be

$$\mathcal{H} := H^{(\frac{1}{2})}(\mathbb{R}^d, \mathbb{R}) \oplus H^{(-\frac{1}{2})}(\mathbb{R}^d, \mathbb{R}) \quad (4.3.1)$$

as a real Hilbert space, endowed with the complex structure $i = \begin{pmatrix} 0 & -A^{-1/2} \\ A^{1/2} & 0 \end{pmatrix}$. We may interpret elements of $\mathcal{H}$ as $(f_0, f_1) = \pi(f_0)\hat{\Omega} - \varphi(f_1)\hat{\Omega}$, where (φ, π) are the distributional initial data of the quantum field φ and $\hat{\Omega}$ is the Minkowski vacuum state.

It is sometimes convenient to use a covariant formulation in spacetime. To this end we can use the advanced $(-)$ and retarded $(+)$ fundamental solutions $E^\pm$ of the Klein-Gordon operator and write $E = E^- - E^+$. We may then define a continuous linear map $D : C_0^\infty(\mathbb{R}^{d+1}, \mathbb{R}) \rightarrow C_0^\infty(\mathbb{R}^d, \mathbb{R}) \oplus C_0^\infty(\mathbb{R}^d, \mathbb{R})$ by setting $Df := (Ef|_{x_0=0}, \partial_0 Ef|_{x_0=0})$. We may interpret $Df \in \mathcal{H}$ as $Df = \varphi(f)\hat{\Omega}$.

To an open region $O \subset \mathbb{R}^d$ we associate the closed real-linear subspace $H_O \subset \mathcal{H}$ defined by

$$H_O := \overline{C_0^\infty(O, \mathbb{R}) \oplus C_0^\infty(O, \mathbb{R})}$$

and the von Neumann algebra $\mathcal{R}(H_O)$ on the Fock space $\mathcal{F}_+(\mathcal{H})$. Using the Reeh-Schlieder theorem one may show that $H_O \subset \mathcal{H}$ is a standard subspace if O and $\mathbb{R} \setminus \overline{O}$ are both non-empty open sets [FG89, Prop. 2.7]. Equivalently, H_O can be associated to the spacetime region $V := D(O)$ that is the domain of dependence of O .

4.3.1 Reference modular Hamiltonians

In Section 4.2.1 we gave expressions for the relative modular Hamiltonian between two coherent states whose one-particle vectors had a difference in $H + H'$ for a standard subspace H and its symplectic complement H' . These relative modular Hamiltonians were expressed in terms of the modular Hamiltonian of a reference state. In this section we will review two key examples for free scalar fields, where the modular Hamiltonian is explicitly known.

Example 4.3.1 (Rindler wedge). *The one-particle modular flow of the Rindler wedge in the x_1 -direction is given by the boost transformation $\Lambda_1^{-2\pi t}$ [BW75]. Here the base region R is the half space with coordinates $(x^1, \vec{x}_\perp)$, where $x^1 > 0$ and $\vec{x}_\perp$ denotes the perpendicular spatial coordinates. The modular flow acting on any element of $\mathcal{H}$ of the form Df with $f \in C_0^\infty(\mathbb{R}^{d+1}, \mathbb{R})$ is*

$$\begin{aligned} \Delta_{H_R}^{it} Df(x) &= Df(\Lambda_1^{2\pi t} x), \\ \Lambda_1^s(x^0, x^1, \vec{x}_\perp) &= (x^0 \cosh(s) + x^1 \sinh(s), x^0 \sinh(s) + x^1 \cosh(s), \vec{x}_\perp). \end{aligned}$$

The relative modular Hamiltonian at one-particle level is given by

$$K_{H_R} f = 2\pi \begin{pmatrix} A^{-\frac{1}{2}}(x^1 A - \partial_1) & 0 \\ 0 & A^{\frac{1}{2}} x^1 \end{pmatrix} f \quad (4.3.2)$$

for any $f = (f_0, f_1) \in C_0^\infty(\mathbb{R}^d, \mathbb{R}) \oplus C_0^\infty(\mathbb{R}^d, \mathbb{R})$. If f is supported away from $\{x^1 = 0\} = \partial R$, then we find from Corollary 4.2.4 that

$$H(W(f)\hat{\Omega}, \hat{\Omega}) = \frac{\pi}{2} \int_{x^1 > 0} [f_0(x^1 A - \partial_1) f_0 + x^1 f_1^2] d^d x \quad (4.3.3)$$

$$\begin{aligned} &= \frac{\pi}{2} \int_{x^1 > 0} x^1 (|\nabla f_0|^2 + m^2 f_0^2 + f_1^2) d^d x \\ &= \pi \int_{x^1 > 0} x^1 \left\langle \varphi_S(f) \hat{\Omega}, T_{00}(x)|_{x^0=0} \varphi_S(f) \hat{\Omega} \right\rangle d^d x, \end{aligned} \quad (4.3.4)$$

where $T_{00}(x)$ is the normal-ordered energy density, cf. [CLR20] for a derivation of this result for more general f .

Example 4.3.2 (Massless scalar field on the double cone). *Similarly, we can consider the massless scalar field for a double cone in $(d+1)$ -dimensional Minkowski space with base $B = \{\|\vec{x}\| < r\}$ a ball of radius $r > 0$. The modular flow is known to be related to that of the Rindler wedge via a conformal mapping [HL82] and the flow acts as [Haa12, Sec. V.4.2],*

$$\Delta_{H_B}^{it} Df(x) = DN(2\pi t, x)^{\frac{1-d}{2}} f(T^{2\pi t} x), \quad (4.3.5)$$

$$T^s(x^0, \vec{x}) = N(s, x^0, \vec{x})^{-1} \left(x^0 \cosh(s) + \frac{r^2 - x^2}{2r} \sinh(s), \vec{x} \right), \quad (4.3.6)$$

$$N(s, x^0, \vec{x}) := \frac{x^0}{r} \sinh(s) + \frac{r^2 - x^2}{2r^2} \cosh(s) + \frac{r^2 + x^2}{2r^2},$$

where we wrote $x^2 = -(x^0)^2 + \|\vec{x}\|^2$ and the Jacobian factor $N(t, x)^{\frac{1-d}{2}}$ is needed to preserve solutions. The relative modular Hamiltonian at one-particle level is given by

$$K_{H_B} f = 2\pi \begin{pmatrix} A^{-\frac{1}{2}} \left(\frac{1}{r} x^j \partial_j - \frac{r^2 - \|\vec{x}\|^2}{2r} \Delta + \frac{d-1}{2r} \right) & 0 \\ 0 & A^{\frac{1}{2}} \frac{r^2 - \|\vec{x}\|^2}{2r} \end{pmatrix} f \quad (4.3.7)$$

for any $f = (f_0, f_1) \in C_0^\infty(\mathbb{R}^d, \mathbb{R}) \oplus C_0^\infty(\mathbb{R}^d, \mathbb{R})$. If f is supported away from $\{\|\vec{x}\| = r\} = \partial B$, then we find from Corollary 4.2.4 that

$$H(W(f)\hat{\Omega}, \hat{\Omega}) = \frac{\pi}{2} \int_B \left[f_0 \left(-\nabla^j \frac{r^2 - \|\vec{x}\|^2}{2r} \nabla_j + \frac{d-1}{2r} \right) f_0 + \frac{r^2 - \|\vec{x}\|^2}{2r} f_1^2 \right] d^d x \quad (4.3.8)$$

$$= \frac{\pi}{2} \int_B \left[\frac{r^2 - \|\vec{x}\|^2}{2r} (|\nabla f_0|^2 + f_1^2) + \frac{d-1}{2r} f_0^2 \right] d^d x. \quad (4.3.9)$$

We refer to [LM23] for more details on the massless modular Hamiltonian.

4.3.2 Estimates for free scalar fields

We now want to apply Theorem 4.1.4 to obtain upper and lower bounds on relative modular Hamiltonians. For this purpose we introduce three open regions $O_1 \subset O_2 \subset O_3 \subset \mathbb{R}^d$ in space such that $\overline{O_i} \subset O_{i+1}$ for $i = 1, 2$ and $\mathbb{R}^d \setminus \overline{O_3} \neq \emptyset$. The Minkowski vacuum $\hat{\Omega}$ is then standard for the three local algebras $\mathcal{R}_i := \mathcal{R}(H_{O_i})$ and therefore also for any coherent states $\Omega = W(f)\hat{\Omega}$ and $\tilde{\Omega} = W(\tilde{f})\hat{\Omega}$ with $f, \tilde{f} \in \mathcal{H} = H^{(\frac{1}{2})}(\mathbb{R}^d, \mathbb{R}) \oplus H^{(-\frac{1}{2})}(\mathbb{R}^d, \mathbb{R})$. For simplicity, we will make the stronger assumption that $f, \tilde{f} \in C_0^\infty(\mathbb{R}^d, \mathbb{R}) \oplus C_0^\infty(\mathbb{R}^d, \mathbb{R})$.

For $i = 1, 2$ we now choose cutoff functions $\eta_i \in C^\infty(\mathbb{R}^d, \mathbb{R})$ with $\eta_i \equiv 1$ on $\overline{O_i}$ and $\eta_i \equiv 0$ on $\mathbb{R}^d \setminus \overline{O_{i+1}}$. We will write $\eta_i f = (\eta_i f_0, \eta_i f_1)$, so $\eta_i f \in C_0^\infty(\mathbb{R}^d, \mathbb{R}) \oplus C_0^\infty(\mathbb{R}^d, \mathbb{R})$ and the Weyl relations (1.3.1) yield

$$\begin{aligned} W(f) &= e^{\frac{i}{2} \text{Im}\langle f, \eta_i f \rangle} W((1 - \eta_i)f) W(\eta_i f) \\ &= e^{-\frac{i}{2} \text{Im}\langle f, \eta_i f \rangle} W(\eta_i f) W((1 - \eta_i)f) \end{aligned}$$

in analogy to (4.2.6). As in Section 4.2.2 we then find

$$W(g_1) K_{\hat{\Omega}}^{(1)} W(-g_1) \leq K_{\tilde{\Omega}, \Omega}^{(2)} \leq W(g_2) K_{\hat{\Omega}}^{(3)} W(-g_2),$$

where we introduced $g_i := (1 - \eta_i)f + \eta_i \tilde{f}$. Here the modular Hamiltonian of the vacuum is second quantised, so we may write $K_{\hat{\Omega}}^{(j)} = d\Gamma(k^{(j)})$ with the abbreviated notation

$$k^{(j)} := K_{H_{O_j}}.$$

If g_1 is in the domain of $k^{(1)}$ and g_2 in that of $k^{(3)}$ we may use (4.2.5) to find

$$K_{\hat{\Omega}}^{(1)} + \frac{1}{2} \langle g_1, k^{(1)} g_1 \rangle - \varphi_S(ik^{(1)} g_1) \leq K_{\tilde{\Omega}, \Omega}^{(2)} \leq K_{\hat{\Omega}}^{(3)} + \frac{1}{2} \langle g_2, k^{(3)} g_2 \rangle - \varphi_S(ik^{(3)} g_2). \quad (4.3.10)$$

For the relative entropy $H^{(2)}(\Omega, \tilde{\Omega}) = \langle \Omega, K_{\tilde{\Omega}, \Omega}^{(2)} \Omega \rangle$ we similarly find

$$\langle \hat{\Omega}, W(h_1) K_{\hat{\Omega}}^{(1)} W(-h_1) \hat{\Omega} \rangle \leq H^{(2)}(\Omega, \tilde{\Omega}) \leq \langle \hat{\Omega}, W(h_2) K_{\hat{\Omega}}^{(3)} W(-h_2) \hat{\Omega} \rangle,$$

where $h_i := g_i - f = \eta_i(\tilde{f} - f)$. If we assume that h_1 is in the domain of $k^{(1)}$ and h_2 in that of $k^{(3)}$ this yields

$$\frac{1}{2} \langle h_1, k^{(1)} h_1 \rangle \leq H^{(2)}(\Omega, \tilde{\Omega}) \leq \frac{1}{2} \langle h_2, k^{(3)} h_2 \rangle. \quad (4.3.11)$$

If the one-particle modular Hamiltonian can be expressed in terms of an energy density, this gives a kind of Bekenstein bound [Bek81; Lon25; HL25].

For a more compact notation below, we denote the upper, resp. lower, bound in (4.3.11) by H^+ , resp. H^- , so that the difference $H^+ - H^-$ determines the estimate quality. Correspondingly, we write $\eta_+ = \eta_2$, $\eta_- = \eta_1$. The coherent states are determined by $h_\pm := \eta_\pm g$ with $g = \tilde{f} - f = (g_0, g_1) \in C_0^\infty(\mathbb{R}^d, \mathbb{R}) \oplus C_0^\infty(\mathbb{R}^d, \mathbb{R})$.

4.3.3 Quality of our general estimates for relative entropies

To analyse the quality of the relative entropy estimates (4.3.11), we take the difference between the upper and the lower bound and investigate a suitable limit when the three regions $O_1 \subset O_2 \subset O_3$ are all wedges, resp. double cones, for a massive, resp. massless, free scalar field. In both cases we will make use of the following lemma.

Lemma 4.3.3. *Let $\mathcal{S} = \{\eta \in C^\infty(\mathbb{R}, \mathbb{R}) \mid \eta \equiv 0 \text{ on } x \leq -1, \eta \equiv 1 \text{ on } x \geq 1\}$ and $E : \mathcal{S} \rightarrow \mathbb{R}$ the linear map defined by*

$$E[\eta] := \int_{-1}^1 (x+1) \eta'(x)^2 dx, \quad (4.3.12)$$

where the prime denotes the derivative. Then $\inf_{\eta \in \mathcal{S}} E[\eta] = 0$.

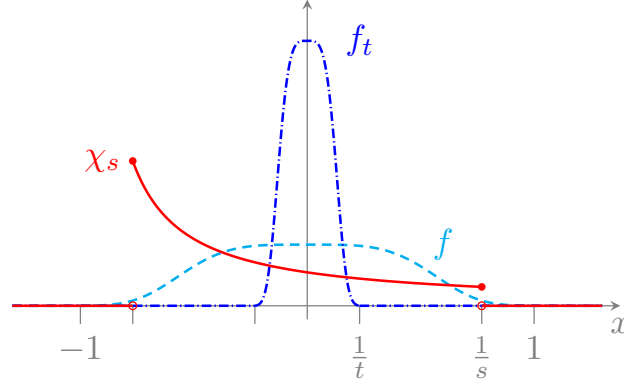


Figure 4.2: The functions χ_s (red solid curve), f (cyan dashed curve) and f_t (blue dash-dotted curve) used in the proof of Lemma 4.3.3.

Proof. It is clear that $E[\eta] \geq 0$ for all $\eta \in \mathcal{S}$. If we view the functional $E[\eta]$ as a Lagrangian, then any extremal value is attained at a solution of the Euler-Lagrange equation $-\partial_x(x+1)\partial_x\eta = 0$ on the interval $(-1, 1)$, i.e., $\eta'(x) = c(x+1)^{-1}$ for some $c \in \mathbb{R}$. Unfortunately, $E[\eta]$ would be infinite for any such solution with $c \neq 0$. Nevertheless, we will show that we can approximate such a solution by functions that make the value of E arbitrarily small.

