ENTROPIC GRADIENT FLOW STRUCTURE OF QUANTUM MARKOV SEMIGROUPS



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Tag der Abgabe: 15. 10. 2019 Tag der öffentlichen Verteidigung: 23. 03. 2020 "It seems to me that the poet has only to perceive that which others do not perceive, to look deeper than others look. And the mathematician must do the same thing."

Sofia Kovalevskaya¹

"Entropy is a figure of speech, then, a metaphor. It connects the world of thermodynamics to the world of information flow. The machine uses both. The Demon makes the metaphor not only verbally graceful, but also objectively true."

Thomas Pynchon²

"Todd, trust math. As in Matics, Math E. First-order predicate logic. Never fail you. Quantities and their relation. Rates of change. The vital statistics of God or equivalent. When all else fails. When the boulder's slid all the way back to the bottom. When the headless are blaming. When you do not know your way about. You can fall back and regroup around math. Whose truth is deductive truth. Independent of sense or emotionality. The syllogism. The identity. Modus Tollens. Transitivity. Heaven's theme song. The night light on life's dark wall, late at night. Heaven's recipe book. The hydrogen spiral. The methane, ammonia, H2O. Nucleic acids. A and G, T and C. The creeping inevibatility. Caius is mortal. Math is not mortal. What it is is: listen: it's true."

David Foster Wallace³

¹Sónya Kovalévsky. *Her Recollections of Childhood*, translated from the Russian by Isabel. F. Hapgood. The Century Co, New York, 1895.

²Thomas Pynchon. *The Crying of Lot 49.* J. B. Lippincott, Philadelphia, 1966.

³David Foster Wallace. Infinite Jest. Little, Brown and Company, New York, 1996.

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ZUSAMMENFASSUNG IN DEUTSCHER SPRACHE

Gegenstand der vorliegenden Arbeit ist die Konstruktion einer nichtkommutativen Transportmetrik, die es erlaubt, spursymmetrische vollständig Markovsche Halbgruppen als Gradientenfluss der Entropie aufzufassen.

Eine vollständig Markovsche Halbgruppe ist eine Halbgruppe von Operatoren P_t auf einer von Neumann algebra \mathcal{M} , die gewisse Stetigkeitseigenschaften haben, die Identität von \mathcal{M} auf sich selbst abbilden und für die die Operatoren

$$P_t \otimes \mathrm{id} \colon \mathscr{M} \otimes M_n(\mathbb{C}) \to \mathscr{M} \otimes M_n(\mathbb{C})$$

für alle $n \in \mathbb{N}$ positive Elemente auf positive Elemente abbilden. Solche Halbgruppen treten under anderem in der Beschreibung von offenen Quantensystemen auf, zu ihnen gehören aber auch klassische Beispiele wie die Halbgruppe, die der diskrete Laplaceoperator auf einem Graph oder der Laplace-Beltrami-Operator auf einer Riemannschen Mannigfaltigkeit erzeugt.

Ein Gradientenfluss eines Funktionals auf einem metrischen Raum ist eine Kurve, die zu jedem Zeitpunkt stets in die Richtung des steilsten Abstieges fließt. Es ist in einer Reihe von Fällen bekannt, dass man die Gradientenflüsse der Boltzmann-Entropie

$$\operatorname{Ent}(\rho) = \int \rho \log \rho \, dm$$

oder ihres nichtkommutativen Analogons, der von Neumann-Entropie, bezüglich geeigneter Transportmetriken als Lösungen von Differentialgleichungen der Form

$$\dot{\rho}_t = -\mathscr{L}\rho_t$$

charakterisieren kann, so zum Beispiel wenn \mathscr{L} der (positive) Laplace-Beltrami-Operator auf einer Riemannschen Mannigfaltigkeit, der Laplace-Operator auf einem endlichen Graphen oder ein Lindblad-Generator auf einer Matrixalgebra ist.

ZUSAMMENFASSUNG IN DEUTSCHER SPRACHE

Ziel dieser Arbeit ist es zu zeigen, dass das gemeinsame zugrundeliegende Prinzip in all diesen Fällen die Markoveigenschaft der von \mathscr{L} erzeugten Halbgruppe ist. Dazu wird für eine gegebene spursymmetrische vollständig Markovsche Halbgruppe eine Transportmetrik auf dem Raum der Dichteoperatoren konstruiert, die die Metriken in den oben genannten Fällen verallgemeinert. Es wird bewiesen, dass unter geeigneten Voraussetzungen die gegebene Halbgruppe der eindeutige Gradientenfluss der von-Neumann-Entropie ist. Als Konsequenzen werden Semikonvexität der Entropie entlang von Geodäten und Funktionalungleichungen für die Halbgruppe diskutiert.

INTRODUCTION

In this thesis, a noncommutative analog of the Wasserstein distance is constructed that allows to view tracially symmetric quantum Markov semigroups as gradient flows of the entropy.

A quantum Markov semigroup (QMS) is a semigroup of operators P_t on a von Neumann algebra \mathcal{M} that have certain continuity properties, map the identity of \mathcal{M} onto itself and for which the operators

$$P_t \otimes \mathrm{id} \colon \mathscr{M} \otimes M_n(\mathbb{C}) \to \mathscr{M} \otimes M_n(\mathbb{C})$$

map positive elements onto positive elements for all $n \in \mathbb{N}$. These semigroups occur for example in quantum statistical mechanics in the study of open quantum systems. In this context, the second law of thermodynamics asserts that the entropy decreases (or increases, depending on the sign convention) in time along the QMS. One natural question is whether one can in some way quantify the rate of entropy dissipation/production.

A gradient flow of the function $S: M \to \mathbb{R}$ on a Riemannian manifold is a semigroup of maps $\Phi_t: M \to M$ such that

$$\frac{d}{dt}\Phi_t = -\nabla S \circ \Phi_t,$$

$$\Phi_0 = \mathrm{id}.$$

In other words, the trajectories $(\Phi_t(x))_{t\geq 0}$ are curves of steepest descent for S. We will show that one can endow the space of density operators of an open quantum system with a (formal) Riemannian structure such that the time evolution of the system follows gradient flow curves of the entropy. In this sense the entropy not only decreases in time, but does so at the highest possible rate, giving a quantitative version of the second law of thermodynamics for Markovian open quantum systems.

The notion of gradient flows has long since been generalized to convex functionals on Hilbert spaces and been used in the theory of partial differential equations. For example, it is well known that the semigroup generated by a positive self-adjoint operator is the gradient flow of the associated quadratic form.

In contrast, the study of gradient flows in metric spaces that are not normed is relatively recent. In the classical (non-quantum) case, the idea of viewing evolution equations as gradient flows of entropy functionals in a suitable metric space goes back to the celebrated article of Jordan, Kinderlehrer and Otto [JKO98]. They showed that solutions of the heat equation

$$\dot{\mu}_t = \Delta \mu_t$$

on \mathbb{R}^d can be obtained as limits of a generalized minimizing movement scheme (now known as JKO scheme) in the space of probability measures with finite second moment endowed with the L^2 -Wasserstein metric

$$W_{2}(\mu,\nu) = \left(\inf \left\{ \int_{\mathbb{R}^{d} \times \mathbb{R}^{d}} |x-y|^{2} d\pi(x,y) \left| (\mathrm{pr}_{1})_{\#} \pi = \mu, (\mathrm{pr}_{2})_{\#} \pi = \nu \right\} \right)^{1/2}$$

This is an instance of an optimal transport problem (see the textbooks [Vil03, Vil09] by Villani for an introduction into this theory) and is often called Monge–Kantorovich formulation of the Wasserstein metric after the founders of this research field.

Shortly after the JKO result, Benamou and Brenier [BB00] gave a dynamic characterization of the Wasserstein distance now known as Benamou–Brenier formula, namely

$$W_{2}(\mu,\nu) = \inf\left\{\int_{0}^{1} \left(\int_{\mathbb{R}^{d}} |v_{t}|^{2} d\mu_{t}\right)^{1/2} dt \left| \dot{\mu}_{t} + \nabla \cdot (\mu_{t}v_{t}) = 0, \, \mu_{0} = \mu, \mu_{1} = \nu\right\}.$$

This lead Otto [Ott01] to the interpretation of the Wasserstein space as a (formal) Riemannian manifold and the heat flow as gradient flow of the entropy in the sense explained above.

The JKO result spawned a lot of subsequent activity, extending the gradient flow characterization to various other geometric settings (see for example [AGS14a, AS18, Erb10, GKO13, Jui14, OS09]) as well as to other evolution equations (see e.g. [Erb16]).

Not the least, the characterization of the heat flow as gradient flow of the entropy played a crucial role in the work of Ambrosio, Gigli and Savaré [AGS14a, AGS14b, AGS15] and Erbar, Kuwada and Sturm [EKS15] that provided an understanding of the connection between synthetic lower bounded Ricci curvature bounds in the sense of Lott–Sturm–Villani [LV09, Stu06a, Stu06b] and Bakry– Émery [BÉ85]. In contrast, for discrete spaces the Monge–Kantorovich formulation of transport distances has turned out not to be useful in this direction: While one can define the Wasserstein distance for probability measures on arbitrary metric spaces, absolutely continuous curves in the Wasserstein space are constant when the metric is discrete. Hence there are simply no non-trivial gradient flows. Similarly, the Wasserstein distance has not lent itself to gradient flow characterizations of evolution equations with non-local generators such a fractional Laplacians.

However, Maas [Maa11], Mielke [Mie11], and Chow, Huang, Li and Zhou [CHLZ12] independently defined a discrete transport metric \mathcal{W} on the set of probability densities over a finite graph such that the heat flow for the graph Laplacian coincides with the gradient flow of the entropy with respect to \mathcal{W} . Instead of the Monge–Kantorovich optimal transport problem, their approach is based on a discrete version of the Benamou–Brenier formula.

Vector fields on a graph are usually identified with functions on the (oriented) edges so that unlike for manifolds, there is not a canonical way to multiply a function on the graph with a vector field to obtain a new vector field. For example, one could define

$$(u\xi)(x,y) := u(x)\xi(x,y)$$

or

$$(u\xi)(x,y) := u(y)\xi(x,y).$$

The key insight in the articles cited above was that one has to take an average of these two products. More precisely, in the simplest case of an unweighted graph, the metric \mathcal{W} is defined as follows:

$$\mathcal{W}(\mu_0,\mu_1)^2 = \inf\left\{\frac{1}{2}\int_0^1 \sum_{(x,y):\ x \sim y} \hat{\mu}_t(x,y)\xi_t(x,y)^2 dt \,\Big| \,\dot{\mu}_t(x) = \frac{1}{2} \sum_{y:\ y \sim x} \hat{\mu}_t(x,y)\xi_t(x,y)\right\}.$$

Here, $\hat{\mu}_t(x, y)$ denotes the logarithmic mean of $\mu_t(x)$ and $\mu_t(y)$, that is,

$$\hat{\mu}_t(x, y) = \int_0^1 \mu_t(x)^{\alpha} \mu_t(y)^{1-\alpha} \, d\alpha.$$

In fact, one can use means other than the logarithmic one to obtain a whole family of discrete transport metrics. But it is only the logarithmic mean that yields the entropic gradient flow structure of the discrete heat equation.

This new metric has already proven to be very fertile. On the one hand, the gradient flow characterization has been generalized to the heat equation for generators of jump processes [Erb14] as well as a variety of other evolution equations on graphs [CLZ19, EM14, EFLS16, LM13]. On the other hand, (variants of)

the metric \mathcal{W} has been used (among other things) to define lower Ricci curvature bounds for graphs [EM12] and to study a new discrete version of the nonlinear Schrödinger equation [CLZ18].

Moreover, recent years have seen new activity in the study of matrix-valued optimal transport with several groups studying a version of the metric \mathcal{W} for matrix algebras (see [CM14, CM17a, CGGT17, CGT18, MM17]); and, independently, Brenier [Bre17, Bre18] discovered a surprising connection between matrix-valued optimal transport and fluid dynamics. Notably, Carlen and Maas [CM14, CM17a] showed that the metric \mathcal{W} allows to view certain quantum Markov semigroups on finite-dimensional algebras as gradient flow of the von Neumann entropy.

Both in the case of graphs and matrix algebras, all work so far has been limited to a finite-dimensional setting and the question of extending it to the infinitedimensional case has been raised in several of the mentioned articles.

The goal of this thesis is to work out Markovianity as crucial structural property shared by all the examples mentioned above and to present an extension of the theory to the infinite-dimensional setting on this basis. More precisely, we give a definition of W and a characterization of tracially symmetric quantum Markov semigroups – a setting that generalizes many of the ones above – as gradient flows of the entropy, based on the first-order differential calculus developed by Cipriani and Sauvageot [CS03]. Despite the attributes "quantum" and "noncommutative", this framework includes the classical (non-quantum or commutative) setting.

In particular, this thesis gives the first unified approach to the results in the local case (for example the heat equation on Euclidean space, manifolds, infinitesimally Riemannian metric measure spaces) on the one hand and non-local case (e.g. heat equation on graphs, for fractional powers of the Laplacian) on the other hand, which could only be treated by analogy until now. Let us stress that such a unified treatment of the local and non-local case is not possible in the finite-dimensional case, since locality is a purely infinite-dimensional phenomenon (incidentally, it did not appear in the seminal work of Beurling–Deny [BD58] on Dirichlet forms, as they only treated the finite-dimensional case).

On the noncommutative side, this setting does not only cover infinite-dimensional quantum systems, but also some classical examples of noncommutative geometry such as the noncommutative heat semigroup on the noncommutative torus. This could open the door to a theory of Ricci curvature for noncommutative spaces, a concept that has been notoriously elusive in noncommutative geometry until now.

Let us shortly comment on the differences to prior work. In contrast to the case of metric measure spaces, many powerful tools coming from the Monge– Kantorovich theory of optimal transport are not available here. Furthermore, in the Benamou–Brenier formulation, the continuity equation depends linearly on the measure density in the local case, while in our setting, it is in general a nonlinear equation in the density.

These problems have already been tackled successfully in the non-local case of graphs and jump processes, however, the necessary analysis of monotonicity and convexity properties turns out more difficult in the noncommutative setting as operator monotonicity and operator convexity are decidedly more rigid notions than their commutative counterparts.

Compared to previous work on matrix-valued optimal transport, we deal not only with operators on an infinite-dimensional space (as opposed to matrices), but mostly with unbounded ones. This requires a careful adaptation of classical tools for operator monotonicity and convexity, which are usually only developed for bounded operators. Furthermore, it is only in the infinite-dimensional case that the full power of the theory of gradient flows in metric spaces is needed.

Among other possible applications, we hope to lay the ground for a systematic study of geodesic convexity of the entropy for infinite-dimensional quantum systems, a topic which has already proven useful for convergence results in the finite-dimensional case [CM17a, CM18].

Moreover, the theory developed here could provide a framework for approximation results of smooth spaces or infinite-dimensional systems by discrete spaces or finite-dimensional systems, which so far have only been treated in some particular cases [GM13, Gar17, GKM18].

Outline and summary of results

In Chapter 1 we recall some basic facts about quantum Dirichlet forms, including the first-order differential calculus of Cipriani and Sauvageot.

Let us first illustrate it with an example. The prototype of a (commutative) Dirichlet form is the Dirichlet energy on \mathbb{R}^n , that is,

$$\mathscr{E}(u)=-\int u\Delta u\,dx.$$

By partial integration, $\mathscr E$ can equivalently be expressed as

$$\mathscr{E}(u) = \int |\nabla u|^2 dx,$$

and ∇ is a derivation in the sense that it satisfies the product rule $\nabla(uv) = u\nabla v + v\nabla u$.

Now, if \mathscr{E} is a quantum Dirichlet form, the first-order differential calculus of Cipriani and Sauvageot (Theorem 1.20) asserts that it can be represented in a

similar way. To be more precise, there exists a Hilbert bimodule \mathcal{H} and an operator ∂ with values in \mathcal{H} such that

$$\mathscr{E}(a) = \|\partial a\|_{\mathscr{H}}^2$$

and ∂ satisfies the product rule $\partial(ab) = a\partial b + (\partial a)b$. One crucial difference of the general case from the Dirichlet energy on \mathbb{R}^n is that the left and right multiplication on \mathcal{H} may be different. For commutative Dirichlet forms, this phenomenon is connected to the nonlocality of the form.

In general, the left and right multiplication L(a) and R(a) on \mathcal{H} are only defined for bounded elements a in the domain of \mathcal{E} . In the last part of Chapter 1 we examine when they can be extended to all of \mathcal{M} . It turns out that this question is closely related to the carré du champ (or square field operator)

$$\Gamma(a)(x) = \langle x \partial a, \partial a \rangle_{\mathcal{H}}.$$

As the main new result of the chapter we characterize when the carré du champ is σ -weakly continuous for all $a \in D(\mathscr{E})$. In the commutative case, this simply means that the energy measure is absolutely continuous with respect to the reference measure. In Theorem 1.32 we show that this property holds if and only if the left and right multiplication have a σ -weakly continuous extension to all of \mathscr{M} . In this case we say that the trace τ is energy dominant. (in the commutative case, this holds if and only if the energy measure is absolutely continuous with respect to the reference measure) For the rest of the thesis we will work under the standing assumption that this property holds.

In Chapter 2 we study a class of means θ . Just as in the discrete case discussed above, the left and right multiplication L and R on the tangent bimodule \mathscr{H} do not coincide in general, and one can take averages of them: If $\theta : [0,\infty)^2 \to [0,\infty)$ is continuous, we define $\hat{\rho} = \theta(L(\rho), R(\rho))$ via the spectral theorem for density operators ρ and denote the associated quadratic form by $\|\cdot\|_{\rho}^2$.

Furthermore, we define \mathscr{A}_{θ} as the space of all bounded elements a in the domain of \mathscr{E} for which $\|\partial a\|_{\rho}^{2}$ is bounded independently of the density operator ρ . Later on, \mathscr{A}_{θ} will play the role of a space of test "functions".

While these definitions make sense for arbitrary continuous functions θ , one needs more structure to obtain interesting results. For this reason we then narrow our focus to functions θ that can be represented by operator means in the sense of Kubo–Ando (Definition 2.17). These functions are closely related to operator monotone functions and admit an integral representation

$$\theta(s,t) = \int_0^1 \frac{st}{\lambda s + (1-\lambda)t} \, d\mu(\lambda)$$

for a Borel probability measure μ . Of special interest for us are the arithmetic mean $AM(s,t) = \frac{1}{2}(s+t)$ and the logarithmic mean

$$LM(s,t) = \frac{s-t}{\log s - \log t}$$

For θ that can be represented by a symmetric operator mean we show that \mathscr{A}_{θ} is a *-algebra (Proposition 2.22) and the map $\rho \mapsto \|\partial a\|_{\rho}^{2}$ is concave and upper semicontinuous for all $a \in \mathscr{A}_{AM}$ (Theorem 2.14). The second result will be crucial for semicontinuity properties of the metric \mathcal{W} discussed next.

In Chapter 3 we construct the noncommutative transport metric \mathcal{W} and analyze some of its basic properties. We first introduce a class of curves in the space of density operators, called admissible curves (Definition 3.4). These are curves (ρ_t) for which the noncommutative continuity equation

$$\dot{\rho}_t = \partial^* (\hat{\rho}_t \xi_t)$$

has a solution (ξ_t) in a suitable weak sense. In the weak formulation of this equation, the algebra \mathscr{A}_{θ} introduced in the previous chapter comes into play. If it exists, the solution (ξ_t) is unique and will be denoted by $(D\rho_t)$.

The metric \mathcal{W} is then defined (Definition 3.12) as the length metric associated with the action functional

$$(\rho_t) \to \int \|D\rho_t\|_{\rho_t}^2 dt$$

on the space of admissible curves. By the Benamou–Brenier formula, this metric coincides with the L^2 -Wasserstein distance if \mathscr{E} is the standard Dirichlet energy on Euclidean space, while it agrees with the nonlocal transport distance constructed in [CHLZ12, Maa11, Mie11] for finite graphs and with the noncommutative transport distance from [CM17a] for tracially symmetric QMS on matrix algebras.

In general, it cannot be ruled out that \mathcal{W} is degenerate or takes the value infinity. While the latter already occurs for the Wasserstein distance on Euclidean space, we will show that \mathcal{W} is non-degenerate under fairly weak assumptions (Proposition 3.20). Furthermore we establish some basic properties such as the convexity of \mathcal{W} (Lemma 3.24) and use the semicontinuity result from the previous chapter to deduce lower semicontinuity of the action functional with respect to pointwise weak convergence in L^1 (Theorem 3.30).

Chapter 4 deals with the von Neumann entropy

$$\operatorname{Ent}(\rho) = \tau(\rho \log \rho)$$

and the Fisher information

$$\mathscr{I}(\rho) = \mathscr{E}(\rho, \log \rho).$$

While the entropy functional is well understood also for infinite-dimensional quantum systems and we mainly rehearse some known facts, less seems to be known about this variant of the Fisher information. In fact, already the expression given above suffers from several regularity issues (not all density operators are in the domain of \mathscr{E} , the logarithm is not a Lipschitz function), and we spend much of this section giving a rigorous definition via approximation and showing that several different approximations yield the same result. We then go on the show that orbits of the QMS (P_t) are admissible curves (Proposition 4.24, Corollary 4.26) with action bounded by the integrated Fisher information and that the entropy dissipation rate along these curves is given by the Fisher information (Proposition 4.25).

In Chapter 5 we introduce the gradient estimate

$$\|\partial P_t a\|_{\rho}^2 \le e^{-2Kt} \|\partial a\|_{P_t \rho}^2, \qquad (\operatorname{GE}(K,\infty))$$

which is a variant of the Bakry-Émery gradient estimate. In fact, if (P_t) is the heat semigroup on a complete Riemannian manifold (M,g), then the gradient estimate reduces to the Bakry-Émery estimate

$$\Gamma(P_t u) \le e^{-2Kt} P_t \Gamma(u)$$

with $\Gamma(f) = |\nabla f|^2$, which is equivalent to $\operatorname{Ric}_g \ge K$.