We choose a parameter $s > 1$ to restrict the extremal function $\eta'(x)$ to the interval $[-s^{-1}, s^{-1}]$ and normalise it with the constant $c_s = \log(s+1) - \log(s-1)$. I.e., we set $\chi_s(x) := (c_s(x+1))^{-1}$ for $|x| < s^{-1}$ and $\chi_s \equiv 0$ for $|x| \geq s^{-1}$, which yields $\int \chi_s(x) dx = 1$, cf. Figure 4.2. Consider any positive function $f \in C_0^\infty(\mathbb{R}, \mathbb{R})$ supported in $[-1, 1]$ and normalised, $\int f(x) dx = 1$, which we rescale to $f_t(x) := tf(tx)$ with a second parameter t such that $t^{-1} \leq 1 - s^{-1}$ or, equivalently, $t \geq \frac{s}{s-1}$. Then f_t is a smooth function supported in $[-t^{-1}, t^{-1}]$ and the convolution $\chi_s * f_t$ is a smooth function supported in $[-1, 1]$. All of these functions are normalised by construction. We now define

$$\eta_{s,t}(x) := \int_{-\infty}^x (\chi_s * f_t)(y) dy ,$$

which is an element in $\mathcal{S}$, and we consider

$$E[\eta_{s,t}] = \int_{-1}^1 \iint_{\mathbb{R}^2} (x+1)\chi_s\left(x - \frac{y}{t}\right) f(y)\chi_s\left(x - \frac{z}{t}\right) f(z) dz dy dx .$$

Because χ_s is continuous at $x \neq \pm s^{-1}$, the integrand converges pointwise to $(x+1)\chi_s(x)^2 f(y)f(z)$ as $t \rightarrow \infty$ at any $x \neq \pm s^{-1}$. Moreover, as $\|\chi_s\|_\infty = \frac{s}{c_s(s-1)}$ the integrand is bounded by $\frac{2s^2}{c_s^2(s-1)^2} f(y)f(z)$, which is integrable on $[-1, 1] \times \mathbb{R}^2$, so by the Dominated Convergence Theorem and the normalisation of all the functions, we find

$$\begin{aligned} \lim_{t \rightarrow \infty} E[\eta_{s,t}] &= \int_{-1}^1 (x+1)\chi_s(x)^2 \iint_{\mathbb{R}^2} f(y)f(z) dz dy dx \\ &= \int_{-1}^1 (x+1)\chi_s(x)^2 dx \\ &= \frac{1}{c_s} \int_{-1}^1 \chi_s(x) dx \\ &= \left(\log \frac{s+1}{s-1} \right)^{-1} . \end{aligned}$$

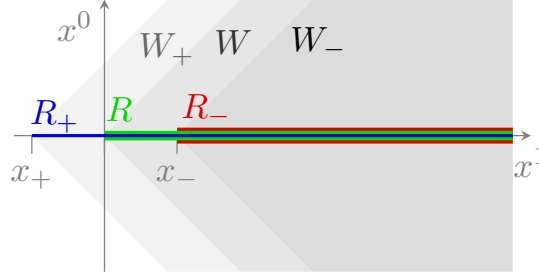


Figure 4.3: Illustration of the nested wedge regions $W_- \subset W \subset W_+$ and their respective half spaces $R_- \subset R \subset R_+$ in the Cauchy hypersurface $\mathbb{R}^d$. Here, only the x^0, x^1 directions are shown and perpendicular spatial coordinates are suppressed.

The result vanishes as $s \rightarrow 1^+$, so we can make $E[\eta_{s,t}]$ as small as we like. $\square$

Note that for any $\eta_+ \in \mathcal{S}$ the function $\eta_-(x) := 1 - \eta_+(-x)$ is also in $\mathcal{S}$, so that the lemma also holds when we replace $\eta'(x)$ by $\eta'(-x)$ in (4.3.12). The derivative η' of any function $\eta \in \mathcal{S}$ is a mollifier, i.e. it has compact support in $[-1, 1]$, is normalised $\int_{-1}^1 \eta'(x) dx = 1$, and the functions $\eta'_\varepsilon(x) := \frac{1}{\varepsilon} \eta'(\frac{x}{\varepsilon})$ are a representation of the Dirac distribution in the limit $\varepsilon \rightarrow 0^+$.

Nested Rindler wedges

As a first example, we consider coherent states over nested Rindler wedge regions $W = D(R)$, $W_\pm = D(R_\pm)$ with bases $R = \{x^1 > 0\}$, $R_\pm := \{x^1 - x_\pm > 0\}$ illustrated in Figure 4.3. It will be convenient to introduce the corresponding weight functions

$$\beta(\vec{x}) = x^1, \quad \beta_\pm(\vec{x}) := x^1 - x_\pm. \quad (4.3.13)$$

The upper and lower bounds $H^\pm$ in (4.3.11) can then be expressed using (4.3.2) as

$$H^\pm = \frac{\pi}{2} \int_{R_\pm} \beta_\pm \left[(\nabla \eta_\pm g_0)^2 + m^2 \eta_\pm^2 g_0^2 + \eta_\pm^2 g_1^2 \right] d^d x \quad (4.3.14)$$

$$= \frac{\pi}{2} \int_{R_+} \beta_+ \eta_+^2 \left[(\nabla g_0)^2 + m^2 g_0^2 + g_1^2 \right] d^d x + \frac{\pi}{2} \int_{R_+ \setminus R_-} \beta_\pm \eta_\pm (\nabla \eta_\pm) \cdot (\nabla g_0^2) d^d x \quad (4.3.15)$$

$$+ \frac{\pi}{2} \int_{R_+ \setminus R_-} \beta_\pm (\nabla \eta_\pm)^2 g_0^2 d^d x, \quad (4.3.16)$$

where we have restricted the integrals to R_+ or $R_+ \setminus R_-$, because $\text{supp } \eta_\pm \subset R_+$ and $\text{supp } \nabla \eta_\pm \subset R_+ \setminus R_-$. We also simplified the expression with the identity $2g_0 \nabla g_0 = \nabla g_0^2$.

Theorem 4.3.4. *For any $f, \tilde{f} \in C_0^\infty(\mathbb{R}^d, \mathbb{R}) \oplus C_0^\infty(\mathbb{R}^d, \mathbb{R})$, the relative entropy between the coherent excitations $\Omega = W(f)\hat{\Omega}$ and $\tilde{\Omega} = W(\tilde{f})\hat{\Omega}$ on the Rindler wedge $W = D(R)$ is*

$$H(\Omega, \tilde{\Omega}) = \frac{\pi}{2} \int_R \beta \left[(\nabla g_0)^2 + m^2 g_0^2 + g_1^2 \right] d^d x \quad (4.3.17)$$

with $(g_0, g_1) := \tilde{f} - f$, which is approximated arbitrarily well by H^+ from above and H^- from below.

Proof. For the simplification of the bounds (4.3.14), we place the two bounding half spaces at equal distances $x_\pm = \mp 2\varepsilon$, see also Figure 4.3. We construct corresponding cutoff functions $\chi_\pm$ that vary only in the x^1 -direction from arbitrary $\tilde{\eta}_\pm \in \mathcal{S}$ as considered in Theorem 4.3.3,

$$\eta_\pm(\vec{x}) := \tilde{\eta}_\pm \left(\frac{x^1}{\varepsilon} \pm 1 \right). \quad (4.3.18)$$

Since the weights (4.3.13) and the cutoffs (4.3.18) only vary with x^1 , we integrate g_0 over all other spatial coordinates to get the function

$$\tau_0(x^1) := \int_{(x^2, x^3, \dots) \in \mathbb{R}^{d-1}} g_0^2 d^{d-1}x ,$$

which is in $C_0^\infty(\mathbb{R}, \mathbb{R})$. We substitute $x = x^1/\varepsilon$ in the second and third integrals of the bounds (4.3.14) and get

$$\begin{aligned} H^\pm &= \frac{\pi}{2} \int_{R_+} \beta_\pm \eta_\pm^2 [(\nabla g_0)^2 + m^2 g_0^2 + g_1^2] d^d x + \frac{\pi\varepsilon}{2} \int_{-2}^2 (x \pm 2) \tilde{\eta}_\pm(x \pm 1) \tilde{\eta}'_\pm(x + 1) \tau'_0(\varepsilon x) dx \\ &\quad + \frac{\pi}{2} \int_{-2}^2 (x \pm 2) \tilde{\eta}'_\pm(x \pm 1)^2 \tau_0(\varepsilon x) dx . \end{aligned}$$

By the Dominated Convergence Theorem the first integral converges to (4.3.17) in the limit $\varepsilon \rightarrow 0^+$, because a dominating function is readily found and $\beta_\pm \rightarrow \beta$ and $\eta_\pm(\vec{x}) \rightarrow \vartheta(x^1)$ converge pointwise, where ϑ is the Heaviside step function. Similarly, the second term converges to 0 and the third term to

$$\frac{\pi}{2} \tau_0(0) \int_{-2}^2 (x \pm 2) \tilde{\eta}'_\pm(x \pm 1)^2 dx = \pm \frac{\pi}{2} \tau_0(0) \int_{-1}^1 (y + 1) \tilde{\eta}'_\pm(\pm y)^2 dy ,$$

where we used the substitution $\pm y := x \pm 1$ and the support properties of $\tilde{\eta}'_\pm$. This integral can be made arbitrarily small by Lemma 4.3.3 and the remarks below it. $\square$

We note that the regularity assumptions on $f, \tilde{f}$ can be weakened considerably without affecting the proof.

Nested double cones for massless fields

In the case of double cones, the arguments are very similar, but now the bases $B_- \subset B \subset B_+$ are d -dimensional balls with radii $0 < r_- < r < r_+$, for simplicity centred around the coordinate origin of $\mathbb{R}^d$. The corresponding weight functions are

$$\beta(\vec{x}) := \frac{r^2 - \|\vec{x}\|^2}{2r} , \quad \beta_\pm(\vec{x}) := \frac{r_\pm^2 - \|\vec{x}\|^2}{2r_\pm} . \quad (4.3.19)$$

The upper and lower bounds $H^\pm$ in (4.3.11) can then be expressed using (4.3.7) as

$$H^\pm = \frac{\pi}{2} \int_{B_+} \beta_\pm [(\nabla \eta_\pm g_0)^2 + \eta_\pm^2 g_1^2] d^d x + \frac{\pi(d-1)}{4r_\pm} \int_{B_+} \eta_\pm^2 g_0^2 d^d x \quad (4.3.20)$$

$$= \frac{\pi}{2} \int_{B_+} \beta_\pm \eta_\pm^2 [(\nabla g_0)^2 + g_1^2] d^d x + \frac{\pi(d-1)}{4r_\pm} \int_{B_+} \eta_\pm^2 g_0^2 d^d x \quad (4.3.21)$$

$$+ \frac{\pi}{2} \int_{B_+ \setminus B_-} \beta_\pm \eta_\pm (\nabla \eta_\pm) \cdot (\nabla g_0^2) d^d x + \frac{\pi}{2} \int_{B_+ \setminus B_-} \beta_\pm (\nabla \eta_\pm)^2 g_0^2 d^d x , \quad (4.3.22)$$

where we have restricted the integrals to B_+ and $B_+ \setminus B_-$, because $\text{supp } \eta_\pm \subset B_+$ and $\text{supp } \nabla \eta_\pm \subset B_+ \setminus B_-$, respectively.

Theorem 4.3.5. *In the massless case, for any $f, \tilde{f} \in C_0^\infty(\mathbb{R}^d, \mathbb{R}) \oplus C_0^\infty(\mathbb{R}^d, \mathbb{R})$, the relative entropy between the coherent excitations $\Omega = W(f)\hat{\Omega}$ and $\tilde{\Omega} = W(\tilde{f})\hat{\Omega}$ on the double cone $D(B)$ with B a ball of radius r is*

$$H(\Omega, \tilde{\Omega}) = \frac{\pi}{2} \int_B \left(\beta [(\nabla g_0)^2 + g_1^2] + \frac{d-1}{2r} g_0^2 \right) d^d x \quad (4.3.23)$$

with $(g_0, g_1) := \tilde{f} - f$, which is approximated arbitrarily well by H^+ from above and H^- from below.

Proof. Similar to the Rindler wedges in Section 4.3.3, we approximate the middle region B symmetrically by balls $B_\pm$ with radii $r_\pm = r \pm 2\varepsilon$ for $0 < \varepsilon < \frac{r}{2}$ and use cutoff functions that are spherically symmetric,

$$\eta_\pm(\vec{x}) := \tilde{\eta}_\pm \left(\frac{r - \|\vec{x}\|}{\varepsilon} \pm 1 \right). \quad (4.3.24)$$

We integrate first over the unit sphere S^{d-1}

$$\tau_0(\|\vec{x}\|) := \int_{S^{d-1}} g_0^2 d\text{vol}_{S^{d-1}},$$

which is a function in $C_0^\infty([0, \infty), \mathbb{R})$. We substitute $s = (r - \|\vec{x}\|)/\varepsilon$ in the second and third integrals of $H^\pm$ and find

$$\begin{aligned} H^\pm &= \frac{\pi}{2} \int_B \eta_\pm^2 \left(\beta_\pm [(\nabla g_0)^2 + g_1^2] + \frac{d-1}{2r_\pm} g_0^2 \right) d^d x \\ &+ \frac{\pi\varepsilon}{2} \int_{-2}^2 \frac{r_\pm^2 - (r - \varepsilon s)^2}{2r_\pm \varepsilon} \tilde{\eta}_\pm(s \pm 1) \tilde{\eta}'_\pm(s \pm 1) \tau'_0(r - \varepsilon s) (r - \varepsilon s)^{d-1} ds \\ &+ \frac{\pi}{2} \int_{-2}^2 \frac{r_\pm^2 - (r - \varepsilon s)^2}{2r_\pm \varepsilon} \tilde{\eta}'_\pm(s \pm 1)^2 \tau_0(r - \varepsilon s) (r - \varepsilon s)^{d-1} ds. \end{aligned}$$

Again, by the Dominated Convergence Theorem the first integral converges to (4.3.23) in the limit $\varepsilon \rightarrow 0^+$, because a dominating function is readily found and $\beta_\pm \rightarrow \beta$ and $\eta_\pm(\vec{x}) \rightarrow \vartheta(r - \|\vec{x}\|)$ converge pointwise. Similarly, the second term converges to 0 and the third term to

$$\frac{\pi}{2} \tau_0(r) r^{d-1} \int_{-2}^2 (s \pm 2) \tilde{\eta}'_\pm(s \pm 1)^2 ds = \pm \frac{\pi}{2} \tau_0(r) r^{d-1} \int_{-1}^1 (y + 1) \tilde{\eta}'_\pm(\pm y)^2 dy,$$

where we used the fact that $\frac{r_\pm^2 - (r - \varepsilon s)^2}{2r_\pm \varepsilon} \rightarrow (s \pm 2)$ pointwise as $\varepsilon \rightarrow 0$, the substitution $\pm y = s \pm 1$ and the support properties of $\tilde{\eta}_\pm$. This integral is the same as in the proof of Theorem 4.3.4, so it can be made arbitrarily small. $\square$

4.4 Towards more general estimates

To conclude this chapter, we shall briefly discuss some open research questions stemming from the results we discussed.

From the discussion in Section 4.1, while in a typical QFT setting of type III local algebras, the class of pairs of states that are susceptible to our scheme is quite large, due to the Connes-Størmer Theorem, it remains an open question whether all pairs of quasi-equivalent, standard states can be handled in this way. We expect that this question can only be addressed by adapting the methods

of [CS78]. It is also unclear whether the converse of this implication is also valid, i.e., whether every non-signalling unitary u and every vector Ω that is standard for the algebras involved, the pair Ω and $u\Omega$ is susceptible to our estimates. For type I factors, we have shown in Counterexample 4.1.5 that this converse implication fails. However, the arguments used there do not extend to the type III case.

Then, our general estimates may also be very nicely combined with spacetime deformation arguments as in [San09]. I.e., we do not need to insist that $V_1 \subset V_2 \subset V_3$, as long as $V_1 \subset D(V_2)$ and $D(V_3) \supset V_2$ and the theory satisfies the time-slice axiom. This could lead to Bekenstein-type bounds on relative entropies, if one starts e.g. with a Minkowski vacuum, whose relative modular Hamiltonian on a double cone is related to the energy density, and one deforms the theory and the states into the future.

In the context of coherent states on CCR algebras, our general estimates simplify and for the particular case of free scalar fields all pairs of coherent excitations of the vacuum are susceptible to our estimates. In Section 4.3 we combined our estimates with a squeezing argument to recover a known formula for the relative entropy on a wedge or a double cone (in the massless case), cf. [CGP19; CLR20; LM23; BCD22]. This implies in particular that the relative entropy can be approximated arbitrarily well by our estimates, suggesting that they might not lose information also in the general case. Analogous limiting arguments for the relative modular Hamiltonians are more difficult to formulate, due to the unboundedness of the operators involved, which complicate the notion of convergence. One possibility would be to investigate convergence of the estimates in (4.3.10) in the graph norm, but we have not pursued this here.

A natural question to ask is whether it is possible to extend our estimates beyond the case of coherent states on CCR algebras. For pairs of general quasi-free states $\omega, \tilde{\omega}$ the situation is already more complicated. If the states are quasi-equivalent and standard for the region V_2 , as in Section 4.1.1, then we may implement both states by standard vectors $\Omega, \tilde{\Omega}$ in the same Hilbert space and there is a Bogolyubov transformation b , implemented by a unitary u_b satisfying $\tilde{\Omega} = u_b\Omega$. As discussed in Section A.3, Bogolyubov unitaries act on Weyl operators (generating local algebras) as $u_b W(f) u_b^* = W(bf)$, say for f supported in some bounded region, so they will not preserve generic local algebras and may in principle allow superluminal signalling. It seems difficult to determine in general whether the pair of states is susceptible to our estimates. (See also [LLR21] for results on states with a single squeezed mode.)

Chapter 5

Conclusions

In this thesis, we have discussed relations between Tomita-Takesaki modular theory and quantum physics through the formalism of algebraic QFT (AQFT), in the endeavour to work towards a clearer characterization of the quantities arising from modular theory and relative modular theory, in particular modular Hamiltonians, relative modular Hamiltonians and thus relative entropies. The main strategy to do so in our work has been to search for relations between such quantities, especially in cases where they are not known, and better understood quantities such as energy densities or modular Hamiltonians when they have been computed, and the way we worked towards such relations has been by means of estimates, i.e. upper or lower bounds.

First, we have presented in Chapter 1 the essentials of the mathematical tools needed for these topics, which are C^* -algebras, von Neumann algebras, Tomita-Takesaki modular theory, and the basics of the theory of symplectic spaces.

Then, in Chapter 2, we used these concepts to explain the main concepts of AQFT, with the perspective of aiming for a greater generality than the standard Haag-Kastler approach, for this reason we employed (whenever appropriate) the locally covariant framework due to Brunetti, Fredenhagen and Verch [BFV03].

Chapter 3 follows the results of [CS25], where the approach has been to estimate differences of functions of modular Hamiltonians for a class of Gaussian states on a Weyl algebra built as perturbations of a suitable Gaussian reference state, bounding them from above with their energies.

Chapter 4 follows [CMS26], where, shifting the focus to relative modular Hamiltonians, the idea was to estimate relative modular Hamiltonians for suitable pairs of states on some local algebra in terms of modular Hamiltonians of a reference state on bigger or smaller algebras, which may be better understood. These abstract estimates offer a link to (the absence of) superluminal signalling in the sense of Sorkin's paradox, they apply to the unitaries generating the dynamical algebra of Buchholz-Fredenhagen for a Lagrangian QFT, and may also be specialized to coherent states for CCR systems. In this last case, focussing on free scalar fields, for wedge regions and (in the massless case) double cones, exact results can be obtained by 'squeezing', i.e. making the upper and lower bounds arbitrarily close, and this corroborates the strength of our general estimates.

Finally, the appendices were dedicated to giving more details about certain mathematical tools needed for some of these topics. In Appendix A, we have discussed the theory of Fock spaces and Bogolyubov transformations, Appendix B was dedicated to the surprisingly complex theory of operator monotone and operator convex functions, and Appendix C discusses some inequalities involving p -norms of operators, such as the Powers-Størmer and van Hemmen-Ando inequalities.

On the basis of our initial goals of working towards improving our understanding of modular Hamiltonians and relative modular Hamiltonians, this thesis has shown that estimates can be a useful mean to work towards this objective, and in some cases they can also be a valuable technique to obtain exact results, or approximate them arbitrarily well. We have discussed in Section 3.2.3 how the approach of Chapter 3 based on perturbations of a reference Gaussian state becomes limited when applied to bounded regions instead of the whole Minkowski spacetime, but could still lead to some local results. Instead, the perspective of Chapter 4 is much broader and provides more general results on abstract von Neumann algebras, which, when applied to local algebras in QFT, hint at the possibility to obtain exact expressions for relative modular Hamiltonians and relative entropies in cases where they are not known. As discussed in Section 4.4, considering coherent states on CCR algebras, we used our techniques to reproduce results for the relative entropy of free fields on wedge regions and we employed the same logic for double cones in the massless case, so a natural development would be to investigate if these ideas could be applied to more general regions or directly to modular Hamiltonians, on the operator level. A broader question would then be to ask whether our estimates could be applied to more general quasi-free states linked by some Bogolyubov transformation, however stepping from Weyl unitaries to operator quadratic in the fields has proven to be quite technically challenging. Nevertheless, developing the tools to estimate relative modular Hamiltonians for more general classes of states would be very valuable in improving our physical understanding of the quantities arising from Tomita-Takesaki modular theory.

Appendix A

Fock spaces and Bogolyubov transformations

In this appendix, we will discuss the generalities and technical details of Fock spaces, thermal (KMS) states and Bogolyubov transformations, for these topics we will follow [BR97, Sec. 5.2 and 5.3] and [RS75, Sec. X.7]. For a comprehensive source on Bogolyubov transformations, we also refer to [DG13].

A.1 Fock space generalities

In this section, we will present the general construction of the Fock space, following Section 5.2.1 of [BR97], considering both the bosonic and fermionic case (in this thesis, only the former will be of use). Let $\mathcal{H}$ be a complex Hilbert space with a complex inner product $\langle, \rangle$ and let $\mathcal{H}^n = \mathcal{H} \otimes \cdots \otimes \mathcal{H} = \mathcal{H}^{\otimes n}$ denote the n -fold tensor product of $\mathcal{H}$ with itself. Then, the Fock space $\mathcal{F}(\mathcal{H})$ will be defined as

$$\mathcal{F}(\mathcal{H}) = \bigoplus_{n \geq 0} \mathcal{H}^n, \quad (\text{A.1.1})$$

where we take $\mathcal{H}^0 = \mathbb{C}$, so an element ψ of $\mathcal{F}(\mathcal{H})$ will be given by a sequence of vectors $(\psi^{(n)})_{n \geq 0}$ with $\psi^{(n)} \in \mathcal{H}^n$. The vector $\Omega = (1, 0, \dots, 0)$, i.e. the zero-particle state, will be the (Fock) vacuum. Then, if we define the operators $P_{\pm}$ on $\mathcal{F}(\mathcal{H})$ as

$$\begin{aligned} P_+(f_1 \otimes f_2 \otimes \cdots \otimes f_n) &= \frac{1}{n!} \sum_{\pi} f_{\pi(1)} \otimes f_{\pi(2)} \otimes \cdots \otimes f_{\pi(n)}, \\ P_-(f_1 \otimes f_2 \otimes \cdots \otimes f_n) &= \frac{1}{n!} \sum_{\pi} \text{sign}(\pi) f_{\pi(1)} \otimes f_{\pi(2)} \otimes \cdots \otimes f_{\pi(n)}, \end{aligned} \quad (\text{A.1.2})$$

for all $f_1, \dots, f_n \in \mathcal{H}$, summing over all permutations π of n indices. By linearity, these operators can be extended to two densely defined operators of norm 1. Then, we can define the bosonic Fock space $\mathcal{F}_+(\mathcal{H})$ and the fermionic Fock space $\mathcal{F}_-(\mathcal{H})$ as

$$\mathcal{F}_{\pm}(\mathcal{H}) := P_{\pm} \mathcal{F}(\mathcal{H}), \quad (\text{A.1.3})$$

and $\mathcal{H}_{\pm}^n := P_{\pm} \mathcal{H}^n$ will be their corresponding n -particle (sub)spaces.

The structure of the Fock space allows the amplification of unitary and self-adjoint operators on $\mathcal{H}$ to $\mathcal{F}_{\pm}(\mathcal{H})$ through second quantization. For a unitary operator U on $\mathcal{H}$, we can define the

operators U_n on $\mathcal{H}_\pm^n$ by setting $U_0 = \mathbb{1}$,

$$U_n (P_\pm (f_1 \otimes \cdots \otimes f_n)) = P_\pm (U f_1 \otimes U f_2 \otimes \cdots \otimes U f_n) \quad (\text{A.1.4})$$

and extending by continuity. Its second quantization will be defined as

$$\Gamma (U) = \bigoplus_{n \geq 0} U_n, \quad (\text{A.1.5})$$

which will still be unitary. For a self-adjoint operator H on $\mathcal{H}$, we can instead define its second quantization $d\Gamma(H)$ from the one of an unitary. Indeed, if $U(t) = e^{itH}$ is a strongly continuous one-parameter group of unitaries, then $\Gamma(U(t)) = e^{itd\Gamma(H)}$. This corresponds to setting $H_0 = 0$,

$$H_n (P_\pm (f_1 \otimes \cdots \otimes f_n)) = P_\pm \left(\sum_{i=1}^n f_1 \otimes f_2 \otimes \cdots \otimes H f_i \otimes \cdots \otimes f_n \right), \quad (\text{A.1.6})$$

on $\mathcal{H}_\pm^n$, for all $f_1, \dots, f_n \in \mathcal{D}(\mathcal{H})$, and extending by continuity. The direct sum of the H_n will be essentially self-adjoint and we get its self-adjoint closure

$$d\Gamma(H) = \overline{\bigoplus_{n \geq 0} H_n}. \quad (\text{A.1.7})$$

As an example, we can define the (*particle*) *number operator* N on $\mathcal{F}(\mathcal{H})$, on the domain

$$\mathcal{D}(N) = \left\{ \psi = \left(\psi^{(n)} \right)_{n \geq 0} / \sum_{n \geq 0} n^2 \left\| \psi^{(n)} \right\|^2 < \infty \right\} \quad (\text{A.1.8})$$

of finite-particle vectors, as the self-adjoint operator

$$N\psi = \left(n\psi^{(n)} \right)_{n \geq 0}, \quad (\text{A.1.9})$$

for any $\psi \in \mathcal{D}(N)$. The number operator has the property to be the second quantization of the one-particle space identity, $N = d\Gamma(\mathbb{1})$.

Now, we can define the C^* -algebras of observables associated respectively with bosons and fermions, through annihilation and creation operators. For any $f \in \mathcal{H}$, we can define operators $a(f)$, $a^*(f)$ on $\mathcal{F}(\mathcal{H})$ by setting $a(f)\psi^{(0)} = 0$, $a^*(f)\psi^{(0)} = f$ and

$$\begin{aligned} a(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_n) &= \sqrt{n}(f, f_1) f_2 \otimes f_3 \otimes \cdots \otimes f_n, \\ a^*(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_n) &= \sqrt{n+1} f \otimes f_1 \otimes \cdots \otimes f_n. \end{aligned} \quad (\text{A.1.10})$$

Extending by linearity, we get two densely defined operators such that

$$\begin{aligned} \left\| a(f)\psi^{(n)} \right\| &\leq \sqrt{n} \|f\| \left\| \psi^{(n)} \right\|, \\ \left\| a^*(f)\psi^{(n)} \right\| &\leq \sqrt{n+1} \|f\| \left\| \psi^{(n)} \right\|, \end{aligned} \quad (\text{A.1.11})$$

with $\psi^{(n)} \in \mathcal{H}^n$. It follows that $a(f)$ and $a^*(f)$ will have well-defined extensions to the domain $\mathcal{D}(\sqrt{N})$ and

$$\begin{aligned} \|a(f)\psi\| &\leq \|f\| \left\| \sqrt{N+1} \psi \right\|, \\ \|a^*(f)\psi\| &\leq \|f\| \left\| \sqrt{N+1} \psi \right\|, \end{aligned} \quad (\text{A.1.12})$$

for any $\psi \in \mathcal{D}(\sqrt{N})$. Also, such operators will be adjoints,

$$\langle a^*(f) \psi, \psi' \rangle = \langle \psi, a(f) \psi' \rangle, \quad (\text{A.1.13})$$

for any $\psi, \psi' \in \mathcal{D}(\sqrt{N})$. Then, we can define bosonic (+) and fermionic (−) annihilation and creation operators $a_{\pm}(f)$, $a_{\pm}^*(f)$ on $\mathcal{F}_{\pm}(\mathcal{H})$ as

$$\begin{aligned} a_{\pm}(f) &:= P_{\pm} a(f) P_{\pm}, \\ a_{\pm}^*(f) &:= P_{\pm} a^*(f) P_{\pm}, \end{aligned} \quad (\text{A.1.14})$$

for any $f \in \mathcal{H}$. As before, we will have that $a_{\pm}(f)$ and $a_{\pm}^*(f)$ are each other's adjoints and, as $a(f)$ leaves $\mathcal{F}_{\pm}(\mathcal{H})$ invariant, we will also have

$$\begin{aligned} a_{\pm}(f) &= a(f) P_{\pm}, \\ a_{\pm}^*(f) &= P_{\pm} a^*(f). \end{aligned} \quad (\text{A.1.15})$$

From their definitions, we can see that the maps $f \longrightarrow a_{\pm}(f)$ are antilinear and $f \longrightarrow a_{\pm}^*(f)$ are linear.

Then, we can check that the creation and annihilation operators will satisfy the canonical commutation relations (CCR) in the bosonic case, i.e.

$$\begin{aligned} [a_+(f), a_+^*(g)] &= \langle f, g \rangle \mathbb{1}, \\ [a_+(f), a_+(g)] &= [a_+^*(f), a_+^*(g)] = 0, \end{aligned} \quad (\text{A.1.16})$$

for $f, g \in \mathcal{H}$, and the canonical anticommutation relations (CAR) in the fermionic case, i.e.

$$\begin{aligned} \{a_+(f), a_+^*(g)\} &= \langle f, g \rangle \mathbb{1}, \\ \{a_+(f), a_+(g)\} &= \{a_+^*(f), a_+^*(g)\} = 0. \end{aligned} \quad (\text{A.1.17})$$

In the main text and in the following sections, we will however focus on the bosonic case, so for simplicity we will drop the index + and consider (with abuse of the general notation) creation and annihilation operators $a(f)$, $a^*(f)$ which will satisfy the CCR (A.1.16).

A quantity that is directly defined from the bosonic creation and annihilation operators is the real linear Segal field, i.e.

$$\varphi_S(f) = \frac{1}{\sqrt{2}} (a^*(f) + a(f)) \quad (\text{A.1.18})$$

for $f \in \mathcal{H}$, of which we will discuss the commutation properties in Section A.4. From Segal fields, we can define the unitary Weyl operators

$$W(f) = e^{i\varphi_S(f)}, \quad (\text{A.1.19})$$

which will satisfy the Weyl relations (1.3.1), which are an ‘exponentiated form’ of the CCR (A.1.16) where the algebra generators are represented by Weyl unitaries.

A.2 Thermal states on bosonic systems

Given this construction of the Fock space, we will now discuss the system described by the bosonic Fock space $\mathcal{F}_+(\mathcal{H})$ over the one-particle space $\mathcal{H}$ and a one-particle Hamiltonian H on $\mathcal{H}$, following [BR97, Sec. 5.2.5]. The dynamics of a bosonic non-interacting system will be described by the second quantization $d\Gamma(H)$ of H .

The time evolution of a vector $\psi \in \mathcal{F}_+(\mathcal{H})$ will be given by $\psi_t = \Gamma(e^{-itH})\psi$ and for operators A on $\mathcal{F}_+(\mathcal{H})$ (the observables) we will have $\tau_t(A) = \Gamma(e^{itH})A\Gamma(e^{-itH})$. Such a dynamics defines a one-parameter group of $*$ -automorphisms of the CCR algebra and we get $\tau_t(W(f)) = W(e^{itH}f)$ for Weyl operators $W(f)$. Then, we can define a Gibbs state at inverse temperature $\beta > 0$ in terms of $d\Gamma(H)$ whenever the operator $e^{-\beta d\Gamma(H)}$ is trace-class. In particular, we have the following result, cf. [BR97, Thm. 5.2.27].

Proposition A.2.1. *Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and let $\beta \in \mathbb{R}$. The following are equivalent:*

- i. $e^{-\beta H}$ is trace-class on $\mathcal{H}$ and $\beta H > 0$;
- ii. $e^{-\beta d\Gamma(H)}$ is trace-class on $\mathcal{F}_+(\mathcal{H})$.

Remark. Note that the implication from point i. to point ii. uses the following estimates. W.l.o.g., let $\beta > 0$ and consider the eigenvalues $\{h_n\}_{n \geq 0}$ of H , taken in increasing order (decreasing if considering $\beta < 0$) and repeating according to multiplicity. Then we have that

$$\mathrm{tr}_{\mathcal{H}_+^m}(e^{-\beta d\Gamma(H)}) \leq \sum_{n_1, n_2, \dots, n_m} e^{-\beta \sum_{p=1}^m h_{n_p}}$$

and so

$$\begin{aligned} 0 \leq \mathrm{tr}(e^{-\beta d\Gamma(H)}) &= \sum_{m \geq 0} \mathrm{tr}_{\mathcal{H}_+^m}(e^{-\beta d\Gamma(H)}) \\ &\leq \prod_{m \geq 0} (1 - e^{-\beta h_m})^{-1} \\ &= \prod_{m \geq 0} \left(1 + e^{-\beta h_m} (1 - e^{-\beta h_m})^{-1}\right) \\ &\leq \exp \left\{ \sum_{m \geq 0} e^{-\beta h_m} (1 - e^{-\beta h_m})^{-1} \right\} \\ &\leq \exp \left\{ (1 - e^{-\beta h_0})^{-1} \mathrm{tr}(e^{-\beta H}) \right\}, \end{aligned}$$

which proves the implication.

Then, assuming that $e^{-\beta d\Gamma(H)}$ is trace-class, we can define the Gibbs equilibrium state as

$$\omega_\beta(A) = \frac{\mathrm{tr}(e^{-\beta d\Gamma(H)}A)}{\mathrm{tr}(e^{-\beta d\Gamma(H)})}, \quad (\text{A.2.1})$$

for $A \in \mathcal{B}(\mathcal{H})$, which will be characterized by the following proposition, cf. [BR97, Prop. 5.2.28].