Among other things, this gradient estimate ensures that the QMS (P_t) has a smoothing effect (Proposition 5.7), namely that it maps $L^2(\mathcal{M}, \tau) \cap \mathcal{M}$ into \mathcal{A}_{θ} . Moreover, it implies the following contraction estimate (Theorem 5.13):

$$\mathcal{W}(P_t\rho, P_t\sigma) \leq e^{-Kt}\mathcal{W}(\rho, \sigma).$$

To give some examples for which the gradient estimate holds, we adapt a technique developed by Carlen and Maas in the finite-dimensional case [CM17a] to deduce the gradient estimate from an intertwining relation (Proposition 5.18).

Chapter 6 is devoted to the announced characterization of tracially symmetric QMS as gradient flows of the entropy. We show (Theorem 6.15) that if τ is a normal faithful tracial state on the separable von Neumann algebra \mathcal{M} and (P_t) is a tracially symmetric QMS on \mathcal{M} , satisfying the gradient estimate $\operatorname{GE}(K,\infty)$ for the logarithmic mean and a technical condition, such that τ is energy dominant, then the evolution variational inequality

$$\frac{1}{2}\frac{d}{dt}\mathcal{W}(P_t\rho,\sigma)^2 + \frac{K}{2}\mathcal{W}(P_t\rho,\sigma)^2 + \operatorname{Ent}(P_t\rho) \leq \operatorname{Ent}(\sigma)$$

holds for all density operators ρ, σ with finite entropy and finite distance and a.e. $t \ge 0$. The technical condition is satisfied for example if the gradient estimate also holds for the arithmetic mean (not necessarily for the same *K*).

As the proof is quite technical, we first prove this result in the special case when (P_t) is ultracontractive (Theorem 6.6) to make the outline of the proof more transparent. The QMS (P_t) is called ultracontractive if it maps $L^1(\mathcal{M}, \tau)$ into \mathcal{M} for all t > 0. This has not only the advantage that one can deal with bounded operators, but also guarantees that the trajectories $t \mapsto P_t a$ are smooth for t > 0(Proposition 6.4).

To prove the general case, some more effort is needed to compensate for the lack of these two properties. As a key technical step, we show that admissible curves between density operators with finite entropy can be approximated by regular ones while at the same time controlling the entropy, Fisher information and action of these curves (Lemma 6.12, Proposition 6.13, Corollary 6.14).

In Chapter 7 we study consequences of the gradient flow characterization. On the one hand, the gradient estimate $GE(K,\infty)$ for K > 0 implies a variety of functional inequalities such as the modified Sobolev inequality (Proposition 7.10)

$$\operatorname{Ent}(\rho) \leq \frac{1}{2K} \mathscr{I}(\rho),$$

which is equivalent to the exponential entropy decay bound (Proposition 7.12)

$$\operatorname{Ent}(P_t \rho) \le e^{-2Kt} \operatorname{Ent}(\rho)$$

and implies the Talagrand inequality (Proposition 7.13)

$$\mathcal{W}(\rho, 1)^2 \leq \frac{2}{K} \operatorname{Ent}(\rho)$$

as well as the Poincaré inequality (Proposition 7.14)

$$\|a - \tau(a)\|_2^2 \leq K \mathscr{E}(a).$$

On the other hand, the gradient flow characterization can be used to prove semi-convexity of the von Neumann entropy along \mathcal{W} -geodesics. The study of convexity properties along geodesics (also called displacement convexity) of functionals on Wasserstein space was initiated by McCann [McC94] and later played a crucial role in the Lott–Villani–Sturm theory of synthetic Ricci curvature for metric measure spaces [LV09, Stu06a, Stu06b].

A priori, it is not even clear if arbitrary density operators with finite distance are joined by a geodesic. However, if the evolution variational inequality holds, then the distance between density operators with finite entropy can be realized as infimum over curves with uniformly bounded entropy (Proposition 7.2). Together with a compactness argument this yields that density operators with finite entropy and finite distance are joined by a \mathcal{W} -geodesic (Theorem 7.15). It follows from an abstract result on gradient flows that the entropy is geodesically K-convex, that is,

$$\operatorname{Ent}(\rho_t) \le (1-t)\operatorname{Ent}(\rho_0) + t\operatorname{Ent}(\rho_1) - \frac{K}{2}t(1-t)\mathcal{W}(\rho_0,\rho_1)^2$$

for every geodesic (ρ_t) in the space of density operators endowed with the metric \mathcal{W} .

The relations between the gradient estimate $GE(K,\infty)$, the evolution variational inequality and geodesic *K*-convexity of the entropy are summarized in Theorem 7.22.

In Chapter 8 a sample of open problems is compiled. Appendices A and B contain some background information on noncommutative L^p spaces for semifinite von Neumann algebras and the various operator topologies used throughout this thesis.

With a few exceptions, the material presented in this thesis is based on a preprint by the author [Wir18].

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CHAPTER 1

QUANTUM MARKOV SEMIGROUPS AND QUANTUM DIRICHLET FORMS

In this chapter two of the main objects of this thesis are introduced, quantum Dirichlet forms and the corresponding symmetric quantum Markov semigroups on noncommutative L^2 spaces.

Quantum Markov semigroups were introduced by Lindblad [Lin76] and Gorini, Kossakowski and Sudarshan [GKS76] in the study of irreversible open quantum systems. Their key insight, motivated by physical considerations, was that the correct assumption on maps constituting the semigroup is not positivity, but complete positivity (both concepts coincide in the commutative case). More recently, quantum Markov semigroups have received growing interest in the context quantum information theory (see for example [KT13, Kin14, RD19])

The counterparts of tracially symmetric quantum Markov semigroups, quantum Dirichlet forms, were first defined by Gross [Gro75] and Albeverio–Høegh-Krohn [AH77] in the tracial case and later extended to the not necessarily tracial case by Goldstein–Lindsay [GL93] and Cipriani [Cip97].

The first two section of this chapter are expository. In Section 1.1 we collect the definitions along with some basic facts, including the correspondence between quantum Dirichlet forms and symmetric quantum Markov semigroups. We also give some examples, which will be taken up later on. In Section 1.2 we review the first-order differential calculus developed by Cipriani–Sauvageot [CS03]. This calculus plays a primal role throughout this thesis.

The results of Section 1.3 are new. We study a noncommutative analog of energy dominant measures. The measure m is called energy dominant for the Dirichlet form \mathscr{E} if the energy measure $\Gamma(f)$ is absolutely continuous with respect

to *m* for all *f* in the domain of \mathscr{E} . In Theorem 1.32 we give a characterization of a noncommutative version of this property in terms of the first-order differential calculus associated with \mathscr{E} . This result will also justify the assumption of energy dominance in the following chapters.

Throughout this chapter let (\mathcal{M}, τ) be a tracial von Neumann algebra. For necessary background material on traces on von Neumann algebras and noncommutative L^p spaces we refer the reader to Appendix A.

1.1 Definitions and basic facts

In this section we introduce quantum Dirichlet forms and quantum Markov semigroups along with some basic properties. In the commutative case, a closed densely defined quadratic form \mathscr{E} on $L^2(X,m)$ is a Dirichlet form if $\mathscr{E}(\tilde{u}) \leq \mathscr{E}(u)$ for all real-valued $u \in L^2(X,m)$, where \tilde{u} denotes the pointwise maximum of u and 1.

To extend this definition to the noncommutative case, one has to make sense of \tilde{a} for $a \in L^2_h(\mathcal{M}, \tau)$. One possibility is to define \tilde{a} via functional calculus, another to define it as the projection onto the cone of self-adjoint elements less or equal 1. in the next lemma we show that both possibilities give the same result.

Recall that for a nonempty, closed, convex subset *C* of a Hilbert space *H* and $x \in H$ there is a unique element $y \in C$ with $||x-y|| = \inf_{z \in C} ||x-z||$. The map $P_C: x \mapsto y$ is called (metric) projection onto *C*. The element $P_C(x)$ can alternatively be characterized as the unique $y \in C$ such that

$$\operatorname{Re}\langle x-y, z-y\rangle \leq 0$$

for all $z \in C$.

We write $\alpha \land \beta = \min\{\alpha, \beta\}$ and $\alpha \lor \beta = \max\{\alpha, \beta\}$ for $\alpha, \beta \in \mathbb{R}$. If *x* is a self-adjoint operator, $x \land \alpha$ stands for the application of the function $\min\{\cdot, \alpha\}$ to *x*, which is the infimum of *x* and $\alpha 1$ in the (commutative) unital *C*^{*}-algebra generated by *x*.

Lemma 1.1. The closure C of $\{x \in L^2_h(\mathcal{M}, \tau) \cap \mathcal{M} \mid x \leq 1\}$ in $L^2(\mathcal{M}, \tau)$ is convex and the projection P_C onto C is given by $P_C(a) = a \land 1$ for all $a \in L^2_h(\mathcal{M}, \tau)$.

Proof. It is easy to see that *C* is convex. For $a \in L_h^2(\mathcal{M}, \tau)$ let $a_n = (a \land 1) \lor (-n)$. Then $a_n \in L_h^2(\mathcal{M}, \tau) \cap \mathcal{M}$, $a_n \leq 1$ and $a_n \to a \land 1$ in $L^2(\mathcal{M}, \tau)$, hence $a \land 1 \in C$. If $b \in \mathcal{M} \cap L_h^2(\mathcal{M}, \tau)$ with $b \leq 1$, then

$$\tau((a - a \land 1)(b - a \land 1)) = \tau((a - 1)_{+}^{1/2}(b - a \land 1)(a - 1)_{+}^{1/2})$$

$$\leq \tau((a - 1)_{+}^{1/2}(1 - a \land 1)(a - 1)_{+}^{1/2})$$

$$= \tau((a - 1)_{+}(a - 1)_{-})$$

$$= 0.$$

For arbitrary $b \in C$, the inequality above follows by continuity. Thus $P_C(a) = a \wedge 1$.

For the next definition recall that a quadratic form on a Hilbert space *H* is a map $Q: H \longrightarrow [0, \infty]$ such that

- $Q(\lambda u) = |\lambda|^2 Q(u)$ for $\lambda \in \mathbb{C}$, $u \in H$, and
- Q(u+v) + Q(u-v) = 2Q(u) + 2Q(v) for $u, v \in H$.

The domain of Q is

$$D(Q) = \{ u \in H \mid Q(u) < \infty \}.$$

The quadratic form Q is called closed if it is lower semicontinuous. The form Q is closed if and only if D(Q) endowed with the norm

$$\|\cdot\|_Q = (\|\cdot\|_H^2 + \|\cdot\|_Q^2)^{1/2}$$

is complete.

For every quadratic form Q on H there exists an associated sesquilinear form q defined as

$$q: D(Q) \times D(Q) \longrightarrow \mathbb{C}, q(u,v) = \frac{1}{4} \sum_{k=0}^{3} i^{k} Q(u+i^{k}v).$$

We will use these two points of view interchangeably and write Q for both of these maps.

The generator \mathcal{L} of a densely defined closed form Q is given by

$$D(\mathcal{L}) = \{ u \in D(Q) \mid \exists v \in H \, \forall w \in D(Q) \colon Q(u, w) = \langle v, w \rangle_2 \},$$

$$\mathcal{L}u = v.$$

The generator is a positive self-adjoint operator on H that uniquely determines the form. Conversely, for every positive self-adjoint operator \mathcal{L} on H there exists a densely defined closed form that is generated by \mathcal{L} .

Definition 1.2 (Markovian form). A quadratic form $\mathscr{E}: L^2(\mathscr{M}, \tau) \longrightarrow [0, \infty]$ is called *real* if $\mathscr{E}(a^*) = \mathscr{E}(a)$ for all $a \in L^2(\mathscr{M}, \tau)$ and *Markovian* if $\mathscr{E}(a \wedge 1) \leq \mathscr{E}(a)$ for all $a \in L^2_h(\mathscr{M}, \tau)$.

Lemma 1.1 shows that the cut-off $a \wedge 1$ can be understood either as an application of functional calculus or as projection in $L^2(\mathcal{M}, \tau)$. By the next lemma (see [DL92, Proposition 2.12] and [CS03, Theorem 10.2]), Markovian forms automatically satisfy a stronger contraction property with respect to Lipschitz functional calculus. **Lemma 1.3.** A closed densely defined real quadratic form $\mathscr{E}: L^2(\mathscr{M}, \tau) \longrightarrow [0, \infty]$ is Markovian if and only if $\mathscr{E}(f(a)) \leq \mathscr{E}(a)$ for all $a \in L^2_h(\mathscr{M}, \tau)$ and all 1-Lipschitz functions $f: \mathbb{R} \longrightarrow \mathbb{R}$ with f(0) = 0.

For $n \in \mathbb{N}$ denote by tr_n the normalized trace on $M_n(\mathbb{C})$ and let $\tau_n = \tau \otimes \operatorname{tr}_n$ on $(\mathcal{M} \otimes M_n(\mathbb{C}))_+ \cong M_n(\mathcal{M})_+$, that is,

$$\tau_n: M_n(\mathcal{M})_+ \longrightarrow [0,\infty], \tau_n((a_{ij})) = \frac{1}{n} \sum_{i=1}^n \tau(a_{ii}).$$

Definition 1.4 (Completely Markovian form). For quadratic form \mathscr{E} on $L^2(\mathscr{M}, \tau)$, the amplification \mathscr{E}_n on $L^2(\mathcal{M}_n(\mathscr{M}), \tau_n)$ is defined by

$$\mathscr{E}_n: L^2(M_n(\mathscr{M}), \tau_n) \longrightarrow [0, \infty], \mathscr{E}_n((a_{ij})) = \sum_{i,j=1}^n \mathscr{E}(a_{ij}).$$

The form \mathscr{E} is called *completely Markovian* if \mathscr{E}_n is Markovian for all $n \in \mathbb{N}$.

A closed, densely defined, real, completely Markovian quadratic form \mathscr{E} on $L^2(\mathscr{M}, \tau)$ is called *completely Dirichlet form* on (\mathscr{M}, τ) .

Now we turn to quantum Markov semigroups. Recall that an (operator) semigroup on a locally convex space E is a family $(T_t)_{t\geq 0}$ of continuous linear maps from E to E such that

- $T_0 = id$,
- $T_s T_t = T_{s+t}$ for $s, t \ge 0$.

The semigroup (T_t) is called strongly continuous if $T_t u \to u$ as $t \to 0$ for all $u \in E$. The generator of the strongly continuous semigroup (T_t) is the operator \mathscr{L} given by

$$D(\mathscr{L}) = \left\{ u \in E \mid \lim_{t \to 0} \frac{1}{t} (u - T_t u) \text{ exists} \right\},$$
$$\mathscr{L}(u) = \lim_{t \to 0} \frac{1}{t} (u - T_t u).$$

If *E* is a Hilbert space and T_t is symmetric and contractive for all $t \ge 0$, then the generator of (T_t) is a positive self-adjoint operator. Conversely, for every positive self-adjoint operator \mathcal{L} there is a unique strongly continuous semigroup with generator \mathcal{L} . See [EN00] for more details on semigroups on Banach spaces and [Yos80] for more information on semigroups on locally convex spaces.

For $p \in [1,\infty)$ we endow $L^p(\mathcal{M},\tau)$ with the norm topology. In the case $p = \infty$ however, strong continuity in the norm topology is too restrictive. For this reason we will always consider the σ -weak topology when talking about semigroups on \mathcal{M} .

Definition 1.5 (Completely sub-Markovian semigroup). Let $p \in [1,\infty]$. A semigroup $(P_t)_{t\geq 0}$ on $L^p(\mathcal{M},\tau)$ is called *positive* if P_t maps $L^p_+(\mathcal{M},\tau)$ into $L^p_+(\mathcal{M},\tau)$ for all $t\geq 0$. The semigroup (P_t) is called *completely positive* if the extension (P_t^n) to $L^2(M_n(\mathcal{M}),\tau_n)$ given by

$$P_t^n: L^p(M_n(\mathcal{M}), \tau_n) \longrightarrow L^p(\mathcal{M}_n, \tau_n), P_t^n((a_{ij})) = (P_t a_{ij})$$

is positive for all $n \in \mathbb{N}$.

A strongly continuous semigroup (P_t) on $L^p(\mathcal{M}, \tau)$ is called *sub-Markovian* if it is positive and $P_t a \leq 1$ for $a \in L^p_h(\mathcal{M}, \tau)$ with $a \leq 1$, and *completely sub-Markovian* if (P_t^n) is sub-Markovian for all $n \in \mathbb{N}$.

Let q be the dual exponent of p. A semigroup (P_t) on $L^p(\mathcal{M}, \tau)$ is called τ -symmetric if

$$\tau(bP_ta) = \tau(aP_tb)$$

for all $a, b \in L^p(\mathcal{M}, \tau) \cap L^q(\mathcal{M}, \tau)$ and $t \ge 0$.

Although originally only defined on a single L^p space, every τ -symmetric sub-Markovian semigroup induces a coherent family of sub-Markovian semigroups on the whole scale of L^p spaces.

Proposition 1.6. Let $p \in [1,\infty]$ and let (P_t) be a τ -symmetric sub-Markovian semigroup on $L^p(\mathcal{M},\tau)$. For all $q \in [1,\infty]$ there exists a unique semigroup $(P_t^{(q)})$ on $L^q(\mathcal{M},\tau)$ such that (P_t) and $(P_t^{(q)})$ coincide on $L^p(\mathcal{M},\tau) \cap L^q(\mathcal{M},\tau)$. Moreover,

(i) $(P_t^{(q)})$ is a sub-Markovian semigroup for all $q \in [1,\infty]$,

(*ii*)
$$||P_t^{(q)}|| \le 2$$
 for all $t \ge 0, q \in [1,\infty]$

(iii)
$$(P_t^{(q)})^* = P_t^{(q')}$$
 for all $t \ge 0$ and $q, q' \in [1,\infty]$ with $1/q + 1/q' = 1$.

Proof. For p = 2 these assertions are proven in [DL92, Propositions 2.2 and 2.14], but the proofs easily extend to $p \in [1,\infty)$. For $p = \infty$, everything but the strong continuity of $(P_t^{(q)})$ works analogously.

Let $a \in L^q(\mathcal{M}, \tau) \cap \mathcal{M}$ and $b \in L^{q'}(\mathcal{M}, \tau) \cap \mathcal{M}$, where 1/q + 1/q' = 1. Since (P_t) is strongly continuous on \mathcal{M} with respect to the σ -weak topology, we have

$$\tau(bP_t^{(q)}a) = \tau(bP_ta) \to \tau(ba).$$

Since $(P_t^{(q)}a)_{t\geq 0}$ is uniformly bounded in $L^q(\mathcal{M}, \tau)$ by (ii), this convergence extends to all $a \in L^q(\mathcal{M}, \tau)$ and $b \in L^{q'}(\mathcal{M}, \tau)$. Thus $(P_t^{(q)})$ is strongly continuous with respect to the weak topology on $L^q(\mathcal{M}, \tau)$. It follows from the general theory of operator semigroups (see [EN00, Theorem I.5.8]) that $(P_t^{(q)})$ is indeed strongly continuous with respect to the norm topology on $L^q(\mathcal{M}, \tau)$. \Box When there is no danger of confusion, we may drop the superscript and simply write (P_t) for all the semigroups acting on the different L^p spaces.

Remark 1.7. Let (P_t) be a τ -symmetric sub-Markovian semigroup on $L^p(\mathcal{M}, \tau)$ with generator \mathscr{L} . For $a \in D(\mathscr{L})$ the curve $(P_t a)_{t \geq 0}$ is the unique classical solution of the initial value problem

$$\dot{x}_t = -\mathscr{L} x_t$$
 for $t > 0$
 $x_0 = a$ (MME)

in $L^p(\mathcal{M}, \tau)$.

For p = 2 it follows from the spectral theorem that $t \mapsto P_t$ has an analytic continuation the the right half-plane {Re z > 0}, and by the noncommutative version of Stein's interpolation (see [Gro72, Proposition 3]) this result extends to $p \in (1,\infty)$. In particular, P_t maps $L^p(\mathcal{M},\tau)$ into $D(\mathcal{L})$ for all t > 0 and therefore $(P_ta)_{t\geq 0}$ solves the initial value problem (MME).

The situation is quite different in the edge cases p = 1 or $p = \infty$. Indeed, P_t may fail to map $L^1(\mathcal{M}, \tau)$ into $D(\mathcal{L})$ for some t > 0 as is witnessed by the Ornstein–Uhlenbeck semigroup on $L^1(\mathbb{R}, \exp(-x^2/2)dx)$ – see [Dav90, Theorem 4.3.5]. The analyticity of (P_t) will be taken up again in Section 6.2.

Definition 1.8 (Quantum Markov semigroup). A completely sub-Markovian semigroup (P_t) on \mathcal{M} is called *conservative* or *quantum Markov semigroup* if $P_t 1 = 1$ for all $t \ge 0$. A τ -symmetric completely sub-Markovian (P_t) on $L^p(\mathcal{M}, \tau)$ is called *completely Markovian* if $(P_t^{(\infty)})$ is conservative.

Remark 1.9. By duality, a τ -symmetric completely sub-Markovian semigroup (P_t) on $L^p(\mathcal{M}, \tau)$ is completely Markovian if and only if the semigroup $(P_t^{(1)})$ on $L^1(\mathcal{M}, \tau)$ is trace-preserving, that is,

$$\tau(P_t^{(1)}a) = \tau(a)$$

for $a \in L^1(\mathcal{M}, \tau)$. Since we study dynamics on density operators in the later chapters, having a trace-preserving semigroup is a natural assumption.

Just as in the commutative case, there is a bijective correspondence between (completely) Dirichlet forms and τ -symmetric (completely) sub-Markovian semigroups. The following result is due to Albeverio–Høegh-Krohn [AH77, Theorems 2.7, 2.8] in finite case and Davies–Lindsay [DL92, Theorems 2.13, 3.3] in the semifinite case.