Proposition A.2.2. *Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and let $\beta \in \mathbb{R}$. Assume that $e^{-\beta H}$ is trace-class and $\beta H > 0$, and let (A.2.1) denote the Gibbs equilibrium state over $\mathcal{B}(\mathcal{F}_+(\mathcal{H}))$. Then, ω_β is the gauge-invariant Gaussian state with two-point function*

$$\omega_\beta(a^*(f)a(g)) = \left\langle g, e^{-\beta H} \left(\mathbb{1} - e^{-\beta H} \right)^{-1} f \right\rangle$$

and so

$$\omega_\beta(W(f)) = \exp \left\{ -\frac{1}{4} \left(f, \left(\mathbb{1} + e^{-\beta H} \left(\mathbb{1} - e^{-\beta H} \right)^{-1} f \right) \right) \right\}.$$

Note that, in this context, *gauge invariance* refers to a global $U(1)$ phase symmetry. Under a gauge transformation by an angle ϑ , the annihilation and creation operators transform as $a(f) \mapsto e^{-i\vartheta}a(f)$ and $a^*(f) \mapsto e^{i\vartheta}a^*(f)$. A state ω is *gauge-invariant* if its expectation values do not change under this transformation. As a consequence, the expectation value of any operator string with an unequal number of creation and annihilation operators must vanish. Then, a gauge-invariant Gaussian state ω is entirely and uniquely determined by a single two-point correlation function $\omega(a^*(f)a(g))$.

Now, this discussion on Gibbs equilibrium states can be subsumed into the characterization of the Kubo-Martin-Schwinger (KMS) states, cf. [BR97, Sec. 5.3.1]. Indeed, if we consider a state ω_β of the form (A.2.1), with $\beta > 0$, $H > 0$ is a self-adjoint on the one-particle Hilbert space $\mathcal{H}$, and $e^{-\beta d\Gamma(H)}$ is trace-class, such a state will formally satisfy the condition

$$\omega_\beta(A\tau_t(B))|_{t=i\beta} = \omega_\beta(BA), \quad (\text{A.2.2})$$

w.r.t. the automorphism group $\tau_t(A) = e^{itH}Ae^{-itH}$, $A, B \in \mathcal{B}(\mathcal{H})$. This condition involves two main elements, which are (i) the analyticity of the functions $t \mapsto \omega_\beta(A\tau_t(B))$ in the strip $0 < \text{Im } t < \beta$, and (ii) the fact that the pair A, B ‘approximately commutes’ within the state ω_β .

These concepts can be made precise by the KMS condition. First, we shall consider the definition of an algebraic dynamical system in a general sense, cf. [San13, Sec. 2]

Definition A.2.3. An algebraic dynamical system $(\mathcal{A}, \tau_t)$ consists of a unital $*$ -algebra $\mathcal{A}$ and a one-parameter group of $*$ -isomorphisms τ_t on $\mathcal{A}$.

The algebra $\mathcal{A}$ may be interpreted as the algebra of observables and τ_t will describe the time evolution. In this context, a state (positive, normalized linear functional) ω on $\mathcal{A}$ is an equilibrium state ω for $(\mathcal{A}, \tau_t)$ if $\tau_t^*\omega := \omega \circ \tau_t = \omega$ for all $t \in \mathbb{R}$. We refer to [San13] for more properties of equilibrium states. For the purpose of our discussion, we will only focus on the characterization of thermal equilibrium states, which is given by the KMS-condition.

Definition A.2.4. A state ω on an algebraic dynamical system $(\mathcal{A}, \tau_t)$ is called a β -KMS state for $\beta > 0$ if it satisfies the KMS-condition at inverse temperature β , i.e. if for all $A, B \in \mathcal{A}$ there is an analytic function F_{AB} on the strip $S_\beta := \mathbb{R} \times i(0, \beta) \subset \mathbb{C}$ with a bounded, continuous extension to $\overline{S_\beta}$ such that

$$\begin{aligned} F_{AB}(t) &= \omega(A\tau_t(B)), \\ F_{AB}(t + i\beta) &= \omega(\tau_t(B)A). \end{aligned} \quad (\text{A.2.3})$$

Then, a β -KMS state ω is called *extremal* if it is an extremal element of the set of all β -KMS states. In addition, if we consider $\mathcal{A}$ to be a C^* -algebra and $t \in \mathbb{R}$, so to have a C^* -dynamical system based on the group $\mathbb{R}$, the requirement that F_{AB} is bounded can be dropped [BR97, Prop. 5.3.7]. In the context of our non-interacting bosonic system, the CCR algebra (or the Weyl algebra) plays the role of the observable algebra $\mathcal{A}$, and the time evolution $\tau_t(A) = \Gamma(e^{itH})A\Gamma(e^{-itH})$ provides the one-parameter group of $*$ -automorphisms. The Gibbs state ω_β defined in (A.2.1) will indeed be a β -KMS state for this specific C^* -dynamical system, cf. [BR97, Prop. 5.3.3].

Physically speaking, the abstract KMS-condition (A.2.3) has the advantage to remain well-defined even for systems with infinitely many degrees of freedom. In such cases, the Hamiltonian typically possesses a continuous spectrum extending to zero and the operator $e^{-\beta d\Gamma(H)}$ ceases to be trace-class, rendering the standard Gibbs state definition (A.2.1) mathematically ill-defined. The KMS-condition instead bypasses the need for a globally defined trace and partition function, being based on the analytic properties of the equilibrium state, cf. [HHW67].

A.3 Bogolyubov transformations

Starting from the Fock space construction of Section A.1, we will now discuss Bogolyubov transformations, following the exposition in [Sol07, Sec. 9]. We refer to [DG13, Ch. 10] for a more technical discussion. We shall again consider a complex Hilbert space $\mathcal{H}$ with inner product $\langle \cdot, \cdot \rangle$ and its bosonic Fock space $\mathcal{F}_+(\mathcal{H})$. We can consider the space $\mathcal{K} = \mathcal{H} \oplus \overline{\mathcal{H}}$, where $\overline{\mathcal{H}}$ is the dual of $\mathcal{H}$, and the complex conjugation $J : \mathcal{H} \rightarrow \overline{\mathcal{H}}$, with $J(f)g = \langle f, g \rangle$, $f, g \in \mathcal{H}$. From J , we can define a canonical complex conjugation $\tilde{J} : \mathcal{K} \rightarrow \mathcal{K}$, which in matrix form will be

$$\tilde{J} = \begin{pmatrix} 0 & J^* \\ J & 0 \end{pmatrix}. \quad (\text{A.3.1})$$

Following Section 8 of [Sol07], we may define the bosonic generalized creation and annihilation operators on $\mathcal{K}$ as

$$\begin{aligned} A(f \oplus Jg) &= a(f) + a^*(g), \\ A^*(f \oplus Jg) &= a^*(f) + a(g), \end{aligned} \quad (\text{A.3.2})$$

with $f, g \in \mathcal{H}$, where a^* and a are the bosonic annihilation and creation operators. These operators are such that $A^*(F) = A(\tilde{J}F)$, for $F \in \mathcal{K}$. With this notation, the CCR can be written as

$$[A(F_1), A^*(F_2)] = \langle F_1, iRF_2 \rangle, \quad (\text{A.3.3})$$

where $R : \mathcal{K} \rightarrow \mathcal{K}$ is defined as

$$R = -i \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}. \quad (\text{A.3.4})$$

Note that, in general, $[A(F_1), A(F_2)] \neq 0$. Then, we will have the following definition.

Definition A.3.1. *A linear bounded isomorphism $T : \mathcal{K} \rightarrow \mathcal{K}$ is called a bosonic Bogolyubov map if*

$$A^*(TF) = A(T\tilde{J}F) \quad (\text{A.3.5})$$

for any $F \in \mathcal{K}$ and

$$[A(TF_1), A^*(TF_2)] = \langle F_1, iRF_2 \rangle \quad (\text{A.3.6})$$

for any $F_1, F_2 \in \mathcal{K}$. Such an operator will give a bosonic Bogolyubov transformation

$$A(F) \rightarrow A(TF). \quad (\text{A.3.7})$$

These conditions are equivalent to

$$\begin{aligned} \tilde{J}TF &= T\tilde{J}F, \\ \langle TF_1, iRTF_2 \rangle &= \langle F_1, iRF_2 \rangle, \end{aligned} \quad (\text{A.3.8})$$

for any $F, F_1, F_2 \in \mathcal{K}$. As we assume T to be invertible, we have that $T^{-1} = -RT^*R$. Then, we can equivalently rewrite the definition of a Bogolyubov map as

Theorem A.3.2. *A linear map $T : \mathcal{K} \rightarrow \mathcal{K}$ is a bosonic Bogolyubov map if and only if*

$$T^*RT = R, \quad TRT^* = R, \quad \tilde{J}T\tilde{J} = T. \quad (\text{A.3.9})$$

Note that these conditions indeed make T a bounded isomorphism. Indeed, from $T^*RT = R$ we get that $(-RT^*R)T = \mathbb{1}$, so T has a left inverse, and from $TRT^* = R$ we have $T(-RT^*R) = \mathbb{1}$, so it has a right inverse as well, so it is an isomorphism. Then, these conditions also require T and its adjoint T^* to be everywhere-defined operators on $\mathcal{K}$, so T is bounded by the Hellinger-Toeplitz theorem, cf. [RS72, Sec. III.5], and T^{-1} is as well, by the bounded inverse theorem, cf. [RS72, Thm. III.11]. The condition $\tilde{J}T\tilde{J} = T$ ensures that T respects the real structure of the space.

Under these conditions, we can see that a Bogolyubov map $T : \mathcal{K} \rightarrow \mathcal{K}$ will have matrix form

$$T = \begin{pmatrix} U & J^*VJ^* \\ V & JUJ^* \end{pmatrix}, \quad \text{with} \quad \begin{cases} U^*U = \mathbb{1} + V^*V, \\ UU^* = \mathbb{1} + J^*VV^*J, \\ V^*JU = U^*J^*V, \end{cases} \quad (\text{A.3.10})$$

where $U : \mathcal{H} \rightarrow \mathcal{H}$ and $V : \mathcal{H} \rightarrow \overline{\mathcal{H}}^{\perp}$.¹ Then, we want to see when such a transformation may be implemented by a unitary map on $\mathcal{F}_+(\mathcal{H})$, in the sense that

Definition A.3.3. *A bosonic Bogolyubov transformation $T : \mathcal{K} \rightarrow \mathcal{K}$ is called unitarily implementable if there exists a unitary transformation*

$$\mathcal{U}_T : \mathcal{F}_+(\mathcal{H}) \rightarrow \mathcal{F}_+(\mathcal{H}) \quad (\text{A.3.11})$$

such that

$$\mathcal{U}_T A(F) \mathcal{U}_T^* = A(TF) \quad (\text{A.3.12})$$

for any $F \in \mathcal{K}$.

We have the following result, originally by Shale [Sha62, Theorem 6.2].

Theorem A.3.4. *A bosonic Bogolyubov transformation $T : \mathcal{K} \rightarrow \mathcal{K}$ of the form (A.3.10) is unitarily implementable if and only if V^*V is trace-class (Shale condition).*

An explicit construction of the unitary implementer $\mathcal{U}_T$ is given by [Sol07, Sec. 9] and [Lil25, Sec. 3.2.1]. Under the Shale condition, we will have that the operator $C = U^*J^*V$, which is self-adjoint by the last condition in (A.3.10), has an eigenbasis $\{f_j\}$ with $Cf_j = \lambda_j f_j$, $\lambda_j \in \mathbb{R}$. Indeed, if V^*V is trace-class, $C^*C = V^*JUJ^*J^*V = V^*J(\mathbb{1} + J^*VV^*J)J^*V = V^*V + (V^*V)^2$ will be trace-class as well. In addition, C commutes with U^*U . Then, we may assume w.l.o.g. that the same basis is also an orthonormal eigenbasis for U^*U , $U^*Uf_j = \mu_j^2 f_j$, noting that $\mu_j > 0$. (Indeed, if C has degenerate eigenvalues, then we may need to change the basis in some higher dimensional eigenspaces of C to obtain an eigenbasis for U^*U .) Then, we can define another orthonormal basis $g_j := \mu_j^{-1}Uf_j$, such that also $J^*Vf_j = \nu_j g_j$, with $\nu_j \in \mathbb{R}$. These eigenvalues will satisfy $\lambda_j = \mu_j \nu_j$ and $\mu_j^2 - \nu_j^2 = 1$ for any j .² This construction forces a decomposition of the operator T into modes by the fact that the new annihilation operators will be

$$\mathcal{U}_T A(f_j \oplus 0) \mathcal{U}_T^* = A(T(f_j \oplus 0)) = A(Uf_j \oplus Vf_j) = \mu_j a(g_j) + \nu_j a^*(g_j) \quad (\text{A.3.13})$$

¹Note that the relation $TRT^* = R$ also requires $UV^* = J^*VU^*J^*$. This follows from the other relations, as from $V^*JU = U^*J^*V$ we get $UV^*JU = UU^*J^*V = (\mathbb{1} + J^*VV^*J)J^*V = J^*V + J^*VV^*V = J^*V(\mathbb{1} + V^*V) = J^*VU^*U$, so $UV^*J = J^*VU^*$ and then $UV^* = J^*VU^*J^*$.

²We are following notations from [Sol07] for the operators and from [Lil25] for the eigenvectors, to avoid confusion with other notations introduced before. In Lill's notation, $u = U$ but $v = J^*VJ^*$, so $C = u^*vJ$, however Solovej calls the vectors $f_j = u_j^{\text{Sol}}$, $g_j = f_j^{\text{Sol}}$ and $g_j^{\text{Sol}} = J^*Vf_j$. The eigenvalues' names are the same in both references.

and the creation operators will be their adjoints. Then, as $U^*U = \mathbb{1} + V^*V$, $V^*V f_j = (\mu_j^2 - 1) f_j = \nu_j^2 f_j$, so we can express the Shale condition as $\sum_j \nu_j^2 < \infty$ and the unitary implementer will be [Lil25, Sec. 2.3.1]

$$\mathcal{U}_T = \exp \left(- \sum_j \frac{\xi_j}{2} \left(a^*(g_j)^2 - a(g_j)^2 \right) \right) \mathcal{U}_{gf}, \quad (\text{A.3.14})$$

where $\sinh \xi_j := \nu_j$ (so $\cosh \xi_j = \mu_j$) and $\mathcal{U}_{gf} : \mathcal{F}_+(\mathcal{H}) \rightarrow \mathcal{F}_+(\mathcal{H})$ is the unitary basis change transformation

$$\mathcal{U}_{gf}(f_{j_1} \otimes \cdots \otimes f_{j_n}) = g_{j_1} \otimes \cdots \otimes g_{j_n}, \quad (\text{A.3.15})$$

for any $j_1, \dots, j_n \in \mathbb{N}$. In addition, we will have that the action of the implementer on the Fock vacuum will be [Sol07, Eq. 61]

$$\mathcal{U}_T \Omega = \left(\prod_j (1 - \tanh^2 \xi_j)^{\frac{1}{4}} \right) e^{-\frac{1}{2} \sum_i \tanh \xi_i a^*(g_i)^2} \Omega. \quad (\text{A.3.16})$$

Note that an operator T of the form (A.3.10) may be written as

$$T = T_d T', \quad T_d = \begin{pmatrix} \alpha & 0 \\ 0 & J\alpha J^* \end{pmatrix}, \quad T' = \begin{pmatrix} U' & J^* V' J^* \\ V' & J U' J^* \end{pmatrix}, \quad (\text{A.3.17})$$

where $U' = |U| = \sqrt{\mathbb{1} + V^*V}$, $V' = J\alpha^* J^* V$ and α is the partial isometry giving the polar decomposition $U = \alpha|U|$. By the fact that we require $T^* R T = R$ and $T R T^* = R$, we will have that α will have range $\mathcal{H}$ and trivial kernel, so it is a unitary isometry and (A.3.17) works. Then, we can see that both T_d and T' will be Bogolyubov maps. Following the previous construction, we can then see that, indicating with primed indices the quantities related to T' , $U'^* U' = U^* U$, $V'^* V' = V^* V$ and $C' = U'^* J^* V' = U^* J^* V = C$, so $\mu'_j = \mu_j$, $\nu'_j = \nu_j$, $f'_j = f_j$ and $g'_j = f_j$, so $g_j = \alpha f_j$. It follows that the basis change map $\mathcal{U}_{gf}$ will be given by the second quantization $\Gamma(\alpha)$ of the unitary α , so the two maps are implemented by the unitaries

$$\mathcal{U}_{T'} = \exp \left(- \sum_j \frac{\xi_j}{2} \left(a^*(f_j)^2 - a(f_j)^2 \right) \right), \quad \mathcal{U}_{T_d} = \mathcal{U}_{gf} = \Gamma(\alpha). \quad (\text{A.3.18})$$

Introducing the operator $X_j := \frac{i}{2} \xi_j \left(a^*(f_j)^2 - a(f_j)^2 \right)$, we can then express this operator as $\mathcal{U}_{T'} = \exp \left(\sum_j i X_j \right)$. As the $\{f_j\}$ form an orthonormal basis for $\mathcal{H}$, we have that $[X_j, X_k] = 0$ for any j, k and thus we can split the exponential into the product of the exponentials relative to each mode, i.e.

$$\mathcal{U}_{T'} = \prod_j e^{i X_j}. \quad (\text{A.3.19})$$

A.4 Commutation properties in Fock spaces

We now want to analyse the action of such exponentials on quantum fields. To start, we shall consider Segal fields (A.1.18). From the CCR (A.1.16), we have that [Rui78, Sec. 2]

$$[\varphi_S(f), \varphi_S(g)] = i \operatorname{Im} \langle f, g \rangle. \quad (\text{A.4.1})$$

From this basic relation, we can derive how generic analytic functions of Segal fields commute.

Proposition A.4.1. *Let $F(x), G(x)$ be analytic, with $F(x) = \sum_{n=0}^{\infty} c_n x^n$ and $G(x) = \sum_{n=0}^{\infty} d_n x^n$. Then,*

$$[F(\varphi_S(f)), G(\varphi_S(g))] = \sum_{n=1}^{\infty} \frac{(i \operatorname{Im} \langle f, g \rangle)^n}{n!} G^{(n)}(\varphi_S(g)) F^{(n)}(\varphi_S(f)), \quad (\text{A.4.2})$$

where $G^{(n)}$ and $F^{(n)}$ are respectively the n -th derivatives of G and F .

Note that we will not consider convergence questions on a suitable domain in Hilbert space and consider these relations to act on finite particle vectors.

Proof. We start by considering powers of fields, for which we get

$$[\varphi_S(f)^n, \varphi_S(g)] = ni \operatorname{Im} \langle f, g \rangle \varphi_S(f)^{n-1}. \quad (\text{A.4.3})$$

We can see this by induction, as the $n = 1$ case is given by (A.4.1), and for $n = 2$ we get

$$\begin{aligned} [\varphi_S(f)^2, \varphi_S(g)] &= \varphi_S(f) [\varphi_S(f), \varphi_S(g)] + [\varphi_S(f), \varphi_S(g)] \varphi_S(f) \\ &= 2i \operatorname{Im} \langle f, g \rangle \varphi_S(f), \end{aligned}$$

so, by induction, we get

$$\begin{aligned} \varphi_S(f)^n \varphi_S(g) &= \varphi_S(f) \varphi_S(f)^{n-1} \varphi_S(g) \\ &= \varphi_S(f) (\varphi_S(g) \varphi_S(f)^{n-1} + (n-1)i \operatorname{Im} \langle f, g \rangle \varphi_S(f)^{n-2}) \\ &= (\varphi_S(g) \varphi_S(f) + i \operatorname{Im} \langle f, g \rangle) \varphi_S(f)^{n-1} + (n-1)i \operatorname{Im} \langle f, g \rangle \varphi_S(f)^{n-1} \\ &= \varphi_S(g) \varphi_S(f)^n + ni \operatorname{Im} \langle f, g \rangle \varphi_S(f)^{n-1}, \end{aligned}$$

which yields (A.4.3).

Now, considering $F(x) = \sum_{n=0}^{\infty} c_n x^n$, we get

$$[F(\varphi_S(f)), \varphi_S(g)] = \sum_{n=0}^{\infty} c_n [\varphi_S(f)^n, \varphi_S(g)] = \sum_{n=0}^{\infty} c_n \cdot ni \operatorname{Im} \langle f, g \rangle \varphi_S(f)^{n-1} = i \operatorname{Im} \langle f, g \rangle F'(\varphi_S(f)).$$

We now want to generalize this expression to powers of $\varphi_S(g)$. To do so, we will use the fact that $[A^n, B] = \sum_{k=1}^n (-1)^{k-1} \binom{n}{k} A^{n-k} \operatorname{ad}_A^k(B)$, where $\operatorname{ad}_A(B) = [A, B]$ and $\operatorname{ad}_A^k(B) = [A, \operatorname{ad}_A^{k-1}(B)]$ are nested commutators (this may be checked by induction). Then, $[B, A^n] = -[A^n, B]$, and considering $A = \varphi_S(g)$ and $B = F(\varphi_S(f))$, we get

$$[F(\varphi_S(f)), \varphi_S(g)^n] = - \sum_{k=1}^n (-1)^{k-1} \binom{n}{k} \varphi_S(g)^{n-k} \operatorname{ad}_{\varphi_S(g)}^k(F(\varphi_S(f))) \quad (\text{A.4.4})$$

We can then see that $\operatorname{ad}_{\varphi_S(g)}^k(F(\varphi_S(f))) = (-i \operatorname{Im} \langle f, g \rangle)^k F^{(k)}(\varphi_S(f))$. Indeed,

$$\begin{aligned} \operatorname{ad}_{\varphi_S(g)}(F(\varphi_S(f))) &= -[F(\varphi_S(f)), \varphi_S(g)] = -i \operatorname{Im} \langle f, g \rangle F'(\varphi_S(f)) \\ \operatorname{ad}_{\varphi_S(g)}^2(F(\varphi_S(f))) &= [\varphi_S(g), \operatorname{ad}_{\varphi_S(g)}(F(\varphi_S(f)))] \\ &= +i \operatorname{Im} \langle f, g \rangle [F'(\varphi_S(f)), \varphi_S(g)] = +(i \operatorname{Im} \langle f, g \rangle)^2 F''(\varphi_S(f)), \end{aligned}$$

so, by induction,

$$\begin{aligned} \operatorname{ad}_{\varphi_S(g)}^k(F(\varphi_S(f))) &= [\varphi_S(g), \operatorname{ad}_{\varphi_S(g)}^{k-1}(F(\varphi_S(f)))] \\ &= -(-i \operatorname{Im} \langle f, g \rangle)^{k-1} [F^{(k-1)}(\varphi_S(f)), \varphi_S(g)] \\ &= (-i \operatorname{Im} \langle f, g \rangle)^k F^{(k)}(\varphi_S(f)). \end{aligned}$$

Substituting this back in (A.4.4), we get

$$\begin{aligned} [F(\varphi_S(f)), \varphi_S(g)^n] &= - \sum_{k=1}^n (-1)^{k-1} \binom{n}{k} \varphi_S(g)^{n-k} (-i \operatorname{Im} \langle f, g \rangle)^k F^{(k)}(\varphi_S(f)) \\ &= \sum_{k=1}^n \binom{n}{k} (i \operatorname{Im} \langle f, g \rangle)^k \varphi_S(g)^{n-k} F^{(k)}(\varphi_S(f)) \end{aligned}$$

and thus, for $G(x) = \sum_{n=0}^{\infty} d_n x^n$,

$$\begin{aligned} [F(\varphi_S(f)), G(\varphi_S(g))] &= \sum_{n=0}^{\infty} d_n [F(\varphi_S(f)), \varphi_S(g)^n] \\ &= \sum_{n=1}^{\infty} d_n \sum_{k=1}^n \binom{n}{k} (i \operatorname{Im} \langle f, g \rangle)^k \varphi_S(g)^{n-k} F^{(k)}(\varphi_S(f)) \\ &= \sum_{k=1}^{\infty} \sum_{n \geq k} d_n \binom{n}{k} (i \operatorname{Im} \langle f, g \rangle)^k \varphi_S(g)^{n-k} F^{(k)}(\varphi_S(f)) \\ &= \sum_{k=1}^{\infty} (i \operatorname{Im} \langle f, g \rangle)^k \left(\sum_{n \geq k} d_n \binom{n}{k} \varphi_S(g)^{n-k} \right) F^{(k)}(\varphi_S(f)) \end{aligned}$$

Observing that $G^{(k)}(x) = \sum_{n=0}^{\infty} d_n \frac{\partial^k}{\partial x^k} x^n$, we have that $\frac{\partial^k}{\partial x^k} x^n = n(n-1) \dots (n-k+1) x^{n-k}$ if $n \geq k$ and zero otherwise. This yields

$$G^{(k)}(x) = \sum_{n \geq k} d_n n(n-1) \dots (n-k+1) x^{n-k} = k! \sum_{n \geq k} d_n \binom{n}{k} x^{n-k},$$

from which the original statement follows. $\square$

A.4.1 Weyl operators

As an example of Proposition A.4.1, by considering $F(x) = e^{ix}$, $G(x) = e^{ix}$, Proposition A.4.1 applied to Weyl operators $W(f) = e^{i\varphi_S(f)}$ yields

$$\begin{aligned} [W(f), W(g)] &= \sum_{k=1}^{\infty} \frac{1}{k!} (i \operatorname{Im} \langle f, g \rangle)^k \cdot i^{2k} e^{i\varphi_S(g)} e^{i\varphi_S(f)} \\ &= \left(\sum_{k=1}^{\infty} \frac{1}{k!} (-i \operatorname{Im} \langle f, g \rangle)^k \right) e^{i\varphi_S(g)} e^{i\varphi_S(f)} \\ &= (e^{-i \operatorname{Im} \langle f, g \rangle} - 1) W(g) W(f), \end{aligned}$$

which can be also directly obtained from the Weyl relations (1.3.1). About Weyl operators, as we have that $[a(f), a^*(f)] = \|f\|^2 \mathbf{1}$ and thus $[a^*(f), a(f)] = -\|f\|^2 \mathbf{1}$, which commutes with $a^*(f)$, $a(f)$ and every other operator, the Baker-Campbell-Hausdorff formula yields

$$\begin{aligned} e^{\frac{i}{\sqrt{2}} a^*(f)} e^{\frac{i}{\sqrt{2}} a(f)} &= e^{\frac{i}{\sqrt{2}} (a^*(f) + a(f)) + \frac{1}{2} \left[\frac{i}{\sqrt{2}} a^*(f), \frac{i}{\sqrt{2}} a(f) \right]} \\ &= e^{\frac{i}{\sqrt{2}} (a^*(f) + a(f)) + \frac{1}{4} \|f\|^2 \mathbf{1}} = e^{\frac{1}{4} \|f\|^2} e^{\frac{i}{\sqrt{2}} (a^*(f) + a(f))}, \end{aligned} \tag{A.4.5}$$

so we get that

$$W(f) = e^{-\frac{1}{4}\|f\|^2} e^{\frac{i}{\sqrt{2}}a^*(f)} e^{\frac{i}{\sqrt{2}}a(f)}. \quad (\text{A.4.6})$$

Given the Fock vacuum Ω , we can observe that $e^{\frac{i}{\sqrt{2}}a(f)}\Omega = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i}{\sqrt{2}}\right)^n a(f)^n \Omega = \Omega$, as only the $n = 0$ term survives, and thus

$$W(f)\Omega = e^{-\frac{1}{4}\|f\|^2} e^{\frac{i}{\sqrt{2}}a^*(f)}\Omega = e^{-\frac{1}{4}\|f\|^2} \sum_{n=0}^{\infty} \frac{i^n}{2^{\frac{n}{2}}n!} a^*(f)^n \Omega. \quad (\text{A.4.7})$$

Given any self-adjoint operator h on $\mathcal{H}$, we get that

$$\begin{aligned} \langle \Omega, W(f)^* d\Gamma(h) W(f) \Omega \rangle &= e^{-\frac{1}{2}\|f\|^2} \sum_{m,n=0}^{\infty} \left(\frac{i^m}{2^{\frac{m}{2}}m!} \right)^* \frac{i^n}{2^{\frac{n}{2}}n!} \langle \Omega, a(f)^m d\Gamma(h) a^*(f)^n \Omega \rangle \\ &= e^{-\frac{1}{2}\|f\|^2} \sum_{n=0}^{\infty} \frac{1}{2^n (n!)^2} \langle \Omega, a(f)^n d\Gamma(h) a^*(f)^n \Omega \rangle. \end{aligned} \quad (\text{A.4.8})$$

As $a^*(f)^n \Omega = \sqrt{n!} f^{\otimes n}$ and $a(f)^n h f \otimes f^{\otimes(n-1)} = \sqrt{n!} \langle f, h f \rangle \|f\|^{2(n-1)} \Omega$, we get

$$\begin{aligned} \langle \Omega, a(f)^n d\Gamma(h) a^*(f)^n \Omega \rangle &= \sqrt{n!} \langle \Omega, a(f)^n d\Gamma(h) f^{\otimes n} \rangle \\ &= \sqrt{n!} \langle \Omega, a(f)^n (h f \otimes \cdots \otimes f + \cdots + f \otimes \cdots \otimes h f) \rangle \\ &= \sqrt{n!} \cdot n \sqrt{n!} \langle f, h f \rangle \|f\|^{2(n-1)} = n \cdot n! \langle f, h f \rangle \|f\|^{2(n-1)}. \end{aligned} \quad (\text{A.4.9})$$

Combining equations (A.4.8) and (A.4.9), we then get

$$\begin{aligned} \langle \Omega, W(f)^* d\Gamma(h) W(f) \Omega \rangle &= e^{-\frac{1}{2}\|f\|^2} \langle f, h f \rangle \sum_{n=1}^{\infty} \frac{n}{2^n n!} \|f\|^{2(n-1)} \\ &= e^{-\frac{1}{2}\|f\|^2} \langle f, h f \rangle \cdot \frac{1}{2} e^{\frac{1}{2}\|f\|^2} = \frac{1}{2} \langle f, h f \rangle. \end{aligned} \quad (\text{A.4.10})$$

More generally, we can also analyse the adjoint action of a Weyl operator on the second quantization of a self-adjoint operator without computing its action on the Fock vacuum. To do so, we can first see that, for $f, g \in \mathcal{H}$,

$$W(f)a(g)W(f)^* = e^{-\frac{1}{4}\|f\|^2} e^{\frac{i}{\sqrt{2}}a^*(f)} e^{\frac{i}{\sqrt{2}}a(f)} a(g)W(f)^* = a(g) - \frac{i}{\sqrt{2}} \langle g, f \rangle, \quad (\text{A.4.11})$$

by the fact that $\left[e^{\frac{i}{\sqrt{2}}a^*(f)}, a(g) \right] = -\frac{i}{\sqrt{2}} \langle g, f \rangle e^{\frac{i}{\sqrt{2}}a^*(f)}$. Then, by taking the adjoint of the previous expression, we also have that

$$W(f)a^*(g)W(f)^* = a^*(g) + \frac{i}{\sqrt{2}} \langle f, g \rangle. \quad (\text{A.4.12})$$

Then, for any unitary u on $\mathcal{H}$ and any $f \in \mathcal{H}$, we have $\Gamma(u)a^*(f)\Gamma(u)^* = a^*(uf)$. Using this identity and its adjoint we find $\Gamma(u)\varphi_S(f)\Gamma(u)^* = \varphi_S(uf)$ and hence

$$\Gamma(u)W(f)\Gamma(u)^* = W(uf). \quad (\text{A.4.13})$$

By the Weyl relations this yields

$$W(-f)\Gamma(u)W(f)\Gamma(u)^* = W(-f)W(uf) = e^{\frac{i}{2}\text{Im}\langle f, uf \rangle} W((u - \mathbf{1})f).$$

Taking $u = e^{ith}$ for a self-adjoint operator h whose domain contains f , we may use Lemma 4.2.1 for $h(t) = (e^{ith} - \mathbb{1})f$ to differentiate w.r.t. t at $t = 0$, which yields

$$W(-f)d\Gamma(h)W(f) - d\Gamma(h) = \frac{1}{2}\langle f, hf \rangle \mathbb{1} + \varphi_S(ihf) \quad (\text{A.4.14})$$

when acting on any finite particle vector in the domain of $d\Gamma(h)$.