Proposition 1.10. Let \mathscr{L} be a positive self-adjoint operator on $L^2(\mathcal{M},\tau)$. The quadratic form generated by \mathscr{L} is (completely) Markovian if and only if the semigroup generated by \mathscr{L} is (completey) sub-Markovian.

1.1. DEFINITIONS AND BASIC FACTS

If the form \mathscr{E} and the semigroup (P_t) have the same generator, we also say that (P_t) is the semigroup associated with \mathscr{E} and vice versa. In the light of Proposition 1.6, the bijective correspondence from the previous proposition extends to L^p . In this sense we also talk about the associated semigroup on L^p .

Since conservativeness of the semigroup will be a standing assumption, we reserve a special name for the associated Dirichlet forms (motivated by the term quantum Markov semigroup for the corresponding semigroup on \mathcal{M}).

Definition 1.11 (Quantum Dirichlet form). A completely Dirichlet form is called *quantum Dirichlet form* if the associated semigroup is conservative.

Example 1.12. Let (X, \mathcal{B}, m) be a localizable measure space (see Example A.2). Every Markovian form on $L^2(X,m)$ is completely Markovian so that Dirichlet forms on $L^2(X,m)$ in the sense of Beurling–Deny [BD58, BD59] can be identified with completely Dirichlet forms on $L^2(L^{\infty}(X,m),\tau_m)$. Analogously, the notions of sub-Markovianity and complete sub-Markovianity coincide in this case.

Example 1.13. With the notation from Example A.3 let A_{ϑ} be the noncommutative torus and τ the unique tracial state on A_{ϑ} . The map

$$\mathscr{A}_{\vartheta} \longrightarrow \mathscr{A}_{\vartheta}, \sum_{m,n} \alpha_{mn} U^m V^n \mapsto \sum_{m,n} e^{-t(m^2 + n^2)} \alpha_{mn} U^m V^n$$

extends to a bounded linear operator P_t on $L^2(A_{\vartheta}, \tau)$, and the family (P_t) is a completely Markovian semigroup, called the *noncommutative heat semigroup* on the noncommutative torus.

The associated quantum Dirichlet form is the closure of

$$\mathcal{A}_{\vartheta} \longrightarrow [0,\infty), \sum_{m,n} \alpha_{mn} U^m V^n \mapsto \sum_{m,n} (m^2 + n^2) |\alpha_{mn}|^2.$$

Example 1.14. With the notation from Example A.4 let $\mathbb{C}\ell(H)$ be the fermionic Clifford algebra and τ the unique tracial state on $\mathbb{C}\ell(H)$. The number operator N on $\mathscr{F}_{-}(H)$ is defined by

$$D(N) = \{(\psi_k) \in \mathscr{F}_-(H) \mid \sum_{k \ge 0} k^2 \|\psi_k\|_{\Lambda^k H}^2 < \infty\},$$
$$N(\psi_k) = (k\psi_k).$$

The operator $\Phi^{-1}N\Phi$ generates a quantum Dirichlet form on $L^2(\mathbb{C}\ell(H), \tau)$, sometimes referred to as Gross's fermionic Dirichlet form (see [Gro72, Gro75]).

The associated quantum Markov semigroup (P_t) acts on \mathscr{A} by

$$P_t\left(\sum_{j_1<\cdots< j_k}\alpha_{j_1\ldots j_k}e_{j_1}\ldots e_{j_k}\right)=\sum_{j_1<\cdots< j_k}e^{-tk}\alpha_{j_1\ldots j_k}e_{j_1}\ldots e_{j_k}.$$

1.2 First-order differential calculus

In this section we review the first-order differential calculus introduced by Cipriani–Sauvageot [CS03]. As a motivating example let (M,g) be a complete Riemannian manifold and \mathscr{E} the Dirichlet energy on M given by

$$\mathscr{E}: W^{1,2}(M) \longrightarrow [0,\infty), \mathscr{E}(u) = \|du\|_{L^2(M;T^*M)}^2.$$

Of course the exterior derivative d satisfies the Leibniz rule

$$d(uv) = udv + vdu.$$

The insight of Cipriani and Sauvageot was that every completely Dirichlet form admits such a representation by a derivation if one allow for different left and right multiplication on the right-hand side of the Leibniz rule.

Let us first introduce the relevant objects. The material is taken from [CS03] with some slight changes in notation. We start with an abstract replacement of the 1-forms in the introductory example.

Definition 1.15 (Symmetric Hilbert bimodule). Let *A* be a C^* -algebra. The opposite algebra A° is the C^* -algebra with same underlying vector space, involution and norm, but with multiplication given by $a \circ b = ba$ for $a, b \in A$.

A symmetric Hilbert bimodule over A is a quadruple (\mathcal{H}, L, R, J) consisting of a Hilbert space \mathcal{H} , commuting non-degenerate *-representations L of A and R of A° on \mathcal{H} , and an anti-linear isometric involution $J: \mathcal{H} \longrightarrow \mathcal{H}$ such that

$$JL(a) = R(a^*)J$$

for all $a \in A$.

The operations L(a) and R(b) are viewed as left and right multiplication of A on \mathcal{H} and accordingly we write $a\xi$ and ξb for $L(a)\xi$ and $R(b)\xi$. Since L and R commute, expressions of the form $a\xi b$ make sense without brackets.

Next we introduce the abstract version of the exterior derivative in the motivating example.

Definition 1.16 (Symmetric derivation). Let (\mathcal{M}, τ) be a tracial von Neumann algebra, $A \subset \mathcal{M}$ a C^* -algebra and (\mathcal{H}, L, R, J) a symmetric Hilbert bimodule over \mathcal{H} . A *derivation* with values in \mathcal{H} is a closed densely defined operator ∂ on $L^2(\mathcal{M}, \tau)$ such that

- $D(\partial) \cap A$ is dense in A,
- $\partial(ab) = L(a)\partial b + R(b)\partial a$ for all $a, b \in D(\partial) \cap A$.

The derivation ∂ is called *real* if $D(\partial)$ is self-adjoint and

$$J\partial a = \partial(a^*)$$

for all $a \in D(\partial)$.

For the ease of notation, we merge the two preceding concepts in the following definition.

Definition 1.17 (First-order differential calculus). Let (\mathcal{M}, τ) be a tracial von Neumann algebra and $A \subset \mathcal{M}$ a C^* -algebra. A first-order differential calculus over A is a quintuple $(\partial, \mathcal{H}, L, R, J)$ such that (\mathcal{H}, L, R, J) is a symmetric Hilbert bimodule over A and ∂ a symmetric derivation on A with values in \mathcal{H} .

An important consequence of the Leibniz rule is a (two-variable) chain rule.

Definition 1.18 (Quantum derivative). The *quantum derivative* of $f \in C^1(I)$ is the function

$$\tilde{f}: I \times I \longrightarrow \mathbb{R}, \, \tilde{f}(s,t) = \begin{cases} \frac{f(s) - f(t)}{s - t} & \text{if } s \neq t, \\ f'(s) & \text{if } s = t. \end{cases}$$

With this notation, the chain rule reads as follows ([CS03, Lemma 7.2]).

Lemma 1.19 (Chain rule). Let $(\partial, \mathcal{H}, L, R, J)$ be a first-order differential calculus. If $f \in C^1(\mathbb{R})$ has bounded derivative and f(0) = 0, then $f(a) \in D(\partial)$ and

$$\partial f(a) = \tilde{f}(L(a), R(a))\partial a.$$

for all $a \in D(\partial)_h$.

If the left and right action coincide, one recovers the usual chain rule $\partial f(a) = f'(a)\partial a$.

The following representation theorem for completely Dirichlet forms by Cipriani and Sauvageot (see [CS03, Theorems 4.7, 8.2, 8.3]) is central to our investigations. It shows the intimate relation between first-order differential calculi and completely Dirichlet forms.

Theorem 1.20. Let (\mathcal{M}, τ) be a tracial von Neumann algebra.

(a) If $A \subset \mathcal{M}$ is a σ -weakly dense C^* -algebra and $(\partial, \mathcal{H}, L, R, J)$ a first-order differential calculus, then the quadratic form \mathscr{E} defined by

$$D(\mathscr{E}) = D(\partial), \mathscr{E}(a) = \|\partial a\|_{\mathscr{H}}^2$$

is a completely Dirichlet form.

(b) If \mathscr{E} is a quantum Dirichlet form on $L^2(\mathcal{M}, \tau)$, then $\mathscr{C} = D(\mathscr{E}) \cap \mathcal{M}$ is a *algebra and there exist a first-order differential calculus $(\partial, \mathcal{H}, L, R, J)$ over $\overline{\mathscr{C}}$ such that $D(\partial) = D(\mathscr{E})$ and

$$\|\partial a\|_{\mathscr{H}}^2 = \mathscr{E}(a)$$

for all $a \in D(\partial)$.

Moreover, if $(\tilde{\partial}, \tilde{\mathcal{H}}, \tilde{L}, \tilde{R}, \tilde{J})$ is another first-order differential calculus with the same properties, then there exists a unitary map $U: \mathcal{H} \longrightarrow \tilde{\mathcal{H}}$ such that

- $U\partial = \tilde{\partial},$
- $UL = \tilde{L}, UR = \tilde{R},$
- $UJ = \tilde{J}U$.

In the sense of this theorem, we can speak of *the* first-order differential calculus associated with \mathscr{E} .

Remark 1.21. Since we require the left and right action in the definition of Hilbert bimodules to be non-degenerate, not every completely Dirichlet form can be represented by a first-order differential calculus in the sense of the previous theorem. However, every completely Dirichlet form can be represented as

$$\mathscr{E}(a) = \|\partial a\|_{\mathscr{H}}^2 + \frac{1}{2}K(aa^* + a^*a),$$

where ∂ is a symmetric derivation and *K* is a weight, the so-called killing weight (see [CS03, Theorem 8.1]).

Remark 1.22. In [CS03], an additional condition called *regularity* is imposed. This property depends not only on the form \mathscr{E} , but also on the choice of some C^* -subalgebra of \mathscr{M} . Every completely Dirichlet form \mathscr{E} is regular with respect to the norm closure of $D(\mathscr{E}) \cap \mathscr{M}$.

In the last part of this section we discuss some examples. Let us start with the example from the beginning of the section.

Example 1.23 (Riemannian manifolds). Let (M, g) be a complete Riemannian manifold and \mathscr{E} the Dirichlet energy given by

$$D(\mathscr{E}) = W^{1,2}(M), \, \mathscr{E}(u) = \|du\|_{L^2(M;T^*M)}^2$$

The first-order differential calculus associated with \mathscr{E} is given by $\mathscr{H} = L^2(M; T^*M)$, $(u\xi)(x) = (\xi u)(x) = u(x)\xi(x)$, $\partial = d$ and $J\xi = \overline{\xi}$.

Example 1.24 (Metric measure spaces). A *metric measure space* is a triple (X, d, m) consisting of a complete separable metric space (X, d) and a Borel measure m on X such that there exists a Lipschitz map $V: X \longrightarrow [0, \infty)$ with

$$\int_X e^{-V^2} dm \le 1$$

Let $\operatorname{Lip}(X, d)$ denote the space of Lipschitz functions on X and $\operatorname{Lip}(f)$ the local Lipschitz constant of $f \in \operatorname{Lip}(X, d)$. The Cheeger energy Ch is the lower semicontinuous relaxation of the convex functional

$$\operatorname{Ch}_{0}: L^{2}(X, m) \longrightarrow [0, \infty], \operatorname{Ch}_{0}(f) = \begin{cases} \frac{1}{2} \int_{X} \operatorname{Lip}(f)^{2} dm & \text{if } f \in \operatorname{Lip}(X, d), \\ \infty & \text{otherwise.} \end{cases}$$

If Ch is a quadratic form, then (X,d,m) is called infinitesimally Hilbertian. In this case the first-order differential calculus associated with 2Ch coincides with first-order differential calculus developed in [Gig14]. For more information on analysis on metric measure spaces see also [AGS14a, AGS14b, AGS15].

Example 1.25 (Weighted graphs). Let X be a countable set, $m: X \longrightarrow (0, \infty)$ and $b: X \times X \longrightarrow [0, \infty)$ such that

- b(x,x) = 0 for all $x \in X$,
- b(x, y) = b(y, x) for all $x, y \in X$,
- $\sum_{y} b(x, y) < \infty$ for all $x \in X$.

The triple (X, b, m) is called a *weighted* graph (compare [KL10, KL12]). Often one allows for an additional killing weight $c: X \longrightarrow [0, \infty)$, but the associated Dirichlet form will never be conservative if $c \neq 0$, so we drop it from the beginning.

The associated Dirichlet form with Neumann boundary conditions is

$$\mathscr{E}^{(N)}\colon \ell^2(X,m) \longrightarrow [0,\infty], \, \mathscr{E}^{(N)}(u) = \frac{1}{2}\sum_{x,y} b(x,y)|u(x) - u(y)|^2.$$

The associated Dirichlet form with Dirichlet boundary conditions $\mathscr{E}^{(D)}$ is the closure of the restriction of $\mathscr{E}^{(D)}$ to $C_c(X)$.

The first-order differential calculus associated with $\mathscr{E}^{(N)}$ is given by

- $\mathcal{H} = \ell^2(X \times X, \frac{1}{2}b),$
- $(u \cdot \xi)(x, y) = u(x)\xi(x, y), \ (\xi \cdot v)(x, y) = \xi(x, y)v(y),$
- $\partial u(x, y) = u(x) u(y)$, and

• $(J\xi)(x,y) = -\overline{\xi(y,x)}.$

The first-order differential calculus associated with $\mathscr{E}^{(D)}$ is obtained by suitable restriction.

Notice that the crucial difference between Example 1.25 on the one hand and Examples 1.23, 1.24 on the other hand is that left and right multiplication on \mathcal{H} coincide for the Dirichlet forms on Riemannian manifolds and metric measure spaces while they differ for graphs. More generally, left and right multiplication coincide in the commutative setting whenever \mathscr{E} is a strongly local regular Dirichlet form (see [IRT12, Theorem 2.7]).

Finally we give some noncommutative examples.

Example 1.26 (Noncommutative torus). Let \mathscr{E} be the quantum Dirichlet form on the noncommutative torus from Example 1.13. With the notation from Example A.3, the maps

$$\begin{split} \partial_1 \colon \mathscr{A}_{\vartheta} &\longrightarrow L^2(A_{\vartheta}, \tau), \sum_{m,n} \alpha_{mn} U^m V^n \mapsto \sum_{m,n} im \alpha_{mn} U^m V^n, \\ \partial_2 \colon \mathscr{A}_{\vartheta} &\longrightarrow L^2(A_{\vartheta}, \tau), \sum_{m,n} \alpha_{mn} U^m V^n \mapsto \sum_{m,n} in \alpha_{mn} U^m V^n, \end{split}$$

are closable in $L^2(A_{\vartheta}, \tau)$.

Let $\partial = \overline{\partial}_1 \oplus \overline{\partial}_2$, let \mathcal{H} be the closed linear hull of $\{(a\partial_1 b, a\partial_2 b) \mid a, b \in \mathcal{A}_{\partial}\}$ in $L^2(A_{\theta}, \tau) \oplus L^2(A_{\theta}, \tau)$ and define the maps L, R and J by L(a)(x, y) = (ax, ay), R(b)(x, y) = (xb, yb) and $J(x, y) = -(x^*, y^*).$

Then $(\partial, \mathcal{H}, L, R, J)$ is the first-order differential calculus associated with \mathscr{E} . *Example* 1.27 (Fermionic Clifford algebra). Let \mathscr{E} be Gross's fermionic Dirichlet form from Example 1.14.

Let a_i be the annihilation operator on $\mathscr{F}_{-}(H)$ characterized by

$$a_i(e_{j_1} \wedge \dots \wedge e_{j_k}) = \frac{1}{\sqrt{k}} \sum_{l=1}^k (-1)^l \langle e_i, e_{j_l} \rangle e_{j_1} \wedge \dots \wedge \widehat{e_{j_l}} \wedge \dots \wedge e_{j_k}$$

and $\gamma: L^{\infty}(\mathbb{C}\ell(H), \tau) \longrightarrow L^{\infty}(\mathbb{C}\ell(H), \tau)$ the grading operator.

The first-order differential calculus for \mathscr{E}_N is given by $\mathscr{H} = \sum_{i\geq 0} L^2(\mathbb{C}\ell(H), \tau)$, $L(x)(\xi_i) = (x\xi_i), R(x)(\xi_i) = (\gamma(x)\xi_i), J(\xi_i) = -(\xi_i^*)$ and $\partial = \bigoplus_{i\geq 0} \Phi^{-1}a_i\Phi$.

1.3 Carré du champ

We saw in the previous section that a quantum Dirichlet form \mathscr{E} induce a firstorder differential calculus. However, the left and right action on the Hilbert bimodule are only defined for elements from the uniform closure of $D(\mathscr{E}) \cap \mathscr{M}$. In

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this section we characterize when these actions can be extended to the entire von Neumann algebra \mathcal{M} . This is necessary to formulate the continuity equation in Chapter 3.

It turns out that this question is closely related to the so-called carré du champ operator defined below. More precisely we show in Theorem 1.32 that the carré du champ $\Gamma(a)$ has a density with respect to τ if and only if the left and right action of $D(\mathcal{E}) \cap \mathcal{M}$ have normal extensions to \mathcal{M} . This provides a characterization of the noncommutative analogue of energy dominant measures.

Throughout the section let (\mathcal{M}, τ) be a tracial von Neumann algebra, \mathscr{E} a quantum Dirichlet form on $L^2(\mathcal{M}, \tau)$, $\mathscr{C} = D(\mathscr{E}) \cap \mathcal{M}$, and $(\partial, \mathcal{H}, L, R, J)$ the associated first-order differential calculus.

Definition 1.28 (Carré du champ). The *carré du champ operators* $\Gamma_{\mathcal{H}}$ and Γ are defined as

$$\Gamma_{\mathscr{H}}: \mathscr{H} \times \mathscr{H} \longrightarrow \mathscr{C}^*, \Gamma(\xi, \eta)(x) = \langle x\xi, \eta \rangle_{\mathscr{H}}$$

and $\Gamma(a,b) = \Gamma_{\mathcal{H}}(\partial a, \partial b)$ for $a, b \in D(\mathcal{E})$.

We write $\Gamma_{\mathscr{H}}(\xi)$ for $\Gamma_{\mathscr{H}}(\xi,\xi)$ and $\Gamma(a)$ for $\Gamma(a,a)$. It follows from the properties of the first-order differential calculus that $\Gamma_{\mathscr{H}}$ and Γ are sesquilinear and $\|\Gamma_{\mathscr{H}}(\xi,\eta)\|_{\mathscr{C}^*} \leq \|\xi\|_{\mathscr{H}} \|\eta\|_{\mathscr{H}}$ for all $\xi, \eta \in \mathscr{H}$.

Remark 1.29. In terms of \mathcal{E} , the carré du champ can be expressed as

$$\Gamma(a)(x) = \frac{1}{2}(\mathscr{E}(a, ax^*) + \mathscr{E}(ax, a) - \mathscr{E}(a^*a, x^*))$$

for all $a, x \in \mathscr{C}$.

Moreover, if $\xi = \sum_i a_i \partial b_i$, then

$$\mathbf{\Gamma}_{\mathscr{H}}(\xi) = \sum_{i,k} a_i \mathbf{\Gamma}(b_i, b_k) a_k^*,$$

which is taken as definition for $\Gamma_{\mathcal{H}}$ in [HRT13] in the commutative case.

Lemma 1.30. If \mathscr{E} is a quantum Dirichlet form on (\mathcal{M}, τ) , then \mathscr{C} is σ -weakly dense in \mathcal{M} .

Proof. Let $(P_t)_{t\geq 0}$ be the quantum Markov semigroup associated with \mathscr{E} . If $a \in L^2(\mathscr{M}, \tau) \cap \mathscr{M}$, then $P_t(a) \in D(\mathscr{E}) \cap \mathscr{M}$ for all t > 0 and $P_t(a) \to a \sigma$ -weakly as $t \searrow 0$. Now the assertions follows from the fact that $L^2(\mathscr{M}, \tau) \cap \mathscr{M}$ is σ -weakly dense in \mathscr{M} .

Remark 1.31. Since \mathscr{C} is a *-algebra, the Kaplansky density theorem (Theorem B.11) asserts that $D(\mathscr{E}) \cap \mathscr{M}_1$ is even strongly dense in \mathscr{M}_1 .

Theorem 1.32 (Characterization energy dominant trace). Let \mathscr{E} be a quantum Dirichlet form on the tracial von Neumann algebra (\mathcal{M}, τ) with associated first-order differential calculus $(\partial, \mathcal{H}, L, R, J)$. The following assertions are equivalent:

- (i) L is σ -weakly continuous
- (ii) R is σ -weakly continuous
- (iii) $\Gamma(a)$ is σ -weakly continuous for all $a \in D(\mathscr{E})$
- (iv) $\Gamma_{\mathcal{H}}(\xi)$ is σ -weakly continuous for all $\xi \in \mathcal{H}$

Proof. (i) \iff (ii): Since multiplication by a fixed bounded operator and taking adjoints are σ -weakly continuous, the equivalence of (i) and (ii) follows from $L(\cdot) = JR(\cdot)^*J$.

(iii) \Longrightarrow (iv): It is easy to see that $\Gamma_{\mathscr{H}}(\xi)$ is σ -weakly continuous for $\xi \in \ln\{a\partial b \mid a, b \in \mathscr{C}\}$. Combined with the fact that the norm limit of σ -weakly continuous functionals is σ -weakly continuous, (iv) follows.

 $(iv) \Longrightarrow (iii)$: obvious.

(i) \Longrightarrow (iii): This is a consequence of the fact that σ -weak convergence implies weak operator convergence.

(iv) \Longrightarrow (i): By Lemma 1.30 and the subsequent remark, the set $D(\mathscr{E}) \cap \mathscr{M}_1$ is σ -weakly dense in \mathscr{M}_1 . Moreover, since $\Gamma_{\mathscr{H}}(\xi)$ is linear and σ -weakly continuous, it is uniformly continuous with respect to the σ -weak topology (see [Rud91, Theorem 1.17]). Thus, by [Bou89, Theorem II.2], for every $\xi \in \mathscr{H}$ there is a unique σ -weakly continuous extension of $\Gamma_{\mathscr{H}}(\xi)$ to \mathscr{M} with the same norm. We continue to write $\Gamma_{\mathscr{H}}(\xi)$ for this extension.