Remark. The last relations may also be obtained for $\mathcal{H}$ separable in the following manner. Considering a self-adjoint operator h on $\mathcal{H}$ and some orthonormal basis $\{e_j\}$ of $\mathcal{H}$, we have that

$$d\Gamma(h) = \sum_{j,k} \langle e_j, he_k \rangle a^*(e_j)a(e_k) = \sum_j a^*(e_j)a \left(\sum_k \langle he_k, e_j \rangle e_k \right) = \sum_j a^*(e_j)a(he_j) \quad (\text{A.4.15})$$

and thus we get the Weyl adjoint action

$$\begin{aligned} W(f)d\Gamma(h)W(f)^* &= \sum_j W(f)a^*(e_j)W(f)^*W(f)a(he_j)W(f)^* \\ &= \sum_j \left(a^*(e_j) + \frac{i}{\sqrt{2}} \langle f, e_j \rangle \right) \left(a(he_j) - \frac{i}{\sqrt{2}} \langle he_j, f \rangle \right) \\ &= \sum_j a^*(e_j)a(he_j) - \frac{i}{\sqrt{2}} (a^*(hf) - a(hf)) + \frac{1}{2} \langle f, hf \rangle \\ &= d\Gamma(h) - \varphi_S(ihf) + \frac{1}{2} \langle f, hf \rangle. \end{aligned} \quad (\text{A.4.16})$$

Indeed, taking the inner product with the vacuum, we can see we recover equation (A.4.10). Note that equation (A.4.15) could be as well written as

$$d\Gamma(h) = \sum_j a^*(he_j)a(e_j), \quad (\text{A.4.17})$$

with which we would get the same results. More generally, if we have that $h = bc^*$, we can see that

$$d\Gamma(bc^*) = \sum_j a^*(be_j)a(ce_j), \quad (\text{A.4.18})$$

as this has the same action of (A.4.15) or (A.4.17) on any $f \in \mathcal{H}$.

A.4.2 Relative entropy of Gibbs states

As an application of the commutation relations of Section A.4.1, we will consider a Gibbs state of the form (A.2.1) and w.l.o.g. let $\beta = 1$, the state will be described by density matrix $\rho = \frac{e^{-d\Gamma(H)}}{\text{tr}(e^{-d\Gamma(H)})}$, with $H > 0$ acting on the one-particle Hilbert space $\mathcal{H}$, with $\text{tr}(e^{-H}) < \infty$. Then, let ω_0 be the vacuum state with GNS-vector Ω , which we may interpret as the zero temperature state, $\beta = \infty$, and let ρ_0 denote its density matrix, i.e. the orthogonal projection onto Ω .

Then, the relative entropy of ρ_0 with respect to ρ will be

$$\begin{aligned} S(\rho_0, \rho) &= \text{tr}(\rho_0 \log \rho_0 - \rho_0 \log \rho) = -\langle \Omega, \log \rho \Omega \rangle \\ &= \langle \Omega, d\Gamma(H) \Omega \rangle + \log \text{tr}(e^{-d\Gamma(H)}) = \log \text{tr}(e^{-d\Gamma(H)}). \end{aligned} \quad (\text{A.4.19})$$

Also note that, using the techniques of the proof of Proposition A.2.1, it can be seen that, given the eigenvalues $\{h_n\}_{n \geq 0}$ of H ,

$$\begin{aligned} S(\rho_0, \rho) &= \log \operatorname{tr} \left(e^{-\operatorname{d}\Gamma(H)} \right) \leq - \sum_n \log \left(1 - e^{-h_n} \right) \\ &\leq \sum_n \frac{e^{-h_n}}{1 - e^{-h_n}} \\ &\leq \frac{\operatorname{tr} (e^{-H})}{1 - e^{-h_0}} < \infty. \end{aligned} \quad (\text{A.4.20})$$

Similarly, we can compute some lower bounds for the relative entropy. Observing that the trace over $\mathcal{H}_+^m$ can be estimated from below by summing not over all basis elements but only on the diagonal ones in the tensor product, we get

$$\begin{aligned} \operatorname{tr} \left(e^{-\operatorname{d}\Gamma(H)} \right) &= 1 + \sum_{m \geq 1} \operatorname{tr}_{\mathcal{H}_+^m} \left(e^{-\operatorname{d}\Gamma(H)} \right) \\ &\geq 1 + \sum_{m \geq 1} \sum_n e^{-mh_n} \\ &= 1 + \sum_n \sum_{m \geq 1} e^{-mh_n} \\ &= 1 + \sum_n \left(\frac{1}{1 - e^{-h_n}} - 1 \right) \\ &= 1 + \sum_n \frac{1}{e^{h_n} - 1}. \end{aligned} \quad (\text{A.4.21})$$

and so

$$S(\rho_0, \rho) = \log \operatorname{tr} \left(e^{-\operatorname{d}\Gamma(H)} \right) \geq \log \left(1 + \sum_n \frac{1}{e^{h_n} - 1} \right). \quad (\text{A.4.22})$$

In analogy with the perturbation notations of Section 3.2.2, if we take as a reference Gibbs state the vacuum, we can see a thermal state at temperature $\beta = 1$ as a perturbation of the vacuum given by the operator (3.2.17)

$$\delta_H = \frac{2}{e^H - \mathbb{1}}, \quad (\text{A.4.23})$$

where in this case we consider a generic positive self-adjoint operator H . (The vacuum indeed corresponds to $\delta_H = 0$, take $H \rightarrow \beta H$ and $\beta \rightarrow \infty$.) Then, we get that

$$\operatorname{tr} \delta_H = \sum_n \frac{2}{e^{h_n} - 1}. \quad (\text{A.4.24})$$

Together with (A.4.22) and (A.4.20), this yields the bounds

$$0 < \log \left(1 + \frac{1}{2} \operatorname{tr} \delta_H \right) \leq S(\rho_0, \rho) \leq \frac{1}{2} \operatorname{tr} \delta_H, \quad (\text{A.4.25})$$

as $\delta_H > 0$. Note that these upper and lower bounds get closer to each other for small $\operatorname{tr} \delta_H$, i.e. for large β . (In the limit $\beta \rightarrow \infty$, everything here converges to zero, we get the vacuum $\rho = \rho_0$.)

If we now consider a unitary operator U acting on the bosonic Fock space $\mathcal{F}_+(\mathcal{H})$, we get that

$$\begin{aligned} S(\rho_0, U\rho U^*) &= -\operatorname{tr}(\rho_0 U(\log \rho) U^*) = \langle \Omega, U d\Gamma(H) U^* \Omega \rangle + \log \operatorname{tr}(e^{-d\Gamma(H)}) \\ &= S(\rho_0, \rho) + \langle \Omega, U d\Gamma(H) U^* \Omega \rangle . \end{aligned} \quad (\text{A.4.26})$$

In particular, we can consider as the unitaries Weyl operators of the form $U^* = W(f) = e^{i\varphi_S(f)}$, with $f \in \mathcal{H}$. In this case, we will have that

$$S(\rho_0, W(f)^* \rho W(f)) = S(\rho_0, \rho) + \langle \Omega, W(f)^* d\Gamma(H) W(f) \Omega \rangle , \quad (\text{A.4.27})$$

so we can compute the scalar product from (A.4.10) and get the expression for the relative entropy

$$S(\rho_0, W(f)^* \rho W(f)) = S(\rho_0, \rho) + \frac{1}{2} \langle f, Hf \rangle . \quad (\text{A.4.28})$$

A.4.3 Operators quadratic in the fields

Now, we want to see what is the action of exponential quadratic in the fields, of the kind (A.3.19). Let's start by considering the action of a single exponential. As $\varphi_S(f) = \frac{1}{\sqrt{2}}(a^*(f) + a(f))$, $f \in \mathcal{H}$, we have that $\varphi_S(if) = \frac{i}{\sqrt{2}}(a^*(f) - a(f))$ and thus

$$\begin{cases} a^*(f) &= \frac{1}{\sqrt{2}}(\varphi_S(f) - i\varphi_S(if)) , \\ a(f) &= \frac{1}{\sqrt{2}}(\varphi_S(f) + i\varphi_S(if)) . \end{cases} \quad (\text{A.4.29})$$

Then, we can write

$$\begin{aligned} a^*(f)^2 - a(f)^2 &= -i(\varphi_S(f)\varphi_S(if) + \varphi_S(if)\varphi_S(f)) \\ &= -i([\varphi_S(if), \varphi_S(f)] + 2\varphi_S(f)\varphi_S(if)) \\ &= -2i\varphi_S(f)\varphi_S(if) - \|f\|^2 \end{aligned} \quad (\text{A.4.30})$$

and thus we get

$$X_j = \xi_j \varphi_S(f_j) \varphi_S(if_j) - \frac{i}{2} \xi_j \|f_j\|^2 , \quad (\text{A.4.31})$$

with $f_j \in \mathcal{H}$. As the latter term is a scalar, for the purpose of computing products of the kind $e^{-iX_j} \varphi_S(h) e^{iX_j}$, $h \in \mathcal{H}$, it is equivalent to consider exponentials of X_j or of $\tilde{X}_j = \xi_j \varphi_S(f_j) \varphi_S(if_j)$. Note that, while X_j is self-adjoint, $\tilde{X}_j$ is not. Then, we can see that

$$\begin{aligned} [i\tilde{X}_j, \varphi_S(h)] &= i\xi_j (\varphi_S(f_j) [\varphi_S(if_j), \varphi_S(h)] + [\varphi_S(f_j), \varphi_S(h)] \varphi_S(if_j)) \\ &= -\xi_j (\operatorname{Im} \langle if_j, h \rangle \varphi_S(f_j) + \operatorname{Im} \langle f_j, h \rangle \varphi_S(if_j)) \\ &= \xi_j \varphi_S(\operatorname{Re} \langle f_j, h \rangle f_j - i \operatorname{Im} \langle f_j, h \rangle f_j) \\ &= \varphi_S(\xi_j \langle h, f_j \rangle f_j) =: \varphi_S(L_j h) , \end{aligned} \quad (\text{A.4.32})$$

where $L_j h := \xi_j \langle h, f_j \rangle f_j$ is an antilinear operator on $\mathcal{H}$. Then, we will have that

$$e^{i\tilde{X}_j} \varphi_S(h) = \varphi_S(e^{L_j} h) e^{i\tilde{X}_j} , \quad (\text{A.4.33})$$

and the same will hold for the X_j , so we obtain the adjoint action of the unitary $\mathcal{U}_j = e^{iX_j}$ as

$$\mathcal{U}_j \varphi_S(h) \mathcal{U}_j^* = \varphi_S(e^{L_j} h) . \quad (\text{A.4.34})$$

To calculate the action of the exponential of L_j , we can see that $L_j^0 h = h$, $L_j h = \xi_j \langle h, f_j \rangle f_j$ and $L_j^2 h = \xi_j^2 \|f_j\|^2 \langle f_j, h \rangle f_j$. More generally, an induction argument shows that, for $n \geq 1$,

$$\begin{cases} L_j^{2n} h &= \xi_j^{2n} \|f_j\|^{4n-2} \langle f_j, h \rangle f_j, \\ L_j^{2n-1} h &= \xi_j^{2n-1} \|f_j\|^{4n-4} \langle h, f_j \rangle f_j, \end{cases} \quad (\text{A.4.35})$$

so

$$\begin{aligned} e^{L_j} h &= h + \sum_{n=1}^{\infty} \frac{1}{(2n)!} \xi_j^{2n} \|f_j\|^{4n-2} \langle f_j, h \rangle f_j + \sum_{n=1}^{\infty} \frac{1}{(2n-1)!} \xi_j^{2n-1} \|f_j\|^{4n-4} \langle h, f_j \rangle f_j \\ &= h + \left(\cosh \left(\xi_j \|f_j\|^2 \right) - 1 \right) \frac{\langle f_j, h \rangle}{\|f_j\|^2} f_j + \sinh \left(\xi_j \|f_j\|^2 \right) \frac{\langle h, f_j \rangle}{\|f_j\|^2} f_j \\ &= h - \frac{\langle f_j, h \rangle}{\|f_j\|^2} f_j + e^{\xi_j \|f_j\|^2} \frac{\operatorname{Re} \langle f_j, h \rangle}{\|f_j\|^2} f_j + i e^{-\xi_j \|f_j\|^2} \frac{\operatorname{Im} \langle f_j, h \rangle}{\|f_j\|^2} f_j. \end{aligned} \quad (\text{A.4.36})$$

Generally speaking, we get that

$$e^{iX_j} \varphi_S(h) e^{-iX_j} = e^{i\tilde{X}_j} \varphi_S(h) e^{-i\tilde{X}_j} = \varphi_S(e^{L_j} h) \quad (\text{A.4.37})$$

and thus, from (A.3.19), we get that

$$\mathcal{U}_{T'} \varphi_S(h) \mathcal{U}_{T'}^* = \varphi_S \left(\prod_j e^{L_j} h \right) = \varphi_S(e^L h), \quad (\text{A.4.38})$$

calling $L := \sum_j L_j$. Note that all L_j commute, so there is no ordering problem in the exponential.

Similarly to the case of Weyl operators, we may compute the action of a second-quantized operator $d\Gamma(h)$ on $\mathcal{U}_T \Omega$, where $\mathcal{U}_T$ is the Bogolyubov implementer given by equations (A.3.14) and (A.3.16). Let's start with the one-dimensional case, i.e. when we have a single exponential in (A.3.16). We will get that, dropping the product and sum indices,

$$\mathcal{U}_T \Omega = (1 - \tanh^2 \xi)^{\frac{1}{4}} \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{1}{2} \tanh \xi \right)^n a^*(g)^{2n} \Omega. \quad (\text{A.4.39})$$

It follows that

$$\begin{aligned} \langle \mathcal{U}_T \Omega, d\Gamma(h) \mathcal{U}_T \Omega \rangle &= \sqrt{1 - \tanh^2 \xi} \sum_{m,n=0}^{\infty} \frac{1}{n!m!} \left(-\frac{1}{2} \tanh \xi \right)^{m+n} \langle \Omega, a(g)^{2m} d\Gamma(h) a^*(g)^{2n} \Omega \rangle \\ &= \sqrt{1 - \tanh^2 \xi} \sum_{n=0}^{\infty} \frac{1}{(n!)^2} \left(-\frac{1}{2} \tanh \xi \right)^{2n} \langle \Omega, a(g)^{2n} d\Gamma(h) a^*(g)^{2n} \Omega \rangle. \end{aligned} \quad (\text{A.4.40})$$

Applying (A.4.9), we get that

$$\langle \Omega, a(g)^{2n} d\Gamma(h) a^*(g)^{2n} \Omega \rangle = 2n(2n!) \|g\|^{2(2n-1)} \langle g, hg \rangle = 2n(2n!) \langle g, hg \rangle, \quad (\text{A.4.41})$$

as $\|g\| = 1$, being the $\{g_j\}$ generally an orthonormal basis for $\mathcal{H}$. Then, we get that

$$\begin{aligned} \langle \mathcal{U}_T \Omega, d\Gamma(h) \mathcal{U}_T \Omega \rangle &= \sqrt{1 - \tanh^2 \xi} \langle g, hg \rangle \sum_{n=0}^{\infty} \frac{1}{(n!)^2} \left(-\frac{1}{2} \tanh \xi \right)^{2n} 2n(2n!) \\ &= 2\sqrt{1 - \tanh^2 \xi} \langle g, hg \rangle \sum_{n=1}^{\infty} n \frac{(2n)!}{4^n (n!)^2} (\tanh \xi)^{2n}. \end{aligned} \quad (\text{A.4.42})$$

Recognizing that

$$(1-x)^{-\frac{1}{2}} = \sum_{n=0}^{\infty} \frac{(2n)!}{4^n (n!)^2} x^n$$

for $|x| < 1$ and thus

$$\frac{1}{2}x(1-x)^{-\frac{3}{2}} = x \frac{d}{dx} (1-x)^{-\frac{1}{2}} = \sum_{n=1}^{\infty} n \frac{(2n)!}{4^n (n!)^2} x^n,$$

we get the expression

$$\begin{aligned} \langle \mathcal{U}_T \Omega, d\Gamma(h) \mathcal{U}_T \Omega \rangle &= \tanh^2 \xi \sqrt{1 - \tanh^2 \xi} (1 - \tanh^2 \xi)^{-\frac{3}{2}} \langle g, hg \rangle \\ &= \sinh^2 \xi \langle g, hg \rangle. \end{aligned} \quad (\text{A.4.43})$$

More generally, from equation (A.3.12), following the notation of Section A.3, we will have that

$$\begin{cases} \mathcal{U}_T A(0 \oplus Jf_1) \mathcal{U}_T^* = \mathcal{U}_T a^*(f_1) \mathcal{U}_T^* = a(J^* V f_1) + a^*(U f_1) \\ \mathcal{U}_T A(f_2 \oplus 0) \mathcal{U}_T^* = \mathcal{U}_T a(f_2) \mathcal{U}_T^* = a(U f_2) + a^*(J^* V f_2). \end{cases} \quad (\text{A.4.44})$$

Then, we get

$$\mathcal{U}_T a^*(f_1) a(f_2) \mathcal{U}_T^* = (a(J^* V f_1) + a^*(U f_1)) (a(U f_2) + a^*(J^* V f_2)). \quad (\text{A.4.45})$$

When considering the vacuum expectation value, only the aa^* term survives and we get

$$\langle \Omega, \mathcal{U}_T a^*(f_1) a(f_2) \mathcal{U}_T^* \Omega \rangle = \langle \Omega, a(J^* V f_1) a^*(J^* V f_2) \Omega \rangle \quad (\text{A.4.46})$$

Now, if we consider a bounded self-adjoint operator h on a separable Hilbert space $\mathcal{H}$ and take an orthonormal basis e_j of $\mathcal{H}$, by equation (A.4.15) we have that $d\Gamma(h) = \sum_j a^*(e_j) a(h e_j)$ and so we can compute

$$\begin{aligned} \langle \Omega, \mathcal{U}_T d\Gamma(h) \mathcal{U}_T^* \Omega \rangle &= \sum_j \langle \Omega, \mathcal{U}_T a^*(e_j) a(h e_j) \mathcal{U}_T^* \Omega \rangle \\ &= \sum_j \langle \Omega, a(J^* V e_j) a^*(J^* V h e_j) \Omega \rangle \\ &= \sum_j \langle a^*(J^* V e_j) \Omega, a^*(J^* V h e_j) \Omega \rangle \\ &= \sum_j \langle J^* V e_j, J^* V h e_j \rangle \\ &= \sum_j \langle V e_j, V h e_j \rangle = \sum_j \langle e_j, V^* V h e_j \rangle \\ &= \text{tr}_{\mathcal{H}}(V^* V h). \end{aligned} \quad (\text{A.4.47})$$

Since we are assuming $V^* V$ to be trace-class and we have that $V^* V f_j = \nu_j^2 f_j = \sinh^2 \xi_j f_j$, with $\sum_j \sinh^2 \xi_j < \infty$, we can take the above trace w.r.t. the orthonormal basis $\{f_j\}$ of $\mathcal{H}$ and so we get

$$\langle \Omega, \mathcal{U}_T d\Gamma(h) \mathcal{U}_T^* \Omega \rangle = \text{tr}_{\mathcal{H}}(V^* V h) = \sum_j \sinh^2 \xi_j \langle f_j, h f_j \rangle. \quad (\text{A.4.48})$$

which generalizes the single mode case of equation (A.4.43), where we had $f = g$. (It may be possible to extend this argument to an unbounded self-adjoint operator h by assuming e_j to be in the domain of h for all j and also $\text{tr}(V^* V h) < \infty$.)