For *L* to be σ -weakly continuous it suffices to show that $\varphi \circ L$ is σ -weakly continuous for all $\varphi \in \mathcal{L}(\mathcal{H})_*$. Every $\varphi \in \mathcal{L}(\mathcal{H})_*$ is of the form $\varphi = \sum_n \langle \cdot \xi_n, \eta_n \rangle_{\mathcal{H}}$ for sequences $(\xi_n), (\eta_n)$ in \mathcal{H} such that $\sum_n (\|\xi_n\|_{\mathcal{H}}^2 + \|\eta_n\|_{\mathcal{H}}^2) < \infty$. We have

$$\sum_{n=1}^{\infty} \|\boldsymbol{\Gamma}_{\mathcal{H}}(\boldsymbol{\xi}_n, \boldsymbol{\eta}_n)\|_{\mathcal{M}^*} \leq \sum_{n=1}^{\infty} \|\boldsymbol{\xi}_n\|_{\mathcal{H}} \|\boldsymbol{\eta}_n\|_{\mathcal{H}} \leq \frac{1}{2} \sum_{n=1}^{\infty} (\|\boldsymbol{\xi}_n\|_{\mathcal{H}}^2 + \|\boldsymbol{\eta}_n\|_{\mathcal{H}}^2).$$

Hence $\sum_{n} \Gamma_{\mathscr{H}}(\xi_{n}, \eta_{n})$ converges absolutely with respect to $\|\cdot\|_{\mathscr{M}^{*}}$ to some $\omega \in \mathscr{M}^{*}$. Since the space \mathscr{M}_{*} of σ -weakly continuous linear functionals is closed in \mathscr{M}^{*} , we have $\omega \in \mathscr{M}_{*}$.

Now let (a_i) be a net in \mathcal{M} such that $a_i \to 0$ σ -weakly. Then

$$\sum_{n} \langle a_i \xi_n, \eta_n \rangle_{\mathscr{H}} = \sum_{n} \Gamma_{\mathscr{H}}(\xi_n, \eta_n)(a_i) = \omega(a_i) \xrightarrow{i} 0.$$

Hence *L* is σ -weakly continuous.

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Definition 1.33. Let \mathscr{E} be a quantum Dirichlet form on the tracial von Neumann algebra (\mathcal{M}, τ) . We say that τ is *energy dominant* if one of the equivalent assertions of Theorem 1.32 holds.

As already seen in the proof of Theorem 1.32, if the trace τ is energy dominant, then for all $\xi \in \mathcal{H}$ the functional $\Gamma_{\mathcal{H}}(\xi)$ has a unique σ -weakly continuous extension to \mathcal{M} with the same norm. Since $D(\mathscr{E}) \cap \mathcal{M}_+$ is σ -weakly dense in \mathcal{M}_+ by Theorem B.4, this extension is still positive.

We denote by $\Gamma_{\mathscr{H}}(\xi)$ the preimage of $\Gamma_{\mathscr{H}}(\xi)$ under the isomorphism

$$L^1(\mathcal{M}, \tau) \longrightarrow \mathcal{M}_*, x \mapsto \tau(x \cdot),$$

that is, $\Gamma_{\mathscr{H}}(\xi)$ is the unique element in $L^1(\mathscr{M}, \tau)$ such that

$$\Gamma_{\mathscr{H}}(\xi)(x) = \tau(x\Gamma_{\mathscr{H}}(\xi))$$

for all $x \in \mathscr{C}$. Similarly we define $\Gamma(a) \in L^1(\mathcal{M}, \tau)$ for $a \in D(\mathscr{E})$.

On the other hand, if τ is energy dominant, also the left and right action L and R have unique σ -weakly continuous extensions \tilde{L} and \tilde{R} to \mathcal{M} and \mathcal{M}° , respectively. These extensions are characterized by

$$\langle \tilde{L}(a)\xi,\eta\rangle_{\mathcal{H}} = \tau(a\Gamma_{\mathcal{H}}(\xi,\eta))$$

for $a \in \mathcal{M}, \xi, \eta \in \mathcal{H}$, and similarly for \tilde{R} .

Since the vector space operations as well as the multiplication and the involution on \mathcal{M} are all (separately) σ -weakly continuous, the extensions \tilde{L} and \tilde{R} are again *-homomorphisms. From now on we will denote these extensions simply by L, R.

Remark 1.34. If \mathscr{E} is a Dirichlet form on $L^2(X,m)$, then Γ is twice the (linear functional induced by the) energy measure as defined in [FOT94, Section 3.2]. In this case, the measure m is energy dominant if and only if $\Gamma(u)$ is absolutely continuous with respect to m for all $u \in D(\mathscr{E})$. This concept was introduced by Kusuoka [Kus89, Kus93] in the study of Dirichlet forms on fractals.

Remark 1.35. In the noncommutative setting, energy dominant traces were studied for example in [JZ15], where the corresponding semigroups were called *non-commutative diffusion semigroups*. We do not adopt this terminology as it conflicts with the well-established definition of diffusion semigroups in the commutative case.

Remark 1.36. For an irreducible local Dirichlet form \mathscr{E} it is always possible to construct an energy dominant measure μ such that \mathscr{E} is closable in $L^2(X,\mu)$, see [HRT13, Theorem 5.1].

In the noncommutative setting, one cannot expect an analogously constructed weight to be tracial.

CHAPTER 2

OPERATOR MEANS AND THE ALGEBRA \mathcal{A}_{θ}

In this chapter we study means of the left and right action on \mathscr{H} , which will later appear both in the action functional and the constraint in the definition of the metric \mathscr{W} . As an important tool we introduce the space \mathscr{A}_{θ} , which will take on the role of a space of test "functions". We prove several continuity properties of these means, which are important technical tools for the remainder of the thesis, especially the semicontinuity property established in Theorem 2.14.

In the later chapters we will focus on the logarithmic mean as it gives the connection to gradient flows of the entropy. In this chapter however we keep the discussion more general since means other than the logarithmic one have also proven useful in the commutative case (see for example [CLLZ17] for an application to evolutionary games).

Throughout this chapter let (\mathcal{M}, τ) be a tracial von Neumann algebra and \mathscr{E} a quantum Dirichlet form on $L^2(\mathcal{M}, \tau)$ with associated first-order differential calculus $(\partial, \mathcal{H}, L, R, J)$. We further assume that τ is energy dominant.

2.1 Multiplication operator and a semicontinuity result

In this section we introduce the multiplication operator $\hat{\rho}$ as an interpolation of the left and right multiplication $L(\rho)$ and $R(\rho)$, and study continuity properties of the map $\rho \mapsto \hat{\rho}$.

Since we assume τ to be energy dominant, the left and right action *L* and *R* extend to \mathcal{M} by Theorem 1.32. Using the spectral theorem, we can even extend them to operators affiliated with \mathcal{M} in the following way.

For self-adjoint $a \in \mathcal{M}$ let

$$a=\int_{\mathbb{R}}\lambda\,de(\lambda)$$

be the spectral decomposition. Since L, R are normal *-homomorphisms, the maps $L \circ e$ and $R \circ e$ are spectral measures on \mathcal{H} and

$$L(a) = \int_{\mathbb{R}} \lambda \, d(L \circ e)(\lambda),$$

and analogously for R(a). This formula obviously extends to self-adjoint operators affiliated with \mathcal{M} . We continue to denote also these extensions by L and R. For arbitrary a affiliated with \mathcal{M} with polar decomposition a = u|a| we define L(a) =L(u)L(|a|) and R(a) = R(|a|)R(u). Again this definition is clearly consistent for $a \in \mathcal{M}$, which justifies the use of the same symbol both for the maps on \mathcal{M} and their extensions to operators affiliated with \mathcal{M} .

It is easy to see that for self-adjoint a, b affiliated with \mathcal{M} the operators L(a) and R(b) commute strongly, that is, the spectral measures of L(a) and R(b) commute. Hence we can make sense of expressions of the form $\theta(L(\rho), R(\rho))$ via functional calculus (see [Sch12, Section 5.5]) for positive self-adjoint ρ affiliated with \mathcal{M} .

Definition 2.1. Let ρ be a positive self-adjoint operator affiliated with \mathcal{M} and let $\theta: [0,\infty)^2 \longrightarrow [0,\infty)$ be measurable. Let *e* denote the joint spectral measure of $L(\rho)$ and $R(\rho)$. The multiplication operator $\hat{\rho}$ is defined by

$$\begin{split} D(\hat{\rho}) &= \left\{ \xi \in \mathcal{H} \left| \int_{[0,\infty)^2} \theta(s,t)^2 d\langle e(s,t)\xi,\xi \rangle_{\mathcal{H}} < \infty \right\}, \\ \langle \hat{\rho}\xi,\eta \rangle_{\mathcal{H}} &= \int_{[0,\infty)^2} \theta(s,t) d\langle e(s,t)\xi,\eta \rangle_{\mathcal{H}}. \end{split} \right. \end{split}$$

Remark 2.2. If \mathcal{M} is commutative, one could alternatively define $\hat{\rho}$ separately for the strongly local and the jump part of \mathcal{E} (recall that one can always regularize \mathcal{E} , even if at the cost of a huge state space). Indeed, in the light of the discussion in [CS03, Section 10.1] it is not hard to see that

$$\begin{split} \|\hat{\rho}^{1/2}u\partial v\|_{\mathscr{H}}^{2} &= \int \theta(\rho(x),\rho(x))|u(x)|^{2}d\Gamma^{(c)}(v)(x) \\ &+ \frac{1}{2}\int \theta(\rho(x),\rho(y))|u(x)|^{2}|v(x)-v(y)|^{2}dJ(x,y). \end{split}$$

However, such a definition would be against the spirit of the present thesis to give a unified treatment of the local and non-local case. Moreover, there is no obvious way to extend this kind of definition to noncommutative Dirichlet forms.

Note that in the strongly local case, $\hat{\rho}$ only depends on the diagonal values of θ .

Lemma 2.3. Assume that $\theta: [0,\infty)^2 \longrightarrow [0,\infty)$ is measurable and increasing in both arguments. For positive self-adjoint ρ affiliated with \mathcal{M} let $\rho_n = \rho \wedge n$. Then $\xi \in D(\hat{\rho}^{1/2})$ if and only if $\sup_n \langle \hat{\rho}_n \xi, \xi \rangle_{\mathcal{H}} < \infty$, and in this case

$$\|\hat{\rho}^{1/2}\xi\|_{\mathscr{H}}^{2} = \sup_{n \in \mathbb{N}} \langle \hat{\rho}_{n}\xi,\xi \rangle_{\mathscr{H}}.$$

Proof. Let $\xi \in \mathcal{H}$ and let *e* be a joint spectral measure for $L(\rho)$ and $R(\rho)$. Then

$$\langle \hat{\rho}_n \xi, \xi \rangle_{\mathscr{H}} = \int_{[0,\infty)^2} \theta(s \wedge n, t \wedge n) d \langle e(s,t)\xi, \xi \rangle.$$

By assumption, $\theta(s \land n, t \land n) \nearrow \theta(s, t)$ for all $s, t \ge 0$. The monotone convergence theorem gives

$$\int_{[0,\infty)^2} \theta(s,t) d\langle e(s,t)\xi,\xi\rangle = \sup_{n\in\mathbb{N}} \langle \hat{\rho}_n\xi,\xi\rangle_{\mathscr{H}}.$$

Thus $\xi \in D(\hat{\rho}^{1/2}) = D(\theta(L(\rho), R(\rho))^{1/2})$ if and only if $\sup_n \langle \hat{\rho}_n \xi, \xi \rangle_{\mathscr{H}} < \infty$, and in this case $\|\hat{\rho}^{1/2}\xi\|_{\mathscr{H}}^2 = \sup_n \langle \hat{\rho}_n \xi, \xi \rangle_{\mathscr{H}}$.

Definition 2.4. For a positive self-adjoint operator ρ affiliated with \mathcal{M} and a measurable function $\theta: [0,\infty)^2 \longrightarrow [0,\infty)$ we define

$$\|\cdot\|_{\rho} \colon \mathscr{H} \longrightarrow [0,\infty], \, \|\xi\|_{\rho} = \begin{cases} \|\hat{\rho}^{1/2}\xi\|_{\mathscr{H}} & \text{if } \xi \in D(\hat{\rho}^{1/2}), \\ \infty & \text{otherwise.} \end{cases}$$

In other words, $\|\cdot\|_{\rho}^{2}$ is the quadratic form generated by ρ . Note that this definition implicitly depends on the choice of θ . Lemma 2.3 shows that if θ is increasing in both arguments, this norm can alternatively be computed as $\|\xi\|_{\rho}^{2} = \sup_{n} \langle \hat{\rho}_{n} \xi, \xi \rangle_{\mathscr{H}}$ for $\xi \in \mathscr{H}$.

Lemma 2.5. Assume that $\theta: [0,\infty)^2 \longrightarrow [0,\infty)$ is continuous, increasing in both arguments and $\theta(s,t) > 0$ for s,t > 0. If ρ is an invertible positive self-adjoint operator affiliated with \mathcal{M} , then the map

$$L^{2}(\mathcal{M},\tau) \longrightarrow [0,\infty], a \mapsto \begin{cases} \|\partial a\|_{\rho}^{2} & \text{if } a \in D(\mathscr{E}) \\ \infty & \text{otherwise} \end{cases}$$

is lower semicontinuous.

Proof. First assume that ρ is bounded. Since ρ is invertible and $\theta(s,t) > 0$ for s,t > 0, the operator $\hat{\rho}$ is also invertible. Thus $\hat{\rho}^{1/2}\partial$ is closed and the lower semicontinuity follows from a standard Hilbert space argument. If ρ is not necessarily bounded, the lower semicontinuity follows from Lemma 2.3 and the first part. \Box

Definition 2.6. Let $\theta : [0,\infty)^2 \longrightarrow [0,\infty)$ be measurable. For $a \in D(\mathscr{E})$ let

$$\|a\|_{\theta}^{2} = \sup_{\rho \in L^{1}_{+}(\mathcal{M},\tau)} \frac{\|\partial a\|_{\rho}^{2}}{\|\rho\|_{1}}$$

The test space \mathscr{A}_{θ} is the set of all $a \in D(\mathscr{E}) \cap \mathscr{M}$ with $||a||_{\theta} < \infty$.

Example 2.7. If \mathscr{E} is a strongly local commutative Dirichlet form on $L^2(X, m)$, then

$$\|\partial f\|_{\rho}^{2} = \int_{X} \theta(\rho(x), \rho(x)) \Gamma(f) dm.$$

In particular, if $\theta(s,s) = s$, then $||f||_{\theta}^2 = ||\Gamma(f)||_{\infty}$ and

$$\mathscr{A}_{\theta} = \{ f \in D(\mathscr{E}) \cap \mathscr{M} \mid \Gamma(f) \in L^{\infty}(X, m) \}.$$

This is the space of test functions used in [AES16]. *Example* 2.8. If θ = AM, the arithmetic mean, then

$$\|\partial a\|_{\rho}^{2} = \frac{1}{2}\tau((\Gamma(a) + \Gamma(a^{*}))\rho)$$

and

$$\mathscr{A}_{\mathrm{AM}} = \{ a \in D(\mathscr{E}) \cap \mathscr{M} \mid \Gamma(a), \Gamma(a^*) \in \mathscr{M} \}.$$

A variant of this algebra (without the assumption $\Gamma(a^*) \in \mathcal{M}$) was introduced in [Cip16, Definition 10.7] under the name *Lipschitz algebra*. By [Cip16, Proposition 10.6] the boundedness of $\Gamma(a)$ is equivalent to the boundedness of the commutator $[D, a^*]$, where

$$D = \begin{pmatrix} 0 & \partial^* \\ \partial & 0 \end{pmatrix}$$

is the Dirac operator acting on $L^2(\mathcal{M},\tau) \oplus \mathcal{H}$. Hence the space \mathcal{A}_{AM} is closely related to spectral triples in Connes' noncommutative geometry [Con94] (compare also Remark 3.21).

Remark 2.9. In general, it does not seem feasible to give a more explicit description of \mathscr{A}_{θ} . Note however that if θ is concave, there exist $\alpha, \beta > 0$ such that $\theta \leq \alpha AM + \beta$ and thus $\mathscr{A}_{AM} \subset \mathscr{A}_{\theta}$.

Lemma 2.10. If $\theta: [0,\infty)^2 \longrightarrow [0,\infty)$ is a symmetric measurable function, then $\|\partial a^*\|_{\rho}^2 = \|\partial a\|_{\rho}^2$ for all $a \in D(\mathcal{E}) \cap \mathcal{M}$ and positive self-adjoint operators ρ affiliated with \mathcal{M} . In particular, \mathcal{A}_{θ} is self-adjoint.

Proof. It follows from the properties of the first-order differential calculus that $J\mathbb{1}_A(L(\rho))\mathbb{1}_B(R(\rho)) = \mathbb{1}_B(L(\rho))\mathbb{1}_A(R(\rho))J$ for all Borel sets $A, B \subset [0,\infty)$. Thus, if *e* denotes the joint spectral measure of $L(\rho)$ and $R(\rho)$, then

$$\begin{split} \|\partial a^*\|_{\rho}^2 &= \int_{[0,\infty)^2} \theta(s,t) d \langle e(s,t) J \partial a, J \partial a \rangle_{\mathcal{H}} \\ &= \int_{[0,\infty)^2} \theta(s,t) d \langle e(t,s) \partial a, \partial a \rangle \\ &= \|\partial a\|_{\rho}^2, \end{split}$$

since θ is symmetric.

Lemma 2.11. If τ is a state and $\theta : [0,\infty)^2 \longrightarrow [0,\infty)$ is continuous, increasing in both arguments and $\theta(s,t) > 0$ for s,t > 0, then $\|\cdot\|_{\theta}$ is lower semicontinuous on $L^2(\mathcal{M},\tau)$.

Proof. By Lemma 2.5 it suffices to show that the supremum in the definition of $\|\cdot\|_{\theta}$ can be taken over all invertible $\rho \in L^1_+(\mathcal{M}, \tau)$.

For $\rho \in L^1_+(\mathcal{M},\tau)$ and $\varepsilon > 0$ let $\rho^{\varepsilon} = \rho + \varepsilon$. Evidently, $\rho^{\varepsilon} \in L^1_+(\mathcal{M},\tau)$ is invertible and $\|\rho^{\varepsilon}\|_1 = \|\rho\|_1 + \varepsilon$. Since θ is increasing in both arguments, one sees as in the proof of Lemma 2.3 that

$$\|\partial a\|_{\rho^{\varepsilon}}^{2} = \|\partial a\|_{\rho+\varepsilon}^{2} \ge \|\partial a\|_{\rho}^{2}.$$

Thus

$$\sup_{\varepsilon > 0} \frac{\|\partial a\|_{\rho^{\varepsilon}}^{2}}{\|\rho^{\varepsilon}\|_{1}} \ge \sup_{\varepsilon > 0} \frac{\|\partial a\|_{\rho}^{2}}{\|\rho\|_{1} + \varepsilon} = \frac{\|\partial a\|_{\rho}^{2}}{\|\rho\|_{1}}.$$

Corollary 2.12. If τ is a state and θ is continuous, increasing in both arguments and $\theta(s,t) > 0$ for s,t > 0, then \mathcal{A}_{θ} is complete in the norm $\|\cdot\|_{\mathcal{M}} + \|\cdot\|_{\theta}$.

Next we study continuity properties of the map $\rho \mapsto \|\hat{\rho}^{1/2} \partial a\|_{\mathscr{H}}^2$. We start with an auxiliary result for bounded θ .

Lemma 2.13. Denote by $\mathscr{C}_h(\mathscr{H})$ the set of all self-adjoint operators on \mathscr{H} . If $\theta: [0,\infty)^2 \longrightarrow [0,\infty)$ is continuous, then the map

$$L^1_+(\mathcal{M},\tau) \longrightarrow \mathscr{C}_h(\mathcal{H}), \rho \mapsto \theta(L(\rho), R(\rho))$$

is continuous with respect to the norm topology on L^1 and the strong resolvent topology on $\mathcal{C}_h(\mathcal{H})$.

If θ is additionally bounded, then the map

$$L^1_+(\mathcal{M},\tau) \longrightarrow [0,\infty), \rho \mapsto \|\xi\|_{\rho}^2$$

is continuous for all $\xi \in \mathcal{H}$.

Proof. Let (ρ_n) be a sequence in $L^1_+(\mathcal{M},\tau)$ and $\rho \in L^1_+(\mathcal{M},\tau)$ such that $\rho_n \to \rho$ in the strong L^1 topology. By Lemma B.9 the sequence (ρ_n) also converges to ρ in the strong resolvent sense. Since L and R are normal *-homomorphisms, $L(\rho_n) \to L(\rho)$ and $R(\rho_n) \to R(\rho)$ in the strong resolvent sense as well.

Now $\theta(L(\rho_n), R(\rho_n)) \to \theta(L(\rho), R(\rho))$ follows from Proposition B.5. As the strong resolvent topology coincides with the strong topology on norm bounded subsets of $\mathscr{L}(\mathscr{H})$, the last part is clear.

Theorem 2.14. If $\theta : [0,\infty)^2 \longrightarrow [0,\infty)$ is continuous, then

$$\Lambda: L^1_+(\mathcal{M}, \tau) \longrightarrow [0, \infty), \rho \mapsto \|\xi\|_{\rho}^2$$

is lower semicontinuous with respect to $\|\cdot\|_1$ for all $\xi \in \mathcal{H}$. If θ is additionally concave, then Λ is continuous for $\xi = \partial a$ with $a \in \mathcal{A}_{AM}$.

In particular, if Λ is concave, then it is weakly upper semicontinuous for $\xi = \partial a$ with $a \in \mathscr{A}_{AM}$.

Proof. For $k \in \mathbb{N}$ let $\theta_k = \theta \land k$. By Lemma 2.13 the map

$$\Lambda_k: L^1_+(\mathcal{M}, \tau) \longrightarrow [0, \infty), \rho \mapsto \langle \theta_k(L(\rho), R(\rho))\xi, \xi \rangle_{\mathcal{H}}$$

is continuous with respect to $\|\cdot\|_1$ for all $\xi \in \mathcal{H}$. Since $\Lambda_k \nearrow \Lambda$ by functional calculus, the map Λ is lower semicontinuous as supremum of continuous maps.

To prove the continuity when $\xi = \partial a$ with $a \in \mathcal{A}_{AM}$, it only remains to show upper semicontinuity. Since θ is concave, there exist $\alpha, \beta \ge 0$ such that $\theta \le \alpha AM + \beta$. Since $a \in \mathcal{A}_{AM}$, we have

$$\|(\alpha \operatorname{AM}(L(\rho), R(\rho)) + \beta)^{1/2} \partial \alpha\|_{\mathcal{H}}^2 = \frac{\alpha}{2} \tau((\Gamma(\alpha) + \Gamma(\alpha^*))\rho) + \beta \mathcal{E}(\alpha),$$

which clearly depends continuously on ρ .

Moreover, the map

$$L^1_+(\mathcal{M},\tau) \longrightarrow [0,\infty), \rho \mapsto \|(\alpha AM + \beta - \theta)^{1/2}(L(\rho), R(\rho))\partial a\|^2_{\mathcal{H}}$$

is lower semicontinuous by the first part. Thus $-\Lambda$ is lower semicontinuous as the sum of two lower semicontinuous maps in this case.

Finally, the weak upper semicontinuity for concave Λ follows from the Hahn-Banach theorem.

Remark 2.15. In general, concavity of θ is not sufficient for concavity of Λ . However, in the next section we will study a class of functions θ for which Λ is concave.

Remark 2.16. Note that for the upper semicontinuity part we need $a \in \mathcal{A}_{AM}$ instead of \mathcal{A}_{θ} . Whether upper semicontinuity still holds for a in the bigger space \mathcal{A}_{θ} is unclear.

2.2 Operator means

In the last section we saw that a crucial property of the multiplication operator is the concavity of the assignment $\rho \mapsto \hat{\rho}$. An important class of functions θ for which this property holds are those that can be represented as an operator mean in the sense of Kubo–Ando [KA80]. In this section we review the definition and a representation theorem for operator means before we turn to the application to the multiplication operator in the next section.

Definition 2.17. Let *H* be an infinite-dimensional Hilbert space. An operator mean is a map $#: \mathscr{L}(H)_+ \times \mathscr{L}(H)_+ \longrightarrow \mathscr{L}(H)_+$ such that

- $x_1 \le x_2$ and $y_1 \le y_2$ imply $x_1 \# y_1 \le x_2 \# y_2$,
- $z(x\#y)z \le (zxz)\#(zyz)$ for $x, y, z \in \mathcal{L}(H)_+$,
- $x_n \searrow x$ and $y_n \searrow y$ imply $x_n \# y_n \searrow x \# y$,
- 1#1 = 1.

If *H* is finite-dimensional, a map $#: \mathscr{L}(H)_+ \times \mathscr{L}(H)_+ \longrightarrow \mathscr{L}(H)_+$ is called operator mean if *H* embeds into an infinite-dimensional Hilbert space *K* such that # extends to an operator mean on *K*.

An operator mean # is called *symmetric* if x#y = y#x for all $x, y \in \mathcal{L}(H)_+$.

We say that a continuous function $\theta : [0,\infty)^2 \longrightarrow [0,\infty)$ can be *represented by a* (*symmetric*) *operator mean* if there exists a (symmetric) operator mean such that $\theta(x, y) = x # y$ for all commuting $x, y \in \mathcal{L}(\mathcal{H})_+$.

Example 2.18. Examples of symmetric operator means include

- the arithmetic operator mean $(x, y) \mapsto \frac{1}{2}(x+y)$,
- the logarithmic operator mean, given by the generating function $f(t) = (t 1)/\log t$ (see Proposition 2.19),
- the harmonic operator mean $(x, y) \mapsto 2(x^{-1} + y^{-1})^{-1}$,

• the geometric operator mean $(x, y) \mapsto x^{1/2} (x^{-1/2} y x^{-1/2})^{1/2} x^{1/2}$.

Two examples of nonsymmetric operator means are

- the left trivial mean $(x, y) \mapsto x$, and
- the right trivial mean $(x, y) \mapsto y$.

There is a close relation between operator means and operator monotone functions. A continuous function $f: I \longrightarrow \mathbb{R}$ is called *operator monotone* if $x \le y$ implies $f(x) \le f(y)$ for all bounded self-adjoint operators x, y with spectrum in I.

Proposition 2.19 ([KA80, Theorem 3.2]). Let H be a Hilbert space. For every operator monotone function $f: (0,\infty) \rightarrow (0,\infty)$ with f(1) = 1 there exists a unique operator mean # such that

$$x # y = x^{1/2} f(x^{-1/2} y x^{-1/2}) x^{1/2}$$

for all invertible $x, y \in \mathcal{L}_+(H)$, and every operator mean arises this way.

In the situation of the proposition above, the operator monotone function f is called the *generating function* of #. An important result of Löwner's seminal work on operator monotone functions (see [Lö34]) is that every operator monotone function admits an integral representation. A variant of this theorem reads as follows.

Proposition 2.20 ([Han80, Theorem 4.9]). A function $f: (0,\infty) \longrightarrow (0,\infty)$ is operator monotone if and only if there exists a finite Borel measure μ on [0,1] such that

$$f(t) = \int_0^1 \frac{t}{\lambda + (1 - \lambda)t} \, d\mu(t)$$

for t > 0.

Corollary 2.21. A function $\theta : [0,\infty)^2 \longrightarrow [0,\infty)$ can be represented by an operator mean if and only if there exists a Borel probability measure μ on [0,1] such that

$$\theta(s,t) = \int_0^1 \frac{st}{\lambda s + (1-\lambda)t} \, d\mu(\lambda)$$

for s, t > 0.

In this case θ is increasing in both arguments, positively homogeneous and satisfies $\theta(s,s) = s$ for $s \ge 0$. The resulting mean is symmetric if and only if $\mu(A) = \mu(1-A)$ for all Borel sets $A \subset [0,1]$.

Conversely, if # is an operator mean with generating function f and one defines θ by $\theta(s,t) = sf(s/t)$ for s,t > 0, then $x # y = \theta(x,y)$ for all commuting $x, y \in \mathcal{L}(\mathcal{H})_+$.

2.3 Multiplication operator induced by an operator mean

After we introduced the multiplication operator $\hat{\rho} = \theta(L(\rho), R(\rho))$ and operator means in the last two sections, we will now discuss some additional properties of the multiplication operator in the case when θ can be represented by an operator mean.

Proposition 2.22. If θ can be represented by a symmetric operator mean, then \mathcal{A}_{θ} is a *-algebra.

Proof. We have already proven that \mathcal{A}_{θ} is self-adjoint in Lemma 2.10. It remains to show that \mathcal{A}_{θ} is an algebra.

Let $a, b \in \mathcal{A}_{\theta}$. By Lemma 2.3 it suffices to show that there exists a constant C > 0 such that $\|\partial(ab)\|_{\rho}^{2} \leq C \|\rho\|_{1}$ for all $\rho \in L^{1}_{+}(\mathcal{M}, \tau) \cap \mathcal{M}$. We can assume without loss of generality $\|a\|_{\mathcal{M}}, \|b\|_{\mathcal{M}} \leq 1$.

By the product rule we have

$$\begin{aligned} \|\partial(ab)\|_{\rho}^{2} &= \|\hat{\rho}^{1/2}(L(a)\partial b + R(b)\partial a)\|_{\mathcal{H}}^{2} \\ &\leq 2\langle L(a^{*})\hat{\rho}L(a)\partial b, \partial b\rangle_{\mathcal{H}}^{2} + 2\langle R(b^{*})\hat{\rho}R(b)\partial a, \partial a\rangle_{\mathcal{H}}. \end{aligned}$$

$$(2.1)$$

Let *f* be the generating function of the operator mean # that is represented by θ . If $x \in \mathcal{M}_+$ is invertible, then

$$\begin{split} L(a^*)(L(x)\#R(x))L(a) &= R(x)^{1/2}L(a^*)f(R(x)^{-1/2}L(x)R(x)^{-1/2})L(a)R(x)^{1/2} \\ &\leq R(x)^{1/2}f(R(x)^{-1/2}L(a^*xa)R(x)^{-1/2})R(x)^{1/2} \\ &= L(a^*xa)\#R(x), \end{split}$$

where the inequality in the second line follows from the operator monotonicity of f (see [Han80]). If x is not necessarily invertible, the same inequality still holds by the continuity property of #.

Thus

$$L(a^*)\hat{\rho}L(a) \leq L(a^*\rho a) \# R(\rho)$$

$$\leq L(a^*\rho a) \# R(\rho) + L(\rho) \# R(a^*\rho a)$$

$$\leq L(a^*\rho a + \rho) \# R(\rho + a^*\rho a),$$

(2.2)

where we used the concavity of operator means ([KA80, Theorem 3.5]) for the last inequality.

Since # is assumed to be symmetric, the inequality

$$R(b^{*})\hat{\rho}R(b) \le L(b^{*}\rho b + \rho) \# R(\rho + b^{*}\rho b)$$
(2.3)

follows analogously.

If we combine (2.1), (2.2) and (2.3), we obtain

$$\begin{aligned} \|\partial(ab)\|_{\rho}^{2} &\leq 2\|\partial a\|_{\rho+b^{*}\rho b}^{2} + 2\|\partial b\|_{\rho+a^{*}\rho a}^{2} \\ &\leq 2\|a\|_{\theta}^{2}\|\rho+b^{*}\rho b\|_{1} + 2\|b\|_{\theta}^{2}\|\rho+a^{*}\rho a\|_{1} \\ &\leq 4(\|a\|_{\theta}^{2} + \|b\|_{\theta}^{2})\|\rho\|_{1}. \end{aligned}$$

Hence $ab \in \mathcal{A}_{\theta}$.

Lemma 2.23. If θ can be represented by a symmetric operator mean, then

$$\|\partial \alpha\|_{\rho}^{2} \leq \frac{1}{2}\tau((\Gamma(\alpha) + \Gamma(\alpha^{*}))\rho)$$

for $a \in D(\mathscr{E})$ and $\rho \in L^1_+(\mathscr{M}, \tau)$.

Proof. By [KA80, Theorem 4.5] we have $\theta \leq AM$. Now it suffices to notice that

$$\langle L(\rho)\partial a, \partial a \rangle_{\mathcal{H}} = \tau(\Gamma(a)\rho)$$

and

$$\langle R(\rho)\partial a, \partial a \rangle_{\mathcal{H}} = \tau(\Gamma(a^*)\rho).$$

Lemma 2.24. Assume that θ can be represented by an operator mean. If $\rho_0, \rho_1 \in L^1_+(\mathcal{M}, \tau)$ with $\rho_0 \leq \rho_1$, then $\|\xi\|_{\rho_0} \leq \|\xi\|_{\rho_1}$ for all $\xi \in \mathcal{H}$.

Proof. If ρ_0, ρ_1 are bounded, then the claim is immediate from the definition of operator means. In the general case let $f_{\varepsilon}(r) = r(1+\varepsilon r)^{-1}$. This function is operator monotone, hence $f_{\varepsilon}(\rho_0) \leq f_{\varepsilon}(\rho_1)$. Moreover, $f_{\varepsilon}(r) \nearrow r$ as $\varepsilon \to 0$ implies $\|\xi\|_{f_{\varepsilon}(\rho_i)} \to \|\xi\|_{\rho_i}$ as $\varepsilon \to 0$ for $i \in \{0, 1\}$. Combining this convergence with the monotonicity in the bounded case, we obtain

$$\|\xi\|_{\rho_0} = \lim_{\varepsilon \to 0} \|\xi\|_{f_\varepsilon(\rho_0)} \le \lim_{\varepsilon \to 0} \|\xi\|_{f_\varepsilon(\rho_1)} = \|\xi\|_{\rho_1}.$$

Corollary 2.25. Assume that θ can be represented by an operator mean. If $\rho_n \to \rho$ in $L^1_+(\mathcal{M}, \tau)$ and $\rho_n \leq \rho$, then $\|\xi\|_{\rho_n} \to \|\xi\|_{\rho}$ for $\xi \in \mathcal{H}$. If moreover $\xi \in D(\hat{\rho}^{1/2})$, then $\xi \in D(\hat{\rho}_n^{1/2})$ for all $n \in \mathbb{N}$ and $\hat{\rho}_n^{1/2}\xi \to \hat{\rho}^{1/2}\xi$ in \mathcal{H} .

Proof. The first part is an immediate consequence of Theorem 2.14 and Lemma 2.24. For the second part first note that $\widehat{\rho_n \wedge N}^{1/2} \to \widehat{\rho \wedge N}^{1/2}$ strongly as $n \to \infty$ by Lemma 2.13.

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Let e_n denote the joint spectral measure of $L(\rho_n)$ and $R(\rho_n)$. Then

$$\begin{split} \|(\hat{\rho}_n^{1/2} - \widehat{\rho_n \wedge N}^{1/2})\xi\|_{\mathscr{H}}^2 &= \int_{[0,\infty)^2} (\theta(s,t)^{1/2} - \theta(s \wedge N, t \wedge N)^{1/2})^2 d\langle e_n(s,t)\xi,\xi \rangle_{\mathscr{H}} \\ &\leq \int_{[0,\infty)^2} (\theta(s,t) - \theta(s \wedge N, t \wedge N)) d\langle e_n(s,t)\xi,\xi \rangle_{\mathscr{H}} \\ &= \|\xi\|_{\rho_n}^2 - \|\xi\|_{\rho_n \wedge N}^2. \end{split}$$

The same holds for ρ_n replaced by ρ . Thus

$$\begin{split} \|(\hat{\rho}_{n}^{1/2} - \hat{\rho}^{1/2})\xi\|_{\mathscr{H}} &\leq \|(\hat{\rho}_{n}^{1/2} - \widehat{\rho_{n} \wedge N}^{1/2})\xi\|_{\mathscr{H}} + \|(\widehat{\rho_{n} \wedge N}^{1/2} - \widehat{\rho \wedge N}^{1/2})\xi\|_{\mathscr{H}} \\ &+ \|(\widehat{\rho \wedge N}^{1/2} - \hat{\rho}^{1/2})\xi\|_{\mathscr{H}} \\ &\leq (\|\xi\|_{\rho_{n}}^{2} - \|\xi\|_{\rho_{n} \wedge N}^{2})^{1/2} + \|(\widehat{\rho_{n} \wedge N}^{1/2} - \widehat{\rho \wedge N}^{1/2})\xi\|_{\mathscr{H}} \\ &+ (\|\xi\|_{\rho}^{2} - \|\xi\|_{\rho \wedge N}^{2})^{1/2}. \end{split}$$

Hence

$$\limsup_{n \to \infty} \|(\hat{\rho}_n^{1/2} - \hat{\rho}^{1/2})\xi\|_{\mathscr{H}} \le 2(\|\xi\|_{\rho}^2 - \|\xi\|_{\rho \wedge N}^2)^{1/2},$$

which goes to zero as $N \to \infty$.

Lemma 2.26. If θ can be represented by an operator mean, then

$$L^1_+(\mathcal{M},\tau) \longrightarrow [0,\infty), \rho \mapsto \|\xi\|^2_{\rho}$$

is concave for all $\xi \in \mathcal{H}$.

Proof. Since operator means are jointly concave by [KA80, Theorem 3.5], the map $\rho \mapsto \|\xi\|_{\rho}^{2}$ is concave on $L^{1}_{+}(\mathcal{M},\tau) \cap \mathcal{M}$. Hence, if $\rho_{0}, \rho_{1} \in L^{1}_{+}(\mathcal{M},\tau)$ and $\lambda > 0$, then

$$\|\xi\|_{(1-\lambda)(\rho_0 \wedge n) + \lambda(\rho_1 \wedge n)}^2 \ge (1-\lambda) \|\xi\|_{\rho_0 \wedge n}^2 + \lambda \|\xi\|_{\rho_1 \wedge n}^2.$$

By Lemma 2.3, the right-hand side converges to $(1 - \lambda) \|\xi\|_{\rho_0}^2 + \lambda \|\xi\|_{\rho_1}^2$ as $n \to \infty$. On the other hand, Lemma 2.24 gives

$$\|\xi\|_{(1-\lambda)\rho_0+\lambda\rho_1}^2 \ge \|\xi\|_{(1-\lambda)\rho_0\wedge n+\lambda\rho_1\wedge n}^2$$

Thus $\rho \mapsto \|\xi\|_{\rho}^2$ is concave.

As mentioned before, we will later focus on the case when θ is the logarithmic mean

$$\mathrm{LM} \colon [0,\infty)^2 \longrightarrow [0,\infty), (s,t) \mapsto \begin{cases} \frac{s-t}{\log s - \log t} & \text{if } s \neq t, \\ s & \text{otherwise.} \end{cases}$$

Alternatively, it can be represented as

$$\mathrm{LM}(s,t) = \int_0^1 s^{\alpha} t^{1-\alpha} \, d\,\alpha.$$

A direct calculation shows that LM can be represented by a symmetric operator mean, namely the logarithmic operator mean from Example 2.18. Thus, all the results from this section are applicable in this case.

It is the following identity that sets the logarithmic mean apart from other possible choices of operator means in our context:

$$LM(L(a), R(a))\partial \log(a) = LM(L(a), R(a))\log(L(a), R(a))\partial a = \partial a$$

This cancellation effect relies only on the chain rule for the first-order differential calculus. It would therefore be natural to consider more general functions θ of the form

$$\theta(s,t) = \frac{s-t}{\psi(s) - \psi(t)}.$$

However, if we additionally require that θ can be represented by an operator mean, then it is not hard to see that ψ is already forced to be the logarithm (up to an additive constant). Thus the choice of the logarithmic mean (and the von Neumann entropy later) is not arbitrary, but a consequence of these two simple structural assumptions.

CHAPTER 3

The Noncommutative Transport Metric \mathcal{W}

In this chapter we define a transport metric on the space of density operators that generalizes both the discrete transport metric \mathcal{W} from [Maa11, Mie11, CHLZ12] and the Wasserstein metric W_2 on Riemannian manifolds.

The study of the optimal transport problem

$$\int_{X \times X} d(x, y)^2 d\pi(x, y) \to \min$$
$$(\mathrm{pr}_1)_{\#} \pi = \mu, (\mathrm{pr}_2)_{\#} \pi = \nu$$

defining the L^2 -Wasserstein metric goes back to the work of Monge [Mon81] and Kantorovich [Kan42, Kan04], who formulated the relaxed problem in the modern form. Especially for the quadratic case metric, the name "Wasserstein metric" is misleading, and some authors prefer to call it *Monge-Kantorovich metric* or some variations of that. More information on the history of the Wasserstein metric as well as optimal transport in general can be found in the bibliographical notes in Villani's book [Vil09].

The Benamou–Brenier formula

$$W_2(\mu,\nu)^2 = \inf\left\{\int_0^1 \int_{\mathbb{R}^n} |v_t|^2 d\mu_t dt \, \Big| \, \dot{\mu}_t + \nabla \cdot (\mu_t v_t) = 0, \\ \mu_0 = \mu, \\ \mu_1 = \nu \right\}$$

reformulates the Wasserstein metric on Borel probability measures over \mathbb{R}^n as dynamical optimization problem. It was found by Benamou and Brenier [BB00] in relation to numerical algorithms for the Wasserstein distance and later generalized to considerably more general settings (see for example [AES16]).

Our construction of the transport metric \mathcal{W} relies on a modification of the Benamou–Brenier formula. As already observed in the articles mentioned above in the case of finite graphs and matrix algebras, the crucial step is to not only replace the action functional in the classical Benamou–Brenier formula, but also the constraint by a suitable noncommutative version of the continuity equation.

While the form of this continuity equation is easily adapted from the previous work on the finite-dimensional case, finding a good weak formulation is still challenging. As it turns out, especially in view of the results in Section 6, the algebra \mathscr{A}_{AM} introduced in the last section is a good choice of test "functions". Among several other useful properties of the metric \mathscr{W} , we will use the continuity properties from the last section to prove lower semicontinuity of the energy functional defining \mathscr{W} (Theorem 3.30).

As usual, (\mathcal{M}, τ) is a tracial von Neumann algebra, \mathscr{E} a quantum Dirichlet form on $L^2(\mathcal{M}, \tau)$ such that τ is energy dominant, and $(\partial, \mathcal{H}, L, R, J)$ the associated first-order differential calculus. We further assume that $\theta: [0, \infty)^2 \longrightarrow [0, \infty)$ is a continuous function that can be represented by a symmetric operator mean. In particular, all results from Section 2 are applicable. All expressions like $\hat{\rho}$, $\|\cdot\|_{\rho}$ etc. are to be understood with respect to this particular choice of θ .

3.1 Admissible curves

In this section we introduce a class of curves in the space of noncommutative probability densities which satisfy a noncommutative version of the continuity equation. These will later be the class of curves to which we can assign a length.

Definition 3.1 (Density operator). A *density operator* is an element ρ of $L^1_+(\mathcal{M}, \tau)$ with $\tau(\rho) = 1$. The space of all density operators over (\mathcal{M}, τ) is denoted by $\mathcal{D}(\mathcal{M}, \tau)$.

Under the map $\rho \mapsto \tau(\cdot \rho)$, the density matrices correspond exactly to the normal states on \mathcal{M} . Of course, if \mathcal{M} is commutative, the density operators over (\mathcal{M}, τ) are just the classical probability densities.