Even more generally, under the same hypotheses, from (A.4.15), (A.4.18) and (A.4.45), we can see that for an orthonormal basis $\{e_j\}$ of $\mathcal{H}$,

$$\begin{aligned}
\mathcal{U}_T d\Gamma(h) \mathcal{U}_T^* &= \sum_j \left(a^*(Ue_j) a(Uhe_j) + a(J^* V e_j) a^*(J^* V he_j) \right. \\
&\quad \left. + a(J^* V e_j) a(Uhe_j) + a^*(Ue_j) a^*(J^* V he_j) \right) \\
&= \sum_j \left(a^*(Ue_j) a(Uhe_j) + a^*(J^* V e_j) a(J^* V he_j) \right. \\
&\quad \left. + a(J^* V e_j) a(Uhe_j) + a^*(Ue_j) a^*(J^* V he_j) \right) + \text{tr}_{\mathcal{H}}(V^* V h) \\
&= \text{tr}_{\mathcal{H}}(V^* V h) + d\Gamma(UhU^*) + d\Gamma(J^* V h V^* J) \\
&\quad + \sum_j \left(a(J^* V e_j) a(Uhe_j) + a^*(Ue_j) a^*(J^* V he_j) \right),
\end{aligned} \tag{A.4.49}$$

where only the trace survives when taking expectation values with the vacuum, giving us equation (A.4.48). Note that, in this computation, we are enabled to move the operator h between a and a^* thanks to equations (A.4.15), (A.4.17) and (A.4.18).

Remark. If we interpret the Bogolyubov transformation T as given by a trace-class perturbation δ , in the style of Section 3.1, we can write $\delta = T^* T - \mathbb{1}$, in which case, calling P_+ and P_- the projections of $\mathcal{K} = \mathcal{H} \oplus \overline{\mathcal{H}}$ respectively on $\mathcal{H}$ and $\overline{\mathcal{H}}$, we have that $V = P_- T P_+$ and so

$$V^* V = P_+ T^* P_- T P_+ = \frac{1}{2} P_+ T^* T P_+ - \frac{i}{2} P_+ R P_+ = \frac{1}{2} P_+ (T^* T - \mathbb{1}) P_+ = \frac{1}{2} P_+ \delta P_+, \tag{A.4.50}$$

as $P_{\pm} = \frac{1}{2}(\mathbb{1} \pm iR)$ and $R P_+ = \frac{1}{2}(R - i\mathbb{1}) = -iP_+$. It follows that

$$(\Omega, \mathcal{U}_T d\Gamma(h) \mathcal{U}_T^* \Omega) = \frac{1}{2} \text{tr}_{\mathcal{H}}(P_+ \delta P_+ h) \leq \frac{1}{2} \|h\| \text{tr}_{\mathcal{H}}(P_+ \delta P_+) \leq \frac{1}{2} \|h\| \text{tr}_{\mathcal{K}} \delta, \tag{A.4.51}$$

assuming h bounded and $\delta \geq 0$.

Appendix B

Operator monotone functions and Loewner's theorem

In this appendix, we will discuss some general aspects of the theory of operator monotone and operator convex functions and their characterization given by Loewner's theorem. We refer to [Sim19] for a comprehensive review on these topics. Operator monotone (or matrix monotone) functions are a generalization of monotonically increasing functions on real numbers to $n \times n$ matrices or operators on some Hilbert space, where the case of general bounded and unbounded operators requires more attention to formulate.

B.1 Operator monotone functions

A function $f : (a, b) \subset \mathbb{R} \mapsto \mathbb{R}$ is said to be *monotonically increasing* if for any $x, y \in (a, b)$ such that $x \leq y$, one has $f(x) \leq f(y)$. Similarly, it will be *monotonically decreasing* if $f(x) \geq f(y)$. We will also speak of *strictly increasing*, resp. *strictly decreasing*, functions if for $x < y$, one has $f(x) < f(y)$, resp. $f(x) > f(y)$. Then, the idea is to generalize these concepts by considering similar relations for functions of $n \times n$ matrices. Indeed, we can say that

Definition B.1.1. A function $f : (a, b) \subset \mathbb{R} \mapsto \mathbb{R}$ is monotone on $n \times n$ matrices if for $A \leq B$ one has $f(A) \leq f(B)$ for all $n \times n$ self-adjoint matrices A, B with spectrum contained in (a, b) .

We will call $\mathcal{M}_n(a, b)$ the set of all such functions. The set of functions monotone for $n \times n$ matrices will contain all matrices monotone for bigger matrices, for any n .

Proposition B.1.2. For any n , $\mathcal{M}_n(a, b) \subset \mathcal{M}_{n-1}(a, b)$.

Proof. Let A, B be $n - 1 \times n - 1$ matrices with eigenvalues in (a, b) . Then, we can define

$$\tilde{A} = \begin{pmatrix} A & 0 \\ 0 & \frac{a+b}{2} \end{pmatrix}, \quad \tilde{B} = \begin{pmatrix} B & 0 \\ 0 & \frac{a+b}{2} \end{pmatrix}.$$

We will have that $A \leq B$ iff $\tilde{A} \leq \tilde{B}$ and $f(A) \leq f(B)$ iff $f(\tilde{A}) \leq f(\tilde{B})$, so if $f \in \mathcal{M}_n(a, b)$ we have that $f \in \mathcal{M}_{n-1}(a, b)$. $\square$

Note that the vice versa does not hold and this inclusion is always strict [Sim19, Ch. 7]. This allows to define

$$\mathcal{M}_\infty(a, b) := \bigcap_{n=1}^{\infty} \mathcal{M}_n(a, b), \tag{B.1.1}$$

i.e. the set of matrix monotone functions for any pair of self-adjoint matrices (of any dimension) with eigenvalues in (a, b) . We will call a function $f \in \mathcal{M}_\infty$ *matrix monotone* or *operator monotone*.

Note that in these definitions we refer to the ordering of matrices given by positivity, $A \leq B$ means that $B - A \geq 0$, it is positive, cf. Section 1.1. In addition, functions of matrices will generally be defined by diagonalization, i.e. if $a \leq \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n \leq b$ are the eigenvalues of A counting multiplicity, there will exist some S satisfying

$$A = S \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} S^{-1}$$

and then if $f : (a, b) \subset \mathbb{R} \mapsto \mathbb{R}$, one has

$$f(A) = S \begin{pmatrix} f(\lambda_1) & & \\ & \ddots & \\ & & f(\lambda_n) \end{pmatrix} S^{-1},$$

this definition is independent of S (which may not be unique). For self-adjoint operators on a infinite-dimensional Hilbert space, $f(A)$ will be more generally given by spectral calculus (given appropriate assumptions on f , e.g. continuity).

These definitions can indeed be generalized to bounded and unbounded operators on a Hilbert space. Indeed, we have that matrix monotone functions will be monotone on bounded operators as well [Sim19, Thm. 2.7].

Theorem B.1.3. *Let A, B be self-adjoint operators on a separable Hilbert space $\mathcal{H}$ with spectrum contained in a bounded interval (a, b) . If $f \in \mathcal{M}_\infty(a, b)$,*

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

This may be also generalized to unbounded intervals (and thus to unbounded operators), which will however require more attention. Let's consider the case $(0, \infty)$, which corresponds to strictly positive operators. A positive unbounded operator A has form domain $\mathcal{D}(|A|^{1/2})$ and, if $A, B \geq 0$ are unbounded, $A \leq B$ means that $\mathcal{D}(|B|^{1/2}) \subset \mathcal{D}(|A|^{1/2})$ and $\langle \xi, A\xi \rangle \leq \langle \xi, B\xi \rangle$ for any $\xi \in \mathcal{D}(|A|^{1/2})$. With this definition, we get the following further generalization [Sim19, Thm. 2.9].

Theorem B.1.4. *If A, B are strictly positive (unbounded) self-adjoint operators such that $A \leq B$ and $f \in \mathcal{M}_\infty(0, \infty)$, then $f(A) \leq f(B)$.*

Before a more general characterization of operator monotone functions, we shall remark that the class of these functions is smaller than it may be naively expected. Indeed, many functions that are monotonically increasing over the reals are not operator monotone, the most immediate example is the following.

Example B.1.5. *Let $f(x) = x^2$ on $[0, \infty)$, which is (strictly) monotonically increasing on this domain. Then, we may consider the 2×2 matrices*

$$Q = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix},$$

which are self-adjoint and positive, as they are projections with spectrum $\{0, 1\}$. We can see that $Q + P \geq P$, however $(Q + P)^2 \not\geq P^2$. Indeed, this is equivalent to checking the positivity of

$$Q^2 + QP + PQ = \begin{pmatrix} 2 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix},$$

which however has eigenvalues $\lambda_1 = 1 + \frac{\sqrt{5}}{2} > 0$ and $\lambda_2 = 1 - \frac{\sqrt{5}}{2} < 0$, so $f \notin \mathcal{M}_2(0, \infty)$.

Considering too large of a class of self-adjoint operators can indeed prove quite limiting, as shown by the following result, cf. [Sim19, Thm 1.1]

Theorem B.1.6. *Let $f : \mathbb{R} \mapsto \mathbb{R}$ be such that $A \leq B \implies f(A) \leq f(B)$ hold for all 2×2 self-adjoint matrices. Then, there exist some $b \in \mathbb{R}$, $a \geq 0$ such that*

$$f(x) = ax + b.$$

Then, to get more interesting classes of operator monotone functions, we should restrict their domains to sets smaller than the whole $\mathbb{R}$.

While $f(x) = x^2$ is not monotone for matrices of any dimension > 1 , a function which shows the opposite behaviour is $f(x) = \sqrt{x}$. To see this, we need the following lemma, cf. [Sim19, Lemma 2.3]

Lemma B.1.7. *Let C, D be strictly positive bounded operators on a Hilbert space $\mathcal{H}$, $0 < C \leq D$. Then, $\|C^{1/2}D^{-1/2}\| \leq 1$.*

Proof. For any $\xi \in \mathcal{H}$, $\langle \xi, C\xi \rangle \leq \langle \xi, D\xi \rangle = \langle D^{1/2}\xi, D^{1/2}\xi \rangle$. As $D > 0$, $D^{\pm 1/2}$ are bijections and so $\eta := D^{1/2}\xi$ is a generic vector¹ in $\mathcal{H}$ and from the previous relations $\langle D^{-1/2}\eta, CD^{-1/2}\eta \rangle \leq \|\eta\|^2$. Then, $\|D^{-1/2}CD^{-1/2}\| \leq 1$ and so $\|C^{1/2}D^{-1/2}\|^2 = \|D^{-1/2}C^{1/2}C^{1/2}D^{-1/2}\| \leq 1$. $\square$

We can then prove that the square root is operator monotone, cf. [Sim19, Thm. 4.4].

Proposition B.1.8. *Let $f(x) = \sqrt{x}$. Then, $f \in \mathcal{M}_\infty(0, \infty)$.*

Proof. We give the proof for bounded operators $0 < A \leq B$. First, for any bounded operators C, D , we have that $\text{Sp}(CD) \cup \{0\} = \text{Sp}(DC) \cup \{0\}$ and their spectral radii coincide, $r(CD) = r(DC)$ [KR97a, Prop. 3.2.8]. In particular, if CD is self-adjoint (but DC may not be), $\|CD\| = r(CD) = r(DC) \leq \|DC\|$. Now, assume that B has a bounded inverse. We have that $B^{-1/4}A^{1/2}B^{-1/4}$ is positive and self-adjoint, and choosing $C = B^{-1/4}$, $D = A^{1/2}B^{-1/4}$ (both bounded), we get $\|B^{-1/4}A^{1/2}B^{-1/4}\| \leq \|A^{1/2}B^{-1/2}\| \leq 1$, where the last step comes from Lemma B.1.7. It follows that $\|A^{1/4}B^{-1/4}\| \leq 1$ and so $\sqrt{A} \leq \sqrt{B}$. For a general bounded B , we may fix an $\varepsilon > 0$ and get $B_\varepsilon = B + \varepsilon \mathbf{1}$. This operator has a bounded inverse, so the previous argument applies to yield $\sqrt{A} \leq \sqrt{B_\varepsilon}$. Taking the limit as $\varepsilon \rightarrow 0$, this gives the desired result. $\square$

For generic functions, it is however difficult to determine by hand whether they are operator monotone or not. Functions in $\mathcal{M}_\infty(a, b)$ are however completely characterized by Loewner's theorem.

¹Note that while $D^{1/2}$ is bounded and has dense range, $D^{-1/2}$ may be unbounded with dense domain. η ranges over this dense domain as ξ ranges over the entire Hilbert space.

Theorem B.1.9 (Loewner). *Let $a < b$, with possibly $a = -\infty$ and/or $b = \infty$, and let $f : (a, b) \mapsto \mathbb{R}$ be a function. The following are equivalent.*

i. $f \in \mathcal{M}_\infty(a, b)$;

ii. *there exists a unique finite measure $d\mu$ on $J : \mathbb{R} \setminus (a, b)$ and constants $c \in \mathbb{R}$, $c' \geq 0$ such that*

$$f(x) = c + c'x + \int_J \frac{1+xy}{y-x} d\mu(y); \quad (\text{B.1.2})$$

iii. *f is the restriction to (a, b) of a function f , analytic in $(\mathbb{C} \setminus \mathbb{R}) \cup (a, b)$, such that*

$$\text{Im}(z) > 0 \implies \text{Im}(f(z)) > 0. \quad (\text{B.1.3})$$

We shall not discuss here the proof of this theorem, which would go far beyond the scope of this appendix and refer to [Sim19]. We will however note that the proof has an ‘easier’ part, which is the implication *iii.* to *i.*, while the converse implication is much harder.

We will note that point *ii.* offers a generalization of Theorem B.1.6, as if $(a, b) = (-\infty, \infty)$, then $J = \emptyset$, so an operator monotone function will have the form $f(x) = ax + c$, not only for 2×2 matrices. Point *iii.* provides a practical criterion to determine whether some function is operator monotone. Indeed, we may check monotonicity by taking our function, extending it to $\mathbb{C}$ and then verifying condition (B.1.3).

Example B.1.10. *As an example, we can test this with the following functions.*

i. $f(x) = \sqrt{x}$, $x \in (0, \infty)$.

We get $f(z) = \sqrt{z}$, analytic in $(\mathbb{C} \setminus \mathbb{R}) \cup (0, \infty)$. Then, with $z = re^{i\vartheta}$, $r > 0$, $\vartheta \in [0, 2\pi)$, we get $f(z) = \sqrt{r}e^{i\vartheta/2}$, so $\text{Im}(z) > 0$ when $\vartheta \in (0, \pi)$. As $f(z) = \sqrt{r}(\cos(\vartheta/2) + i\sin(\vartheta/2))$, $\text{Im} f(z) = \sqrt{r}\sin(\vartheta/2) > 0$ when $\vartheta \in (0, \pi)$, so (B.1.3) is satisfied and $f \in \mathcal{M}_\infty(0, \infty)$, as expected from Proposition B.1.8.

ii. $f(x) = \log x$, $x \in (0, \infty)$.