Definition 3.2 (Hilbert space \mathscr{H}_{ρ}). For $\rho \in \mathscr{D}(\mathscr{M}, \tau)$ let $\tilde{\mathscr{H}}_{\rho}$ be the Hilbert space obtained from $D(\hat{\rho}^{1/2})$ after separation and completion with respect to $\|\cdot\|_{\rho}$. Let \mathscr{H}_{ρ} be the closure of $\partial \mathscr{A}_{AM}$ in $\tilde{\mathscr{H}}_{\rho}$.

If $(\rho_t)_{t\in I}$ is a curve in $\mathscr{D}(\mathscr{M}, \tau)$, we say that a curve $(\xi_t)_{t\in I}$ with $\xi_t \in \mathscr{H}_{\rho_t}$ is measurable if $t \mapsto \|\xi_t\|_{\rho_t}$ is measurable and $t \mapsto \langle \xi_t, \partial a \rangle_{\rho_t}$ is measurable for all $a \in \mathscr{A}_{AM}$. The space of all a.e.-equivalence classes of measurable curves (ξ_t) such that $\int_I \|\xi_t\|_{\rho_t}^2 dt < \infty$ is denoted by $L^2(I;(\mathscr{H}_{\rho_t})_{t\in I})$. The space $L^2_{\text{loc}}(I;(\mathscr{H}_{\rho_t})_{t\in I})$ is defined accordingly. *Remark* 3.3. If there exists a countable subset E of \mathscr{A} such that ∂E is dense in \mathscr{H}_{ρ_t} for all $t \in I$, then $(\mathscr{H}_{\rho_t})_{t \in I}$ is a measurable field of Hilbert spaces in the sense of [Tak02, Definition 8.9] and $L^2(I; (\mathscr{H}_{\rho_t})_{t \in I})$ is just a different notation for the direct integral $\int_I^{\oplus} \mathscr{H}_{\rho_t} dt$.

Definition 3.4 (Admissible curves). A curve $(\rho_t)_{t \in I}$ in $\mathcal{D}(\mathcal{M}, \tau)$ is *admissible* if $t \mapsto \tau(\rho_t a)$ is locally absolutely continuous for all $a \in \mathscr{A}_{AM}$ and there exists $\xi \in L^2_{loc}(I; (\mathscr{H}_{\rho_t})_{t \in I})$ such that for all $a \in \mathscr{A}_{AM}$ the continuity equation

$$\frac{d}{dt}\tau(a\rho_t) = \langle \partial a, \xi_t \rangle_{\rho_t} \tag{CE}$$

holds for a.e. $t \in I$.

If it exists, such an element $\xi \in L^2_{\text{loc}}(I; (\mathcal{H}_{\rho_t})_{t \in I})$ is necessarily unique since $\partial \mathscr{A}_{\text{AM}}$ is dense in \mathcal{H}_{ρ_t} for all $t \in I$, and we write $D\rho = \xi$ in this case.

A couple of remarks are in order. First, the definition of absolutely continuous functions allows for an integral characterization of admissible curves that will be useful later on.

Remark 3.5. Let $(\rho_t)_{t \in I}$ be a curve in $\mathscr{D}(\mathscr{M}, \tau)$. It is easy to see that (ρ_t) is admissible if and only if there exists a $c \in L^2_{loc}(I)$ such that

$$|\tau(a\rho_t) - \tau(a\rho_s)| \le \int_s^t c(r) \|\partial a\|_{\rho_r} dr$$

for all $s, t \in I$ and $a \in \mathscr{A}_{AM}$, and in this case, $r \mapsto \|D\rho_r\|_{\rho_r}$ is the minimal function c with this property.

Remark 3.6. First rudiments of a solution theory of equations of similar type based on the noncommutative differential calculus have been developed in [Zae16].

Remark 3.7. If \mathscr{E} is the standard Dirichlet energy on a complete Riemannian manifold (M,g), then (CE) reduces to the classical continuity equation

$$\dot{\rho}_t + \operatorname{div}(\rho_t \xi_t) = 0$$

(weakly in duality with the bounded Lipschitz functions).

Accordingly, if (M,g) has lower bounded Ricci curvature, then a curve $(\rho_t)_{t \in I}$ of probability densities is admissible if and only if it is in $AC^2_{loc}(I;(P_2(M), W_2))$ by [Erb10, Proposition 2.5]. Compare also Example 3.17 and Proposition 7.4.

Finally, let us also discuss two possible variants of the definition of admissible curves.

Remark 3.8. Instead of restricting to $\xi_t \in \mathscr{H}_{\rho_t}$ in (CE), one might want to take $\xi_t \in \widetilde{\mathscr{H}}_{\rho_t}$. This is no longer unique, but if it exists, the orthogonal projection η_t of ξ_t onto \mathscr{H}_{ρ_t} still satisfies (CE) and $\|\eta_t\|_{\rho_t} \leq \|\xi_t\|_{\rho_t}$. Instead of minimizing over all admissible curves (ρ_t) with unique "velocity vector field" $(D\rho_t)$ in the definition \mathscr{W} below, one can therefore equivalently minimize over all pairs of curves (ρ_t, ξ_t) satisfying (CE), where we only assume $\xi_t \in \widetilde{\mathscr{H}}_{\rho_t}$.

Remark 3.9. Since the definition of the multiplication operator $\hat{\rho}$ uses the mean θ , it might appear more natural to replace \mathscr{A}_{AM} by the bigger space \mathscr{A}_{θ} both in the definition of \mathscr{H}_{ρ} and the weak continuity equation (CE). The crucial point is that the upper semicontinuity property from Theorem 2.14 is only guaranteed for \mathscr{A}_{AM} .

However, under suitable conditions on the Dirichlet form \mathscr{E} we introduce in Chapter 5, the closure of $\partial \mathscr{A}_{\theta}$ in $\tilde{\mathscr{H}}_{\rho}$ coincides with \mathscr{H}_{ρ} and the duality in the continuity equation can be extended to $a \in \mathscr{A}_{\theta}$ so that both of these possible definitions finally yield the same result.

Under strong conditions on the curve (ρ_t) , the duality in (CE) can be extended beyond to $D(\mathscr{E})$.

Lemma 3.10. Assume that $\mathscr{A}_{AM} \subset D(\mathscr{E})$ is dense. If $(\rho_t)_{t \in I}$ is an admissible curve in $\mathscr{D}(\mathscr{M}, \tau)$ such that

$$\sup_{J \subset I} \|\rho_t\|_{\mathcal{M}} < \infty$$

for all compact $J \subset I$, then $t \mapsto \tau(\rho_t a)$ is locally absolutely continuous for all $a \in D(\mathscr{E})$ and

$$\frac{d}{dt}\tau(a\rho_t) = \langle \partial a, D\rho_t \rangle_{\rho_t}$$

for a.e. $t \in I$.

Proof. Let (a_k) be a sequence in \mathscr{A}_{AM} such that $a_k \to a$ w.r.t. $\|\cdot\|_{\mathscr{E}}$. Since $\rho_t \in \mathscr{D}(\mathscr{M},\tau) \cap \mathscr{M} \subset L^2(\mathscr{M},\tau)$, we have $\tau(a_k\rho_t) \to \tau(a\rho_t)$ as $k \to \infty$. On the other hand, since $\hat{\rho}_t$ is bounded and $\partial a_k \to \partial a$, we also have $\langle \partial a_k, D\rho_t \rangle_{\rho_t} \to \langle \partial a, D\rho_t \rangle_{\rho_t}$ as $k \to \infty$. Moreover,

$$|\langle \partial a_k, D\rho_t \rangle_{\rho_t}| \leq \|\rho_t\|_{\mathcal{M}}^{1/2} \mathscr{E}(a_k)^{\frac{1}{2}} \|D\rho_t\|_{\rho_t}.$$

Since $(\mathscr{E}(a_k))_k$ is bounded and $t \mapsto \|\rho_t\|_{\mathscr{M}}$ is bounded on compact intervals, we can apply the dominated convergence theorem to get

$$\tau(a(\rho_t - \rho_s)) = \lim_{k \to \infty} \tau(a_k(\rho_t - \rho_s)) = \lim_{k \to \infty} \int_s^t \langle \partial a_k, D \rho_r \rangle_{\rho_r} dr = \int_s^t \langle \partial a, D \rho_r \rangle_{\rho_r} dr.$$

From this equality, both the claimed absolute continuity and the identity for the derivative follow easily. $\hfill \Box$

3.2 The transport metric \mathcal{W}

In this section we introduce the transport metric \mathcal{W} as a length metric with a length functional defined on the class of admissible curves.

Strictly speaking, the map \mathcal{W} will not be a metric since it might be degenerate and take the value infinity. Let us therefore recall the following extended concept of metrics.

Definition 3.11 (Extended pseudometric). Let X be a set. An *extended pseudo*metric on X is a map $d: X \times X \longrightarrow [0, \infty]$ such that

- d(x,x) = 0 for $x \in X$,
- d(x, y) = d(y, x) for $x, y \in X$,
- $d(x, y) \le d(x, z) + d(z, y)$ for $x, y, z \in X$.

An extended pseudometric *d* is an *extended metric* if d(x, y) = 0 implies x = y.

Definition 3.12 (Transport metric \mathcal{W}). The extended pseudometric \mathcal{W} on $\mathcal{D}(\mathcal{M}, \tau)$ is defined by

$$\mathcal{W}: \mathcal{D}(\mathcal{M}, \tau) \times \mathcal{D}(\mathcal{M}, \tau) \longrightarrow [0, \infty], \\ \mathcal{W}(\bar{\rho}_0, \bar{\rho}_1) = \inf \left\{ \int_0^1 \|D\rho_t\|_{\rho_t} dt \, \middle| \, (\rho_t) \text{ admissible}, \rho_0 = \bar{\rho}_0, \rho_1 = \bar{\rho}_1 \right\}.$$

Remark 3.13. If we endow $\mathcal{D}(\mathcal{M}, \tau)$ with the topology induced by the seminorms $\tau(a \cdot)$ for $a \in \mathcal{A}_{AM}$, then the class of admissible curves together with the map that sends an admissible curve $(\rho_t)_{t \in I}$ to $\int_I ||D\rho_t||_{\rho_t} dt$ is a length structure in the sense of [BBI01, Chapter 2] and \mathcal{W} is the associated length metric. The topological condition from their definition is verified in Proposition 3.20.

Remark 3.14. Contrary to the Wasserstein metric, but also the metric \mathcal{W} defined for certain jump processes in [Erb14], we define \mathcal{W} only on densities. This is enough to study gradient flows of the entropy, which is only finite on measures with density anyway, but it would be interesting to see if there is an extension of \mathcal{W} to a larger class of states.

Remark 3.15. A different approach to noncommutative analogues of the Wasserstein distances, which relies on approximation by commutative subalgebras, has been studied in [Zae15]. Contrary to our construction, if the algebra \mathcal{M} is commutative, the metric W_2 defined by Zaev is the usual L^2 -Wasserstein distance. In particular, in some examples it coincides and in some examples it is different from the metric constructed here. It is not clear if there is any deeper connection between these two approaches in the noncommutative case. *Example* 3.16. Let (X, b, m) be a weighted graph and $\mathscr{E}^{(N)}$ as in Example 1.25. Then

$$\|\xi\|_{\rho}^{2} = \frac{1}{2} \sum_{x,y} b(x,y) \theta(\rho(x),\rho(y)) |\xi(x,y)|^{2}$$

for $\rho \in \mathscr{P}(X,m)$ and $\xi \in \ell^2(X \times X, \frac{1}{2}b)$. In particular, if X is finite, this norm coincides with the one defined in [Maa11]. Consequently, our metric \mathscr{W} coincides with the metric \mathscr{W} defined in [Maa11] for finite graphs.

Example 3.17. If \mathscr{E} is the standard Dirichlet energy on \mathbb{R}^n , then

$$\|\partial u\|_{\rho}^{2} = \int_{\mathbb{R}^{n}} |\nabla u|^{2} \rho \, dx$$

and the definition of \mathcal{W} coincides with the Benamou–Brenier formulation [BB00] of the L^2 -Wasserstein distance.

Example 3.18. More generally, let \mathscr{E} be a strongly local regular Dirichlet form on $L^2(X,m)$ and assume that m is energy dominant. Then

$$\|\partial u\|_{\rho}^{2} = \int_{X} \Gamma(u)\rho \, dm.$$

In this case \mathcal{W} coincides with the metric $\mathcal{W}_{\mathscr{E}}$ defined in [AES16, Definition 10.4]. This in turn was shown in [AES16, Theorem 12.5] to coincide with the L^2 -Wasserstein distance \mathcal{W}_2 if (X, d, m) is an RCD (K, ∞) space and \mathscr{E} is twice the Cheeger energy (see also [AGS14b] for the relevant definitions).

Note that in the last two examples the transport metric \mathcal{W} does not depend on the choice of the mean θ . That is because if \mathscr{E} is strongly local, only the values of θ on the diagonal matter, and these are already determined by the assumption that θ can be represented by an operator mean.

If one is only interested in the commutative case, one might want to relax the condition of operator concavity of θ to mere concavity. In this case, θ does not necessarily reduce to the identity on the diagonal. Metrics of this type (in the strongly local case) were studied in [DNS09, CLSS10].

Example 3.19. Let \mathcal{M} be a finite-dimensional von Neumann algebra, tr the normalized trace on \mathcal{M} , and (P_t) a quantum Markov semigroup on \mathcal{M} . Under the assumption that (P_t) satisfies the quantum detailed balance condition, Carlen and Maas [CM17a] defined a *Riemannian* metric on the space $\mathcal{D}_+(\mathcal{M}, \text{tr})$ of strictly positive density matrices. Let us shortly summarize their construction.

Given $\omega = (\omega_1, \dots, \omega_n) \in \mathbb{R}^n$ and $c = (c_1, \dots, c_n) \in \mathbb{R}^n$ (which are canonically associated with (P_t)) and a density matrix ρ , they define

$$[\rho]_{\omega_j}: L^2(\mathcal{M}, \mathrm{tr}) \longrightarrow L^2(\mathcal{M}, \mathrm{tr}), [\rho]_{\omega_j} = \int_0^1 (e^{-\omega_j/2} L_\rho)^s (e^{\omega_j/2} R_\rho)^{1-s} ds,$$

where L_{ρ} and R_{ρ} are the left and right multiplication with ρ on \mathcal{M} . Further, $[\rho]_{\omega} = [\rho]_{\omega_1} \oplus \cdots \oplus [\rho]_{\omega_n}$.

The norm of a tangent vector $\dot{\rho}_0$ is defined by

$$g(\dot{\rho}_0, \dot{\rho}_0) = \inf_{V} \sum_{j=1}^n c_j \langle V_j, [\rho_0]_{\omega_j} V_j \rangle_{L^2(\mathcal{M}, \mathrm{tr})}$$

where the infimum is taken over all V satisfying a continuity equation of the form

$$\dot{\rho}_0 = \operatorname{div}([\rho_0]_{\omega}V).$$

In the case when (P_t) is tracially symmetric and $\theta = LM$, one has $c_j = 1$, $\omega_j = 0$ for all $j \in \{1, ..., n\}$, and it is easily checked that L, R, div etc. coincide with the operations obtained from the first- order differential calculus. Therefore, $[\rho]_0 = \hat{\rho}$ and the distance function induced by g coincides with \mathcal{W} .

However, it should be stressed that the class of quantum Markov semigroups satisfying the detailed balance condition is larger than the class of tracially symmetric ones, so we do not fully recover the construction from [CM17a]. It is an interesting open question how one can generalize the construction of the metric W to the case of infinite-dimensional quantum Markov semigroups satisfying the detailed balance condition or, more generally, KMS-symmetric quantum Markov semigroups. The latter is open even in the finite-dimensional case.

We conclude this section with some basic properties of \mathcal{W} . the first one is a sufficient condition to make \mathcal{W} non-degenerate.

Proposition 3.20. If $\rho_0, \rho_1 \in \mathcal{D}(\mathcal{M}, \tau)$ and $a \in \mathcal{A}_{AM}$, then

$$|\tau(a(\rho_0 - \rho_1))|^2 \le \|a\|_{\theta}^2 \mathcal{W}(\rho_0, \rho_1)^2 \le \|a\|_{AM}^2 \mathcal{W}(\rho_0, \rho_1)^2$$

In particular, if \mathcal{A}_{AM} is σ -weakly dense in \mathcal{M} , then \mathcal{W} is non-degenerate.

Proof. We can assume that $\mathcal{W}(\rho_0, \rho_1) < \infty$, otherwise there is nothing to prove. Let $(\rho_t)_{t \in [0,1]}$ be an admissible curve connecting ρ_0 and ρ_1 . By definition $\|\partial a\|_{\rho_t}^2 \le \|a\|_{\theta}^2$ for all $t \in [0,1]$. Thus

$$|\tau(a(\rho_1 - \rho_0))| \leq \int_0^1 |\langle \partial a, D\rho_t \rangle_{\rho_t} | dt \leq ||a||_{\theta} \int_0^1 ||D\rho_t|| dt$$

Taking the infimum over all admissible curves connecting ρ_0 and ρ_1 yields the first inequality.

The second inequality follows directly from the first an Lemma 2.23. Finally, the last claim is an immediate consequence of the first inequality. \Box

Remark 3.21. According to [Cip16, Proposition 10.6], the seminorm

$$\|\cdot\|_{\mathrm{AM}} \colon \mathscr{A}_{\mathrm{AM}} \longrightarrow [0,\infty), a \mapsto \left(\frac{1}{2}(\|\Gamma(a) + \Gamma(a^*)\|_{\mathscr{M}})\right)^{1/2}$$

is a Lipschitz seminorm in the spirit of [Con89, Rie99]. The induced metric W_{Γ} on $\mathcal{D}(\mathcal{M}, \tau)$ given by

$$W_{\Gamma}(\rho,\sigma) = \sup\{|\tau(a(\rho-\sigma))|: a \in \mathcal{A}_{AM}, ||a||_{AM} \le 1\}$$

is a noncommutative analogue of the L^1 -Wasserstein distance (depending on the context, it is also called Connes distance or spectral distance).

The following lemma is standard.

Lemma 3.22. If $(\rho_s)_{s \in [0,1]}$ is an admissible curve with $D\rho_s \neq 0$ for a.e. $s \in [0,1]$, then (ρ_s) can be reparametrized so that the resulting curve $(\sigma_t)_{t \in I}$ has constant speed and

$$\int_0^1 \|D\sigma_t\|_{\sigma_t}^2 dt \leq \int_0^1 \|D\rho_s\|_{\rho_s}^2 ds.$$

Proof. By assumption, the map

$$[0,1] \longrightarrow [0,1], s \mapsto \frac{\int_0^s \|D\rho_r\|_{\rho_r} dr}{\int_0^1 \|D\rho_r\|_{\rho_r} dr}$$

is continuous and strictly increasing, hence a homeomorphism. Denote its inverse by θ and let $\sigma_t = \rho_{\theta(t)}$. It is immediate from the definition that σ is admissible and $D\sigma_t = \dot{\theta}(t)D\rho_{\theta(t)}$ for a.e. $t \in [0, 1]$. Note that

$$\dot{\theta}(t) = \frac{\int_0^1 \|D\rho_r\|_{\rho_r} dr}{\|D\rho_{\theta(t)}\|_{\rho_{\theta(t)}}}.$$

Thus (σ_t) has constant speed and

$$\int_0^1 \|D\sigma_t\|_{\sigma_t}^2 dt = \left(\int_0^1 \|D\rho_r\|_{\rho_r} dr\right)^2 \le \int_0^1 \|D\rho_r\|_{\rho_r}^2 dr.$$

Corollary 3.23. The pseudometric \mathcal{W} can alternatively be calculated as

$$\mathcal{W}(\bar{\rho}_{0},\bar{\rho}_{1})^{2} = \inf\left\{\int_{0}^{1} \|D\rho_{t}\|_{\rho_{t}}^{2} dt \left| (\rho_{t}) admissible, \rho_{0} = \bar{\rho}_{0}, \rho_{1} = \bar{\rho}_{1}\right\}$$

Lemma 3.24 (Convexity of the squared distance). For $\rho_j^i \in \mathcal{D}(\mathcal{M}, \tau)$, $i, j \in \{0, 1\}$, let $\rho_t^i = (1-t)\rho_0^i + t\rho_1^i$ for $i \in \{0, 1\}$, $t \in [0, 1]$. Then

$$\mathcal{W}^{2}(\rho_{t}^{0},\rho_{t}^{1}) \leq (1-t)\mathcal{W}^{2}(\rho_{0}^{0},\rho_{0}^{1}) + t\mathcal{W}^{2}(\rho_{1}^{0},\rho_{1}^{1})$$

for all $t \in [0, 1]$.

Proof. We can assume that $\mathcal{W}(\rho_0^0, \rho_0^1), \mathcal{W}(\rho_1^0, \rho_1^1) < \infty$. For $j \in \{0, 1\}$ let $(\rho_j^s)_{s \in [0, 1]}$ be admissible curves connecting ρ_j^0 and ρ_j^1 and let $\xi_j^s = D_s \rho_j^s$. Define $\rho_t^s = (1-t)\rho_0^s + t\rho_1^s$ for $s, t \in [0, 1]$. Obviously, $s \mapsto \tau(a\rho_t^s)$ is locally absolutely continuous for all $a \in \mathscr{A}_{AM}$ and $t \in [0, 1]$.

We will show that the map

$$\partial \mathscr{A}_{\mathrm{AM}} \longrightarrow \mathbb{C}, \, \partial a \mapsto \frac{d}{ds} \tau(a \rho_t^s)$$

is well-defined and continuous with respect to $\|\cdot\|_{\rho_t^s}$: Indeed,

$$\begin{split} \frac{\left|\frac{d}{ds}\tau(a\rho_{t}^{s})\right|^{2}}{\left\|\partial a\right\|_{\rho_{t}^{s}}^{2}} &= \frac{\left|(1-t)\frac{d}{ds}\tau(a\rho_{0}^{s})+t\frac{d}{ds}\tau(a\rho_{1}^{s})\right|^{2}}{\left\|\partial a\right\|_{\rho_{t}^{s}}^{2}} \\ &= \frac{\left|(1-t)\langle\partial a,\xi_{0}^{s}\rangle_{\rho_{0}^{0}}+t\langle\partial a,\xi_{1}^{s}\rangle_{\rho_{1}^{s}}\right|^{2}}{\left\|\partial a\right\|_{\rho_{t}^{s}}^{2}} \\ &\leq \frac{\left|(1-t)\langle\partial a,\xi_{0}^{s}\rangle_{\rho_{0}^{0}}+t\langle\partial a,\xi_{1}^{s}\rangle_{\rho_{1}^{s}}\right|^{2}}{(1-t)\left\|\partial a\right\|_{\rho_{0}^{s}}^{2}+t\left\|\partial a\right\|_{\rho_{1}^{s}}^{2}} \\ &\leq (1-t)\frac{\left|\langle\partial a,\xi_{0}^{s}\rangle_{\rho_{0}^{0}}\right|^{2}}{\left\|\partial a\right\|_{\rho_{0}^{s}}^{2}}+t\frac{\left|\langle\partial a,\xi_{1}^{s}\rangle_{\rho_{1}^{s}}\right|^{2}}{\left\|\partial a\right\|_{\rho_{1}^{s}}^{2}} \\ &\leq (1-t)\left\|\xi_{0}^{s}\right\|_{\rho_{0}^{s}}^{2}+t\left\|\xi_{1}^{s}\right\|_{\rho_{1}^{s}}^{2}. \end{split}$$

For the first inequality we used Lemma 2.26, while the second inequality follows from the convexity of the function $(x, y) \mapsto \frac{y^2}{x}$. Thus, $(\rho_t^s)_{s \in [0,1]}$ is admissible for every $t \in [0,1]$ and $(D_s \rho_t^s)_{s \in [0,1]}$ satisfies

$$\|D_{s}\rho_{t}^{s}\|_{\rho_{t}^{s}}^{2} = \sup_{a \in \mathscr{A}_{AM}} \frac{|\langle \partial a, D_{s}\rho_{t}^{s} \rangle_{\rho_{t}^{s}}|^{2}}{\|\partial a\|_{\rho_{t}^{s}}^{2}} \le (1-t)\|D_{s}\rho_{0}^{s}\|_{\rho_{0}^{s}}^{2} + t\|D_{s}\rho_{1}^{s}\|_{\rho_{1}^{s}}^{2}.$$

Therefore

$$\mathcal{W}^{2}(\rho_{t}^{0},\rho_{t}^{1}) \leq (1-t) \int_{0}^{1} \|D_{s}\rho_{0}^{s}\|_{\rho_{0}^{s}}^{2} ds + t \int_{0}^{1} \|D_{s}\rho_{1}^{s}\|_{\rho_{1}^{s}}^{2} ds$$

Taking the infimum over all admissible curves $(\rho_j^s)_{s \in [0,1]}$ connecting ρ_j^0 and ρ_j^1 yields the assertion.

Definition 3.25. Let (X,d) be an extended metric space. A curve $\gamma: I \longrightarrow X$ is called *p*-locally absolutely continuous if there exists a positive function $g \in L^p_{loc}(I)$ such that

$$d(\gamma_s, \gamma_t) \le \int_s^t g(r) dr \tag{AC}_p$$

for all $s, t \in I$. We write $AC_{loc}^{p}(I;(X,d))$ for the space of all *p*-locally absolutely continuous curves in (X,d). If $\gamma \in AC_{loc}^{p}(I;(X,d))$, then the *metric speed*

$$|\dot{\gamma}_t|_d := \lim_{h \to 0} \frac{d(\gamma_{t+h}, \gamma_t)}{|h|}$$

exists for a.e. $t \in I$ and $|\dot{\gamma}|_d$ is the minimal $g \in L^p_{loc}(I)$ such that (AC_p) holds.

It is immediate from the definition that every admissible curve $(\rho_t)_{t \in I}$ belongs to $\operatorname{AC}^2_{\operatorname{loc}}(I;(\mathscr{D}(\mathscr{M},\tau),\mathscr{W}))$ and $|\dot{\rho}_t|_{\mathscr{W}} \leq \|D\rho_t\|_{\rho_t}$ for a.e. $t \in I$.

Corollary 3.26 (Convexity squared metric speed). Let $(\rho_t^i)_{t \in I}$, $i \in \{0, 1\}$, be locally absolutely continuous curves in $(\mathcal{D}(\mathcal{M}, \tau), \mathcal{W})$ and $\rho^s = (1-s)\rho^0 + s\rho^1$ for $s \in [0, 1]$. Then ρ^s is locally absolutely continuous and

$$|\dot{\rho}^{s}|_{\mathcal{W}}^{2} \leq (1-s)|\dot{\rho}^{0}|_{\mathcal{W}}^{2} + s|\dot{\rho}^{1}|_{\mathcal{W}}^{2}$$

for all $s \in [0, 1]$.

At the present stage we cannot say much about when the distance \mathcal{W} between two density matrices is finite. However, if \mathcal{E} satisfies some functional inequalities, we get estimates on \mathcal{W} .

Proposition 3.27. Assume that τ is a state. If \mathscr{E} satisfies the Poincaré inequality with constant $c_P > 0$, that is,

$$\|a - \tau(a)\|_2^2 \le c_P^2 \mathscr{E}(a)$$

for all $a \in D(\mathcal{E})$, then

$$\mathcal{W}(\rho_0,\rho_1) \leq \frac{c_P}{\lambda} \|\rho_1 - \rho_0\|_2$$

for all $\rho_0, \rho_1 \in \mathcal{D}(\mathcal{M}, \tau) \cap L^2(\mathcal{M}, \tau)$ with $\rho_0, \rho_1 \ge \lambda^2 > 0$

Proof. Let $\rho_t = (1-t)\rho_0 + t\rho_1$ and notice that $\rho_t \ge \lambda^2$ implies $\hat{\rho}_t \ge \lambda^2$. For all $a \in \mathscr{A}_{AM}$ we have

$$\begin{aligned} |\tau(a(\rho_t - \rho_s))| &= |t - s| |\tau((a - \tau(a))(\rho_1 - \rho_0))| \\ &\leq c_P |t - s| \|\rho_1 - \rho_0\|_2 \|\partial a\|_{\mathscr{H}} \\ &\leq \frac{c_P}{\lambda} \|\rho_1 - \rho_0\|_2 \int_s^t \|\partial a\|_{\rho_r} dr. \end{aligned}$$

Hence $(\rho_r)_{r \in [0,1]}$ is admissible with $\|D\rho_r\|_{\rho_r} \leq \frac{c_P}{\lambda} \|\rho_1 - \rho_0\|_2$.

Remark 3.28. Qualitatively, this result can be rephrased as follows: The form \mathscr{E} satisfies a Poincaré inequality if and only if ker ∂ is spanned by 1 and ∂^* has closed range. In this case, if (ρ_t) is the linear interpolation between two density matrices in L^2 , then

$$\dot{\rho}_t = \partial^* \eta_t$$

has a solution $\eta_t \in \mathcal{H}$. If ρ_t is additionally bounded away from zero, then there is a solution ξ_t to

$$\hat{\rho}_t \xi_t = \eta_t,$$

and (ρ_t) satisfies the continuity equation for the vector field (ξ_t) .

Remark 3.29. One typical problem for length spaces we have not touched upon yet is the existence of geodesics, that is, length-minimizing curves for a given start and endpoint. A length space is called geodesic if any two points with finite distance are joined by a geodesic. This property is one of the advantages of the metric \mathcal{W} in the finite-dimensional case compared to the Wasserstein distance, with the geometry of the geodesics an object of recent attention (see [GLM17, EMW19]).

Unfortunately, $(\mathcal{D}(\mathcal{M},\tau),\mathcal{W})$ can fail to be geodesic even in the commutative case, as was pointed out to the author by Erbar. However, we will see in Chapter 6 that (under suitable conditions) the subset of all density matrices with finite entropy is indeed geodesic, and this is enough for the study of geodesic convexity of the entropy.

3.3 Lower semicontinuity of the action

In this section we prove that the action functional appearing in the definition of \mathcal{W} is lower semicontinuous with respect to pointwise weak convergence in L^1 and show some first consequences. This property will later be important for several approximation arguments.

Theorem 3.30 (Lower semicontinuity of the action). If $L^1(\mathcal{M}, \tau)$ is separable, then the action functional

$$E: \mathscr{D}(\mathscr{M},\tau)^{[0,1]} \longrightarrow [0,\infty], (\rho_t) \mapsto \begin{cases} \int_0^1 \|D\rho_t\|_{\rho_t}^2 dt & \text{if } (\rho_t) \text{ is admissible,} \\ \infty & \text{otherwise} \end{cases}$$

is lower semicontinuous with respect to pointwise weak convergence in $L^{1}(\mathcal{M}, \tau)$.

Proof. Let (ρ^n) be a sequence in $\mathscr{D}(\mathscr{M},\tau)^{[0,1]}$ and $\rho: [0,1] \longrightarrow \mathscr{D}(\mathscr{M},\tau)$ such that $\rho_t^n \to \rho_t$ weakly in L^1 for all $t \in [0,1]$. Otherwise passing to subsequence, we may assume that $(E(\rho^n))_n$ is convergent. Moreover, if the limit is infinite, there is nothing to prove, so we assume additionally that $\sup_n E(\rho^n) < \infty$. In particular, the curve $(\rho_t^n)_t$ is admissible for all $n \in \mathbb{N}$.

Fix $a \in \mathscr{A}_{AM}$. Since $\rho_t^n \to \rho_t$ weakly for all $t \in [0, 1]$, we have

$$|\tau(a(\rho_t - \rho_s))| = \lim_{n \to \infty} |\tau(a(\rho_t^n - \rho_s^n))| \le \liminf_{n \to \infty} \int_s^t \|D\rho_r^n\|_{\rho_r^n} \|\partial a\|_{\rho_r^n} dr.$$

Let $c^n: [0,1] \longrightarrow [0,\infty)$, $c^n(r) = \|D\rho_r^n\|_{\rho_r^n}$. By assumption, (c^n) is bounded in $L^2([0,1])$, hence we may assume that $c^n \to c$ weakly in $L^2([0,1])$.

Note that the separability of $L^1(\mathcal{M},\tau)$ implies that the weak L^1 -topology restricted to $\mathcal{D}(\mathcal{M},\tau)$ is metrizable (see [DS88, Theorem V.5.1]). Since $\rho \mapsto \|\partial a\|_{\rho}$ is upper semicontinuous (Theorem 2.14), there is a decreasing sequence (G_k) of weakly continuous functions on $\mathcal{D}(\mathcal{M},\tau)$ such that

$$\|\partial a\|_{\rho} = \inf_{k \in \mathbb{N}} G_k(\rho)$$

for all $\rho \in \mathcal{D}(\mathcal{M}, \tau)$. Moreover, we can assume that $G_k \leq ||a||_{\theta}$ for all $k \in \mathbb{N}$.

Let $g^n(r) = G_k(\rho_r^n)$ and $g(r) = G_k(\rho_r)$. The dominated convergence theorem gives $g^n \to g$ strongly in $L^2([0,1])$.

Hence

$$|\tau(a(\rho_t - \rho_s))| \leq \lim_{n \to \infty} \int_s^t c^n(r) g^n(r) dr = \int_s^t c(r) g(r) dr = \int_s^t c(r) G_k(\rho_r) dr$$

for all $k \in \mathbb{N}$.

Finally, another application of the dominated convergence theorem yields

$$|\tau(a(\rho_t - \rho_s))| \leq \lim_{k \to \infty} \int_s^t c(r) G_k(\rho_r) dr = \int_s^t c(r) \|\partial a\|_{\rho_r} dr$$

This inequality implies that (ρ_t) is admissible and $\int_0^1 \|D\rho_t\|_{\rho_t}^2 dt \le \|c\|_{L^2([0,1])}^2$. Thus

$$\int_0^1 \|D\rho_t\|_{\rho_t}^2 dt \le \|c\|_{L^2([0,1])}^2 \le \liminf_{n \to \infty} \int_0^1 \|D\rho_t^n\|_{\rho_t^n}^2 dt.$$

Remark 3.31. The separability of $L^1(\mathcal{M}, \tau)$ is equivalent to each of the following properties:

- (i) The σ -weak topology on the unit ball of \mathcal{M} is metrizable.
- (ii) \mathcal{M} is separable in the strong operator topology.

(iii) \mathcal{M} has a faithful normal representation on a separable Hilbert space.

A von Neumann algebra with one of these properties is often called *separable* (this property is of course not equivalent to the separability in the norm topology, which only holds for finite-dimensional von Neumann algebras).

Lemma 3.32. If \mathscr{A}_{AM} is σ -weakly dense in \mathscr{M} and $L^1(\mathscr{M}, \tau)$ is separable, then every admissible curve is measurable in $L^1(\mathscr{M}, \tau)$.

Proof. Let A be the uniform closure of \mathscr{A}_{AM} . By Kaplansky's density theorem (see Theorem B.11), $A \cap \mathscr{M}_1$ is σ -weakly dense in \mathscr{M}_1 . Since $L^1(\mathscr{M}, \tau)$ is separable, the σ -weak topology is metrizable on \mathscr{M}_1 . Thus, for every $a \in \mathscr{M}$ there exists a sequence (a_k) in A such that $a_k \to a \sigma$ -weakly.

If (ρ_t) is an admissible curve, then $t \mapsto \tau(\rho_t a_k)$ is continuous for all $k \in \mathbb{N}$. Therefore $t \mapsto \tau(\rho_t a)$ is measurable as pointwise limit of a sequence of continuous functions. Using once more the separability of $L^1(\mathcal{M}, \tau)$, we conclude that (ρ_t) is measurable in $L^1(\mathcal{M}, \tau)$ due to Pettis' measurability theorem (see [DU77, Theorem II.2]).

Lemma 3.33. Assume that \mathscr{A}_{AM} is σ -weakly dense in \mathscr{M} and $L^1(\mathscr{M}, \tau)$ is separable. If $(\rho_t)_{t \in [0,1]}$ is an admissible curve in $\mathscr{D}(\mathscr{M}, \tau)$, then there exists a family of admissible curves $(\rho_t^{\varepsilon}) \in C^{\infty}([0,1]; L^1(\mathscr{M}, \tau))$ such that $\rho_0^{\varepsilon} = \rho_0$, $\rho_1^{\varepsilon} = \rho_1$ for $\varepsilon > 0$, and

$$\begin{split} \limsup_{\varepsilon \to 0} &\int_0^1 \|D\rho_t^\varepsilon\|_{\rho_t^\varepsilon}^2 dt \le \int_0^1 \|D\rho_t\|_{\rho_t}^2 dt, \\ \limsup_{\varepsilon \to 0} &\sup_{t \in [0,1]} \|D\rho_t^\varepsilon\|_{\rho_t^\varepsilon}^2 \le \underset{t \in [0,1]}{\mathrm{essup}} \|D\rho_t\|_{\rho_t}^2. \end{split}$$

In particular, the infimum in the definition of W can alternatively be taken over L^1 -smooth admissible curves.

Proof. Let $(\rho_t)_{t \in [0,1]}$ be an admissible curve. Extend it to a curve $(\rho_t)_{t \in \mathbb{R}}$ by setting $\rho_t = \rho_0$ for t < 0 and $\rho_t = \rho_1$ for t > 1. Note that the extended curve is still admissible with $D\rho_t = 0$ for $t \in (-\infty, 0) \cup (1, \infty)$.

Let $(\eta_{\varepsilon})_{\varepsilon>0}$ be a mollifying kernel on \mathbb{R} with $\operatorname{supp} \eta_{\varepsilon} \subset (-\varepsilon, \varepsilon)$ and set

$$\rho_t^{\varepsilon} = \int_{\mathbb{R}} \eta_{\varepsilon}(s) \rho_{t-s} \, ds,$$

where the integral is to be understood as Pettis integral in $L^1(\mathcal{M}, \tau)$. The measurability of (ρ_t) is guaranteed by Lemma 3.32.

The curve $(\rho_t^{\varepsilon})_{t \in \mathbb{R}}$ is in $C^{\infty}(\mathbb{R}; L^1(\mathcal{M}, \tau))$ and satisfies $\rho_t^{\varepsilon} = \rho_0$ for $t \leq -\varepsilon$ and $\rho_t^{\varepsilon} = \rho_1$ for $t \geq 1 + \varepsilon$. Moreover, if $a \in \mathcal{A}_{AM}$, then

$$\begin{aligned} |\tau(a(\rho_t^{\varepsilon} - \rho_s^{\varepsilon}))| &\leq \int_{\mathbb{R}} \eta_{\varepsilon}(r) |\tau(a(\rho_{t-r} - \rho_{s-r}))| dr \\ &\leq \int_{\mathbb{R}} \eta_{\varepsilon}(r) \int_{s-r}^{t-r} \|\partial a\|_{\rho_u} \|D\rho_u\|_{\rho_u} du dr \\ &= \int_s^t \int_{\mathbb{R}} \eta_{\varepsilon}(r) \|\partial a\|_{\rho_{u-r}} \|D\rho_{u-r}\|_{\rho_{u-r}} dr du \\ &\leq \int_s^t \left(\int_{\mathbb{R}} \eta_{\varepsilon}(r) \|\partial a\|_{\rho_{u-r}}^2 dr \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}} \eta_{\varepsilon}(r) \|D\rho_{u-r}\|_{\rho_{u-r}}^2 dr \right)^{\frac{1}{2}} du \end{aligned}$$

Since $\rho \mapsto \|\partial a\|_{\rho}^{2}$ is upper semicontinuous and concave by Lemmas 2.14, 2.26, we can apply the vector-valued version of Jensen's inequality (see [Per74, Theorem 3.10]) to get

$$\int_{\mathbb{R}} \eta_{\varepsilon}(r) \|\partial a\|_{\rho_{u-r}}^2 dr \leq \|\partial a\|_{\rho_u^{\varepsilon}}^2.$$

Thus $(\rho_t^{\varepsilon})_{t \in \mathbb{R}}$ is admissible and

$$\|D\rho_t^{\varepsilon}\|_{\rho_t^{\varepsilon}}^2 \leq \int_{\mathbb{R}} \eta_{\varepsilon}(r) \|D\rho_{t-r}\|_{\rho_{t-r}}^2 dr.$$

for a.e. $t \in [0, 1]$.

Finally one can reparametrize (ρ_t^{ε}) in such a way that $\rho_0^{\varepsilon} = \rho_0$, $\rho_{\varepsilon}^1 = \rho_1$ and the claimed inequalities are retained.

Remark 3.34. Mollifying in the time variable to restrict minimization problems to smooth curves is a standard argument, but the nonlinearity of $\|\xi\|_{\rho}$ in ρ requires some additional care in our case. In particular, the upper semicontinuity of $\rho \mapsto \|\partial a\|_{\rho}^{2}$ is crucial here, because the vector-valued version of Jensen's inequality may fail otherwise (see [Per74]).

CHAPTER 4

VON NEUMANN ENTROPY AND FISHER INFORMATION

In this chapter we introduce two important quantities for the gradient flow characterization of the heat flow, namely the (von Neumann) entropy and the Fisher information or entropy production, and carefully analyze convexity and continuity properties of these two as well as some related functionals.

The conception of entropy in thermodynamics goes back to Clausius [Cla65, Cla67], who also introduced the term *Entropie* (German for entropy). While Clausius' concept of entropy was phenomenological, Boltzmann [Bol71, Bol77] and Gibbs [Gib02] later gave a statistical interpretation in terms of microstates of the system, and in various contexts, the quantity is called Boltzmann or Gibbs entropy.

The extension of the concept of entropy to quantum mechanical systems has to be credited to von Neumann [Neu27] (see also Petz's survey [Pet01] about von Neumann's work on quantum mechanical entropy). Anecdotally, von Neumann is also responsible for Shannon's use of the term entropy for a closely related concept in his foundational work in information theory [Sha48], which is now known as Shannon entropy. Later, von Neumann's concept of quantum entropy was generalized to relative entropy of arbitrary normal states on von Neumann algebras by Araki [Ara76, Ara78]. To avoid confusion with notions of entropy in other fields of mathematics and also to stress the close connection of the noncommutative framework to quantum statistical mechanic, we use the term von Neumann entropy.

The name Fisher information stems from a closely related concept in statistics. It is named after Ronald Fisher, in whose work it is featured prominently (see for example [Fis22, Fis24, Fis34]), although it had already been studied by Edgeworth [Edg08] before.

Since then, various notions of quantum fisher information have been put forward (see the textbooks [Hel76, Kho82] for an early version occurring in the quantum Cramér–Rao inequality and [CL07] for a structural approach generating a family of quantum Fisher information functionals). The quantity we call Fisher information in this thesis appears as the derivative of the entropy along heat flow curves (Proposition 4.25). It is therefore sometimes also called entropy production or entropy dissipation (depending on the sign convention), and as such was first introduced in the context of quantum Markov semigroups by Spohn [Spo78].

Most of this chapter is quite technical and concerned with the rigorous definitions of entropy and Fisher information and some continuity properties. The main exception is Proposition 4.24, which asserts that heat flow curves are admissible and relates their length with the Fisher information. This foreshadows the close relation between entropy, heat flow and the metric \mathcal{W} , which we will exploit for the gradient flow characterization in the next section.

Throughout this chapter let (\mathcal{M}, τ) be a tracial von Neumann algebra, \mathscr{E} a quantum Dirichlet form on $L^2(\mathcal{M}, \tau)$, $(\partial, \mathcal{H}, L, R, J)$ the associated first-order differential calculus and assume that τ is energy dominant. We further assume that θ can be represented by a symmetric operator mean. Denote by $(P_t)_{t\geq 0}$ the quantum Markov semigroup associated with \mathscr{E} and by $\mathscr{L} = \partial^* \partial$ its generator.

4.1 Trace functionals

In this section we study functionals on $L^1_+(\mathcal{M},\tau)$ of the form $a \mapsto \tau(f(a))$ with a focus on convexity, semicontinuity and differentiability. As discussed before, there is a distinct gap between convex functions and operator convex functions. Moreover, simple examples like the square function show that the derivative of the operator function $a \mapsto f(a)$ at a_0 does not equal $f'(a_0)$ in general (for more details on the differentiability of the operator function $a \mapsto f(a)$ in noncommutative L^p spaces see [dPS04]). All these problems can be partially rectified when taking the trace of the operator function.