Proceeding as before, we get $f(z) = \log z = \log(re^{i\vartheta}) = \log r + i\vartheta$, where $\vartheta \in (0, \pi)$ if $\text{Im} z > 0$. Then, $\text{Im} f(z) = \vartheta > 0$ for $\vartheta \in (0, \pi)$, so the logarithm is operator monotone.

iii. $f(x) = x^2$, $x \in (0, \infty)$.

In this instance, we get $f(z) = r^2e^{i2\vartheta}$, so for $\vartheta \in (0, \pi)$ we have $\text{Im} f(z) = r^2\sin(2\vartheta)$, which may be negative. Indeed, the example fails as this function is not operator monotone, as discussed earlier.

Points i. and iii. can be generalized as follows.

iv. $f(x) = x^\alpha$, with $\alpha \in \mathbb{R}$, $x \in (0, \infty)$.

$f(z) = r^\alpha e^{i\alpha\vartheta}$, so for $\vartheta \in (0, \pi)$ we have that $\text{Im} f(z) = r^\alpha \sin(\alpha\vartheta) > 0$ iff $0 \leq \alpha \leq 1$, f is operator monotone only in this range.

v. $f(x) = -x^\alpha$, with $\alpha \in \mathbb{R}$, $x \in (0, \infty)$.

$f(z) = r^\alpha e^{i(\alpha\vartheta + \pi)}$, so for $\vartheta \in (0, \pi)$ we have that $\text{Im} f(z) = r^\alpha \sin(\alpha\vartheta + \pi) > 0$ iff $-1 \leq \alpha \leq 0$, f is operator monotone only in this range.

B.2 Operator convex functions

We shall now briefly discuss some aspects of convex functions and their generalization to matrices and operators. A function $f : (a, b) \subset \mathbb{R} \mapsto \mathbb{R}$ is *convex*, resp. *concave*, if for any $x, y \in (a, b)$ and $t \in [0, 1]$,

$$f(tx + (1 - t)y) \leq tf(x) + (1 - t)f(y),$$

resp. $\geq$. We generalize these concepts with the following definition.

Definition B.2.1. Let $f : (a, b) \mapsto \mathbb{R}$. We say that f is convex on n -matrices, $f \in \mathcal{C}_n(a, b)$, if for all self-adjoint $n \times n$ matrices A, B with spectrum in (a, b) , we have that

$$f(tA + (1 - t)B) \leq tf(A) + (1 - t)f(B), \quad (\text{B.2.1})$$

for all $t \in [0, 1]$.

Similarly to monotone functions, we have that $\mathcal{C}_n \supset \mathcal{C}_{n+1}$ and we may define the set

$$\mathcal{C}_\infty(a, b) := \bigcap_n \mathcal{C}_n(a, b)$$

of the *matrix convex* or *operator convex* functions. As for monotone functions, if $f \in \mathcal{C}_\infty(a, b)$, it will also be convex for operators on a Hilbert space with spectrum in (a, b) . If f satisfies (B.2.1) with the sign reversed, we say that f is *matrix concave* or *operator concave* and write $-f \in \mathcal{C}_\infty(a, b)$.

For differentiable functions $f \in C^1(\mathbb{R}, \mathbb{R})$, f is convex iff f' is monotonically increasing. This fact generalizes in the following way to operators. Let $f : (a, b) \mapsto \mathbb{R}$ and $y \in (a, b)$, then we define

$$f_y^{(1)}(x) := \begin{cases} \frac{f(x) - f(y)}{x - y} & \text{if } x \neq y, \\ f'(x) & \text{if } x = y. \end{cases}$$

Then, we get the following results, cf. [Sim19, Thm. 9.1 and Thm. 9.2].

Theorem B.2.2 (Bendat-Kraus-Sherman-Uchiyama). Let $f \in C^1((a, b), \mathbb{R})$. The following are equivalent:

- i. $f \in \mathcal{C}_\infty(a, b)$;
- ii. for all $y \in (a, b)$, $f_y^{(1)} \in \mathcal{M}_\infty(a, b)$;
- iii. for one $y \in (a, b)$, $f_y^{(1)} \in \mathcal{M}_\infty(a, b)$.

For twice differentiable functions, we get the following result.

Theorem B.2.3. Let $f \in C^2((a, b), \mathbb{R})$. For any n , the following are equivalent:

- i. $f \in \mathcal{C}_n(a, b)$;
- ii. for all $y \in (a, b)$, $f_y^{(1)} \in \mathcal{M}_n(a, b)$.

It is generally more difficult to evaluate whether some function is operator convex than operator monotone. As an example, while the function $f(x) = x^\alpha \in \mathcal{M}_\infty(0, \infty)$ iff $\alpha \in [0, 1]$, we have that $f \in \mathcal{C}_\infty(0, \infty)$ (operator convex) iff $\alpha \in [-1, 0] \cup [1, 2]$, $-f \in \mathcal{C}_\infty(0, \infty)$ (operator concave) iff $\alpha \in [0, 1]$, and neither otherwise [Sim19, Thm. 9.9, Ex. 9.13 and Ex. 10.4]. As a comparison, f as a real-valued function is convex if $\alpha \leq 0$ or $\alpha \geq 1$ and concave for $0 \leq \alpha \leq 1$. Instead, $f(x) = -x^\alpha \in \mathcal{M}_\infty(0, \infty)$ iff $-1 \leq \alpha \leq 0$ and the convexity/concavity conditions are swapped.

Another result for real-valued functions is that if f is concave and non-negative on $(0, \infty)$, then f is monotonically increasing [Sim19, Prop. 10.1]. This can be generalized on the operator level as follows [Sim19, Thm. 10.2].

Theorem B.2.4.

- i. if $-f \in \mathcal{C}_n(0, \infty)$ and $f \geq 0$, then $f \in \mathcal{M}_n(0, \infty)$;
- ii. if $f \in \mathcal{M}_{2n}(0, \infty)$, then $-f \in \mathcal{C}_n(0, \infty)$.

In particular, if $f \geq 0$, then $-f \in \mathcal{C}_\infty(0, \infty)$ iff $f \in \mathcal{M}_\infty(0, \infty)$.

It can be seen that all the above conditions are necessary. Indeed, $f(x) = -x^2 \in -\mathcal{C}_\infty(0, \infty)$ but is not even monotonically increasing (as a real-valued function), so in point i. we need $f \geq 0$. Point i. cannot be generalized to a finite interval, as for example $f(x) = 1 - x^2 > 0$ for $x \in (0, 1)$ and $-f \in \mathcal{C}(0, 1)$, but is not even monotonically increasing. Also, $f(x) = (2 - x)^{-1} \in \mathcal{M}_\infty(0, 1)$ is positive and $f \in \mathcal{C}_\infty(0, 1)$, so point ii. needs a semi-infinite interval as well.

We will conclude this section by presenting a result linking operator convexity to operator inequalities, the Hansen-Jensen-Pedersen inequality, cf. [Sim19, Thm 11.1].

Theorem B.2.5 (Hansen-Jensen-Pedersen). *Let $f : (a, b) \subset \mathbb{R} \mapsto \mathbb{R}$, with possibly $a = -\infty$ and/or $b = \infty$, be a continuous function, and let $\mathcal{H}$ be an infinite-dimensional separable Hilbert space. Then, the following are equivalent:*

- i. $f \in \mathcal{C}_\infty(a, b)$;
- ii. for any finite collection of bounded self-adjoint operators $\{X_j\}_{j=1}^n$ with spectra in (a, b) and any collection of bounded operators $\{A_j\}_{j=1}^n$ with $\sum_{j=1}^n A_j^* A_j = \mathbb{1}$, we have that

$$f\left(\sum_{j=1}^n A_j^* X_j A_j\right) \leq \sum_{j=1}^n A_j^* f(X_j) A_j; \quad (\text{B.2.2})$$

- iii. for any isometry V on $\mathcal{H}$ and any self-adjoint operator X with spectrum in (a, b) ,

$$f(V^* X V) \leq V^* f(X) V; \quad (\text{B.2.3})$$

- iv. for any self-adjoint projection P and any self-adjoint operator X with spectrum in (a, b) ,

$$f(PXP) \leq P f(X) P. \quad (\text{B.2.4})$$

Appendix C

Operator inequalities

In this section, we will present a number of inequalities satisfied by p -norms of operators which will come into play throughout the text.

C.1 Generalities on p -norms

Let $\mathcal{H}$ be a complex Hilbert space and $T \in \mathcal{B}(\mathcal{H})$ a bounded operator on $\mathcal{H}$. For $p \in [1, \infty)$, we define the *Schatten p -norm* of T as

$$\|T\|_p := (\operatorname{tr}(|T|^p))^{\frac{1}{p}}, \quad (\text{C.1.1})$$

where $|T| = \sqrt{T^*T}$ and we refer to Section 1.1 for generalities on the operator trace. For $p = 1$, this yields the trace norm $\|\cdot\|_1 = \operatorname{tr}|\cdot|$, and for $p = 2$, the Hilbert-Schmidt norm $\|\cdot\|_2 = \|\cdot\|_{\text{HS}}$. In the limit $p \rightarrow \infty$, we get the usual operator norm $\|\cdot\| = \|\cdot\|_\infty$.

As the name implies, for $p \in [1, \infty]$, the p -norm is indeed a norm, which will be unitarily invariant, i.e. U, V unitaries on $\mathcal{H}$, $\|UTV\|_p = \|T\|_p$, sub-multiplicative, i.e. $\|ST\|_p \leq \|S\|_p \|T\|_p$, and monotone under p , i.e. for $1 \leq p \leq p' \leq \infty$, $\|T\|_1 \geq \|T\|_p \geq \|T\|_{p'} \geq \|T\|_\infty$, cf. [Sch70]. Note that it is also possible to generalize (C.1.1) to $p \in (0, 1)$ through functional calculus, which will be still well-defined but will yield a seminorm, for which the triangle inequality fails. We refer to [Sim79] for more general properties of p -norms.

C.2 p -norm inequalities

Now, we will review some inequalities involving the p -norms of operators, with particular attention to the trace norm and the Hilbert-Schmidt norm. A first standard result is the Powers-Størmer inequality, cf. [PS70, Lemma 4.1].

Theorem C.2.1 (Powers-Størmer). *Let A, B be positive operators over some Hilbert space. Then,*

$$\left\| \sqrt{A} - \sqrt{B} \right\|_{\text{HS}}^2 \leq \operatorname{tr} |A - B|.$$

This inequality can in fact be generalized beyond the Hilbert-Schmidt and trace norms, through the following results by Kittaneh, cf. [Kit86, Thm. 2 and Cor. 2]

Theorem C.2.2 (Kittaneh). *Let A, B be bounded operators over some Hilbert space such that $A + B \geq \pm X$, where X is a self-adjoint operator. Then, for $1 \leq p \leq \infty$,*

$$\|AX + XB\|_p \geq \|X\|_{2p}^2.$$

Choosing $X = A - B$, this yields the following result.

Theorem C.2.3 (generalized Powers-Størmer inequality). *Let A, B be positive operators over some Hilbert space. Then, for $1 \leq p \leq \infty$,*

$$\|A - B\|_{2p}^2 \leq \|A^2 - B^2\|_p.$$

Another standard result is the van Hemmen-Ando inequality, cf. [HA80, Prop. 2.1] and [Kit87, Thm. 5], where the original result by van Hemmen and Ando is the $p = 1$ case.

Theorem C.2.4 (generalized van Hemmen-Ando inequality). *Let A and B be positive, bounded operators on some Hilbert space. For any $\alpha \geq 0$ such that $\sqrt{A} + \sqrt{B} \geq \alpha \mathbb{1}$ one has*

$$\alpha \|\sqrt{A} - \sqrt{B}\|_p \leq \|A - B\|_p$$

for any p -norm with $1 \leq p \leq \infty$.

Note that the condition $\sqrt{A} + \sqrt{B} \geq \alpha \mathbb{1}$, which for $\alpha > 0$ is e.g. implied by at least one of the two operators being greater than $\alpha \mathbb{1}$, is indeed necessary for this theorem to hold. For example, consider the $p = 1$ case. If we assume the hypotheses of the Powers-Størmer inequality, i.e. $A, B \geq 0$, we could take A, B to be two positive trace-class operators, so $\sqrt{A}, \sqrt{B}$ will be Hilbert-Schmidt. For generic operators, this can yield a finite RHS for the van Hemmen-Ando inequality but an infinite LHS, this case is accounted for by $\alpha = 0$.

In addition, the van Hemmen-Ando inequality has been further generalized beyond the square root to operator monotone functions (see Section B.1) by Kittaneh and Kosaki, cf. [KK87, Thm. 3.1].

Theorem C.2.5 (Kittaneh-Kosaki). *Let A and B be positive, bounded operators on some Hilbert space $\mathcal{H}$, such that $A \geq a \mathbb{1} \geq 0$ and $B \geq b \mathbb{1} \geq 0$. Then, for any operator monotone function f , any operator X on $\mathcal{H}$, and $1 \leq p \leq \infty$, one has*

$$\|f(A)X - Xf(B)\|_p \leq C(a, b) \|AX - XB\|_p,$$

where

$$C(a, b) = \begin{cases} \frac{f(a) - f(b)}{a - b} & \text{if } a \neq b; \\ f'(a) & \text{if } a = b. \end{cases}$$

Another result of this kind is a generalization of the inequality of arithmetic and geometric means (AM-GM inequality) to the operator case by Kosaki, cf. [Kos98, Thm. 1 and App. A].

Theorem C.2.6 (operator AM-GM inequality). *Let A, B, X be bounded operators on some Hilbert space, with A, B positive. For any unitarily invariant norm $\|\cdot\|$, one has*

$$\|\sqrt{A}X\sqrt{B}\| \leq \frac{1}{2} \|AX + XB\|.$$

Note that the arithmetic mean-geometric mean inequality of Theorem C.2.6 applies in particular when $\|\cdot\|$ is any p -norm.

Another result that will be of interest to us is the following, given by Kittaneh in [Kit85].

Theorem C.2.7 (Kittaneh). *Let N be a normal operator on a Hilbert space $\mathcal{H}$ and let f be a function defined on the spectrum of N , $\text{Sp}(N)$. If $|f(x) - f(x')| \leq k|x - x'|$ for any $x, x' \in \text{Sp}(N)$ and some $k \geq 0$, then*

$$\|f(N)X - Xf(N)\|_{\text{HS}} \leq k \|NX - XN\|_{\text{HS}},$$

for any $X \in \mathcal{B}(\mathcal{H})$.

This result leads to the following corollary, cf. [Kit85, Cor. 2].

Corollary C.2.8. *Let N and M be normal operators on $\mathcal{H}$ and let f be a function defined on the union of the spectra of N and M . If $|f(x) - f(x')| \leq k|x - x'|$ for any $x, x' \in \text{Sp}(N) \cup \text{Sp}(M)$ and some $k \geq 0$, then*

$$\|f(N)X - Xf(M)\|_{\text{HS}} \leq k\|NX - XM\|_{\text{HS}},$$

for any $X \in \mathcal{B}(\mathcal{H})$. In particular,

$$\|f(N) - f(M)\|_{\text{HS}} \leq k\|N - M\|_{\text{HS}}.$$

Note that results of the form

$$\|f(A) - f(B)\|_p \leq C\|A - B\|_p,$$

with $C > 0$ finite, are known to exist for Lipschitz functions for $1 < p < \infty$ [PS11; Cas+14]. Note that the $p = 1$ case (considered in [Kre53]) fails, as a counterexample was found in [Far72].

Similarly, for α -Hölder functions with $0 < \alpha < 1$, one has that

$$\|f(A) - f(B)\|_p \leq C\|A - B\|_p^\alpha,$$

for any $p > 0$ [AP10; HSZ22], with $C > 0$ finite.

Unfortunately, the constant C in these general estimates for Lipschitz and Hölder continuous functions is in general unknown and it may not equal the Lipschitz or Hölder constant. Explicit constants are only known for specific examples, e.g. if $p = 2$ and $f(x) = \sqrt{x}$, we recover Theorem C.2.1 with $C = 1$. A general estimate for the operator norm, $p = \infty$, is given by [NF10] with $C = c \cdot k$, where k is the α -Hölder constant, $0 < \alpha < 1$, and $c = 2^{1-\alpha} + 4\pi\sqrt{2}(1 - 2^{\alpha-1})^{-2}$.

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