We first note that the functional $a \mapsto \tau(f(a))$ inherits monotonicity and convexity from f (see [BK90], Lemma 4 and Theorem 14). Note that if f is a continuous convex function, then there exists an affine function l such that $f \ge l$. In particular, $\tau(f(a))$ is well-defined for $a \in L^1(\mathcal{M}, \tau)$ if τ is finite.

Proposition 4.1. Assume that τ is finite. If $f : [0,\infty) \longrightarrow \mathbb{R}$ is a continuous convex (resp. monotone) function, then the trace functional

$$L^1_+(\mathcal{M},\tau) \longrightarrow (-\infty,\infty], a \mapsto \tau(f(a))$$

is convex (resp. monotone).

Next we turn to lower semicontinuity. The proof of the following proposition adapts the proof strategy for the lower semicontinuity of integral functionals in the commutative case (see for example [But89, Theorem 3.4.1]).

Proposition 4.2 (Lower semicontinuity of convex trace functionals). Assume that τ is finite. If $f: I \longrightarrow \mathbb{R}$ is a continuous convex function, then

$$F: L^{1}(\mathcal{M}, \tau)_{I} \longrightarrow (-\infty, \infty], a \mapsto \tau(f(a))$$

is weakly lower semicontinuous.

Proof. Since f is continuous and convex, by [Roc97, Theorem 12.1] there is a sequence (f_i) of affine functions such that $f = \sup_i f_i$. Fix $n \in \mathbb{N}$. For $j \in \{1, ..., n\}$ let

$$E_{j} = \{t \in I \mid \max_{1 \le i < j} f_{i}(t) < f_{j}(t), \max_{j < i \le n} f_{i}(t) \le f_{j}(t)\}.$$

In particular, $f_j(t) = \max_{1 \le i \le n} f_i(t)$ for $t \in E_j$, and $I = \bigsqcup_j E_j$.

Let (a_k) be a sequence in $L^1(\mathcal{M}, \tau)_I$ converging weakly to $a \in L^1(\mathcal{M}, \tau)_I$. In particular, $f_j(a_k) \to f_j(a)$ weakly for all $j \in \mathbb{N}$.

Hence

$$\begin{split} \liminf_{k \to \infty} \tau(f(a_k)) &= \liminf_{k \to \infty} \sum_{j=1}^n \tau(\mathbb{1}_{E_j}(a)f(a_k)) \\ &\geq \liminf_{k \to \infty} \sum_{j=1}^n \tau(\mathbb{1}_{E_j}(a)f_j(a_k)) \\ &= \sum_{j=1}^n \tau(\mathbb{1}_{E_j}(a)f_j(a)) \\ &= \sum_{j=1}^n \tau\left(\mathbb{1}_{E_j}(a)\max_{1 \le i \le n} f_i(a)\right) \\ &= \tau\left(\max_{1 \le i \le n} f_i(a)\right). \end{split}$$

Since $f_1(a)$ is integrable, $\tau(\max_{1 \le i \le n} f_i(a)) \nearrow \tau(f(a))$. This proves the claim. \Box

Now we turn to differentiability. We begin with an auxiliary lemma.

Lemma 4.3. Assume that τ is finite. Let $(a_t)_{t \in I}$ be an L^1 -differentiable curve in $L^1_h(\mathcal{M}, \tau)$. Assume that there exists R > 0 such that $||a_t||_{\mathcal{M}} < R$ for all $t \in I$. If $f \in C^1((-R, R))$, then the map

$$F: I \longrightarrow \mathbb{R}, t \mapsto \tau(f(a_t))$$

is differentiable with derivative $F'(t) = \tau(f'(a_t)\dot{a}_t)$.

Proof. By approximation in C^1 we can assume that f is a polynomial, and by linearity, even that f is a monomial. Observe that

$$\tau(x^{k+1} - y^{k+1}) = \tau\left(\left(\sum_{j=0}^{k} x^{k-j} y^j\right)(x - y)\right)$$

for all $x, y \in \mathcal{M}$ and $k \ge 0$ (of course it is crucial here that τ is a trace). Thus

$$\frac{1}{h}\tau(a_{t+h}^{k+1}-a_t^{k+1}) = \sum_{j=0}^k \tau\left(a_{t+h}^{k-j}a_t^j\left(\frac{a_{t+h}-a_t}{h}\right)\right).$$

Since (ρ_t) is uniformly bounded and L^1 -continuous, we have $|\rho_{t+h}^j - \rho_t^j| \to 0$ as $h \to 0$ in L^1 and, by a standard approximation argument, also σ -weakly. Hence

$$\begin{aligned} \left| \tau \left(a_{t+h}^{k-j} a_t^j \left(\frac{a_{t+h} - a_t}{h} \right) - a_t^k \dot{a}_t \right) \right| &\leq \left| \tau \left(a_{t+h}^{k-j} a_t^j \left(\frac{a_{t+h} - a_t}{h} - \dot{a}_t \right) \right) \right| \\ &+ \left| \tau ((a_{t+h}^{k-j} - a_t^{k-j}) a_t^j \dot{a}_t) \right| \\ &\leq R^k \tau \left(\left| \frac{a_{t+h} - a_t}{h} - \dot{a}_t \right| \right) \\ &+ \left| \tau ((a_{t+h}^{k-j} - a_t^{k-j}) a_t^j \dot{a}_t) \right| \\ &\to 0, h \to 0. \end{aligned}$$

All put together, we have proven that

$$\frac{1}{h}(F(t+h) - F(t)) = \frac{1}{h}\tau(a_{t+h}^{k+1} - a_t^{k+1}) \to \tau((k+1)a_t^k \dot{a}_t)$$

as $h \rightarrow 0$.

Lemma 4.4 (Klein's inequality). Assume that τ is finite. Let $f : [0,\infty) \longrightarrow \mathbb{R}$ be a convex C^1 Lipschitz function. If $a_0, a_1 \in L^1_+(\mathcal{M}, \tau)$, then $f(a_0), f(a_1) \in L^1(\mathcal{M}, \tau)$ and

$$\tau(f(a_1) - f(a_0)) \le \tau(f'(a_1)(a_1 - a_0)).$$

Proof. If $a_0, a_1 \in L^1_+(\mathcal{M}, \tau) \cap \mathcal{M}$, we can adapt the proof of the finite-dimensional case (see [Car10, Theorem 2.11]): Let

$$\varphi \colon [0,1] \longrightarrow \mathbb{R}, t \mapsto \tau(f(ta_0 + (1-t)a_1)).$$

By Lemma 4.3 the map φ is differentiable with derivative

$$\varphi'(t) = \tau(f'(ta_0 + (1-t)a_1)(a_0 - a_1)).$$

Moreover, φ is convex by Proposition 4.1. Hence

$$\varphi(1) - \varphi(0) \ge \frac{\varphi(t) - \varphi(0)}{t}$$

Letting $t \searrow 0$ yields the desired inequality.

Now let $a_0, a_1 \in L^1_+(\mathcal{M}, \tau)$ be arbitrary. We already know that the inequality holds for a_0, a_1 replaced by $a_0 \wedge n$, $a_1 \wedge n$. It remains to show that both sides converge to the correct limit as $n \to \infty$.

Since f' is bounded and increasing, $||f'(a_1 \wedge n)||_{\mathscr{M}} \leq ||f'||_{\infty}$ for all $n \in \mathbb{N}$ and $f'(a_1 \wedge n) \to f'(a_1)$ σ -weakly as $n \to \infty$. It is elementary that $a_0 \wedge n \to \rho_0$ and $a_1 \wedge n \to a_1$ in L^1 . Put together, we get

$$\tau(f'(a_1 \wedge n)(a_1 \wedge n - a_0 \wedge n)) \to \tau(f'(a_1)(a_1 - a_0)).$$

For the left-hand side it suffices to note that the operator map $a \mapsto f(a)$ is continuous in the strong L^1 -topology by Proposition B.7.

As a corollary we obtain a partial generalization of Lemma 4.3 for trace functionals induced by convex functions.

Lemma 4.5. Assume that τ is finite. If $f: [0,\infty) \longrightarrow \mathbb{R}$ is a convex C^1 Lipschitz function and $(a_t)_{t \in I}$ is a (locally) absolutely continuous curve in $L^1_+(\mathcal{M},\tau)$, then $(\tau(f(a_t)))_{t \in I}$ is (locally) absolutely continuous and

$$\frac{d}{dt}\tau(f(a_t)) = \tau(f'(a_t)\dot{a}_t)$$

for a.e. $t \in I$.

Proof. By Klein's inequality we have

$$\tau(f'(a_s)(a_t - a_s)) \le \tau(f(a_t) - f(a_s)) \le \tau(f'(a_t)(a_t - a_s))$$

for all $s, t \in I$. Thus

$$|\tau(f(a_t) - f(a_s))| \le ||f'||_{\infty} ||a_t - a_s||_1.$$

Since $(a_t)_{t \in I}$ is (locally) absolutely continuous, so is $(\tau(f(a_t)))_{t \in I}$.

Now assume that $t \in I$ is a point of differentiability for both the curves $(a_t)_{t \in I}$ and $(\tau(f(a_t)))_{t \in I}$. By Klein's inequality,

$$\frac{d}{dt}\tau(f(a_t)) = \lim_{s \neq t} \frac{1}{t-s}\tau(f(a_t) - f(a_s)) \le \lim_{s \neq t}\tau\left(f'(a_t)\frac{a_t - a_s}{t-s}\right) = \tau(f'(a_t)\dot{a}_t),$$

and

$$\frac{d}{dt}\tau(f(a_t)) = \lim_{s \searrow t} \frac{1}{t-s}\tau(f(a_t) - f(a_s)) \ge \lim_{s \nearrow t}\tau\left(f'(\rho_t)\frac{a_t - a_s}{t-s}\right) = \tau(f'(a_t)\dot{a}_t).$$

This settles the claim.

The same argument shows that (local) Lipschitz continuity of the curve (a_t) implies (local) Lipschitz continuity $t \mapsto \tau(f(a_t))$.

Remark 4.6. The related question of Lipschitz continuity of the operator function $a \mapsto f(a)$ on $L^p(\mathcal{M}, \tau)$ has been addressed in a series of articles (see for example [dPWS02, dPS04, PS08, PS11]). Notably, if 1 , then Lipschitz continuity of the scalar function <math>f is equivalent to Lipschitz continuity of the operator function $a \mapsto f(a)$ on L^p , at least for the classical Schatten classes (see [PS11, Theorem 1]). In contrast, the absolute value is in general neither Lipschitz on L^1 [Dav88, Corollary 11] nor on \mathcal{M} [Kat73].

4.2 Entropy

After the discussion of general trace functionals in the last section, we focus now on the special case $f(\lambda) = \lambda \log \lambda$.

Definition 4.7 (Von Neumann entropy). The von Neumann entropy is defined as

Ent:
$$\mathscr{D}(\mathscr{M},\tau) \longrightarrow [-\infty,\infty], \operatorname{Ent}(\rho) = \begin{cases} \tau(\rho \log \rho) & \text{if } (\rho \log \rho)_+ \in L^1(\mathscr{M},\tau), \\ \infty & \text{otherwise.} \end{cases}$$

Its domain of definition is $D(\text{Ent}) = \{\rho \in \mathcal{D}(\mathcal{M}, \tau) \mid \text{Ent}(\rho) \in \mathbb{R}\}$. Here and in the following, the expression $\rho \log \rho$ is to be understood as $f(\rho)$ for the (continuous) function

$$f: [0,\infty) \longrightarrow \mathbb{R}, \lambda \mapsto \begin{cases} \lambda \log \lambda & \text{if } \lambda > 0, \\ 0 & \text{if } \lambda = 0. \end{cases}$$

Remark 4.8. Since $f : \lambda \mapsto \lambda \log \lambda$ is convex, the von Neumann entropy is a convex functional by Proposition 4.1. In fact, f is even operator convex [Car10, Theorem 2.6].

Remark 4.9. If τ is a state, an application of Jensen's inequality shows that $\text{Ent} \ge 0$. Furthermore, Ent is lower semicontinuous in this case by Proposition 4.2. In contrast, if $\tau(1) = \infty$, the entropy can be rather ill-behaved already in the commutative case (see e.g. [Stu06a, Example 4.4]). For that reason, we will from now on concentrate on the finite case. However, we believe that this assumption is not essential and that similar modifications as in [AGS14a] should also work in our setting.

Remark 4.10. Some authors, especially in the physics community, define the entropy with the opposite sign. We choose the sign in such a way that the entropy is positive if τ is a state and the semigroup (P_t) is a gradient flow of Ent instead of –Ent.

As discussed above, the entropy is lower semicontinuous with respect to the weak L^1 topology if τ is a state. We will later also need lower semicontinuity with respect to the topology induced by \mathcal{W} . To prove it, we first establish a variational formulation of the entropy. In the noncommutative case, it is (along with the idea of the proof presented here) originally due to Petz [Pet88]. We just adapt it to be applicable in duality with \mathcal{A}_{AM} instead of \mathcal{M} .

Proposition 4.11 (Variational formula for the entropy). Assume that τ is a state. If \mathscr{A} is a σ -weakly dense *-subalgebra of \mathscr{M} , then

$$\operatorname{Ent}(\rho) = \sup\{\tau(a\rho) - \log\tau(e^a) \mid a \in \mathcal{A}_+\}$$

for all $\rho \in \mathcal{D}(\mathcal{M}, \tau)$.

Proof. Step 1: The inequality

$$\operatorname{Ent}(\rho) \ge \sup \tau(a\rho) - \log \tau(e^a) \mid a \in \mathcal{M}_+ \}$$

holds for invertible $\rho \in \mathcal{D}(\mathcal{M}, \tau)$.

Let $x = \log(\rho \wedge n)$, $y = a - \log \tau(e^a)$ with $a \in \mathcal{M}_+$. By Klein's inequality (Lemma 4.4) we have

$$\begin{aligned} 0 &\leq \tau(e^{y} - e^{x} - e^{x}(y - x)) \\ &= \tau \left(\frac{e^{a}}{\tau(e^{a})} - \rho \wedge n - (\rho \wedge n)(a - \log \tau(e^{a}) - \log(\rho \wedge n)) \right) \\ &= \tau((\rho \wedge n)\log(\rho \wedge n)) - (\tau(a(\rho \wedge n)) - \log \tau(e^{a})) + 1 - \tau(\rho \wedge n)) \end{aligned}$$

By monotone convergence we obtain

$$0 \le \tau(\rho \log \rho) - \tau(a\rho) - \log \tau(e^a).$$

Step 2: The equality

$$\operatorname{Ent}(\rho) = \sup\{\tau(a\rho) - \log\tau(e^a) \mid a \in \mathcal{M}_+\}$$

holds for all $\rho \in \mathcal{D}(\mathcal{M}, \tau)$.

Let $\rho_n = (1 + 1/n)^{-1}(\rho + 1/n) \in \mathcal{D}(\mathcal{M}, \tau)$. By convexity and Step 1 we have

$$\operatorname{Ent}(\rho) \ge \frac{n+1}{n} \operatorname{Ent}(\rho_n) \ge \frac{n+1}{n} (\tau(a\rho_n) - \log \tau(e^a)) \to \tau(a\rho) - \log \tau(e^a)$$

for $a \in \mathcal{M}_+$.

For the converse inequality first let $a_n = \log(n+1)\rho_n$. This operator is positive, but not necessarily bounded. We have

$$\liminf_{n \to \infty} (\tau(a_n \rho_n) - \log \tau(e^{a_n})) = \liminf_{n \to \infty} (\log(n+1) + \tau(\rho_n \log \rho_n) - \log(n+1)) \ge \operatorname{Ent}(\rho),$$

where the last inequality follows from the lower semicontinuity of Ent.

To see that one can take the supremum over $a \in \mathcal{M}_+$, it suffices to notice that $\tau((a \wedge m)\rho) \rightarrow \tau(a\rho)$ and $\tau(e^{a \wedge m}) \rightarrow \tau(e^a)$ as $m \rightarrow \infty$.

Step 3: The equality

$$\operatorname{Ent}(\rho) = \sup\{\tau(a\rho) - \log\tau(e^a) \mid a \in \mathcal{A}_+\}$$

holds for all $\rho \in \mathcal{D}(\mathcal{M}, \tau)$.

Let $a \in \mathcal{M}_+$. Since $\mathcal{A} \subset \mathcal{M}$ is σ -weakly dense, the unit ball of \mathcal{A} is strongly dense in the unit ball of \mathcal{M} by the Kaplansky density theorem (see Theorem B.11). Thus there is a net (a_i) in \mathcal{A}_+ with $||a_i||_{\mathcal{M}} \leq ||a||_{\mathcal{M}}$ such that $a_i \to a$ strongly. By the continuity of the functional calculus, (e^{a_i}) converges strongly to e^a .

Thus

$$\sup\{\tau(a\rho) - \log\tau(e^{a}) \mid a \in \mathcal{A}_{+}\} = \sup\{\tau(a\rho) - \log\tau(e^{a}) \mid a \in \mathcal{M}_{+}\}$$

and the claimed equality follows from Step 2.

For the next corollary recall that a convex function is called *proper* if it is not identically ∞ .

Corollary 4.12. If τ is a state and $\mathscr{A}_{AM} \subset \mathscr{M}$ is σ -weakly dense, then Ent is a proper lower semicontinuous convex functional on $(\mathscr{D}(\mathscr{M},\tau),\mathscr{W})$.

Proof. Let (ρ_n) be a sequence in $\mathscr{D}(\mathscr{M}, \tau)$ such that $\mathscr{W}(\rho_n, \rho) \to 0$. It follows from Proposition 3.20 that $\tau(a\rho_n) \to \tau(a\rho)$ for all $a \in \mathscr{A}_{AM}$.

Combined with Proposition 4.11 we infer that Ent is the supremum of affine, continuous functions on $(\mathcal{D}(\mathcal{M},\tau),\mathcal{W})$, hence lower semicontinuous and convex. Since Ent(1) = 0, the entropy is also proper.

4.3 Lipschitz functions operating on Dirichlet forms

Since \mathscr{E} is a quantum Dirichlet form, 1-Lipschitz functions C with C(0) = 0 operate on the quadratic form \mathscr{E} in the sense that $\mathscr{E}(C(a)) \leq \mathscr{E}(a)$. In this short section we collect some results for Lipschitz functions operating on the bilinear form \mathscr{E} , that is, estimates for $\mathscr{E}(C_1(a), C_2(a))$. These results will be useful in the next section for a rigorous definition of the Fisher information.

Lemma 4.13. If $a \in D(\mathcal{E})_h$ and $C_1, C_2 : \mathbb{R} \longrightarrow \mathbb{R}$ are increasing Lipschitz functions with $C_1(0) = C_2(0) = 0$, then

$$\mathscr{E}(C_1(a), C_2(a)) \ge 0.$$

Proof. Since $C_1(s) - C_1(t)$ and $C_2(s) - C_2(t)$ have the same sign,

$$|(C_1(s) - C_2(s)) - (C_1(t) - C_2(t))| \le |(C_1(s) + C_1(t)) - (C_2(s) + C_2(t))|$$

for all $s, t \in \mathbb{R}$. Hence there exists a 1-Lipschitz function $C : \mathbb{R} \longrightarrow \mathbb{R}$ with C(0) = 0 such that $C \circ (C_1 + C_2) = C_1 - C_2$. Thus

$$\mathscr{E}(C_1(a), C_2(a)) = \frac{1}{4} (\mathscr{E}(C_1(a) + C_2(a)) - \mathscr{E}(C_1(a) - C_2(a))) \ge 0.$$

Remark 4.14. If C_1, C_2 in the previous lemma are continuously differentiable, we can also use the chain rule to get

$$\mathscr{E}(C_1(a), C_2(a)) = \langle (\tilde{C}_1 \tilde{C}_2)(L(a), R(a))\partial a, \partial a \rangle_{\mathscr{H}} \ge 0.$$

Remark 4.15. The short proof of Lemma 4.13 was suggested to us by S. Puchert, replacing a quite involved proof arguing by approximation of \mathscr{E} .

Corollary 4.16. Let $C, C_1, C_2 : \mathbb{R} \longrightarrow \mathbb{R}$ be increasing Lipschitz functions satisfying $C(0) = C_1(0) = C_2(0) = 0$ and $|C_1(s) - C_1(t)| \le |C_2(s) - C_2(t)|$ for all $s, t \in \mathbb{R}$. Then

$$\mathscr{E}(C(a), C_1(a)) \le \mathscr{E}(C(a), C_2(a))$$

for all $a \in D(\mathcal{E})_h$.

Lemma 4.17. Let \mathscr{E} be a quantum Dirichlet form on $L^2(\mathcal{M}, \tau)$, denote by $\mathscr{L}^{(p)}$ the generator of the associated semigroup on $L^p(\mathcal{M}, \tau)$ for $p \in [1, \infty)$, and let $a \in D(\mathscr{L}^{(p)})$.

If $C_1, C_2: \mathbb{R} \longrightarrow \mathbb{R}$ are increasing 1-Lipschitz functions and there exists a constant $\alpha > 0$ such that $|C_i(t)| \le \alpha |t|^{p-1}$ for $t \in \mathbb{R}$, $i \in \{1,2\}$, then $C_1(\alpha), C_2(\alpha) \in D(\mathscr{E})$ and

$$\mathscr{E}(C_1(a), C_2(a)) \leq \tau(C_1(a)\mathscr{L}^{(p)}a).$$

Proof. First note that $C_i(a) \in L^p(\mathcal{M}, \tau) \cap L^q(\mathcal{M}, \tau) \subset L^2(\mathcal{M}, \tau)$, where q is the dual exponent of p. To prove $C_i(a) \in D(\mathcal{E})$, it suffices to show

$$\frac{1}{t}\tau(C_i(a)(C_i(a) - P_tC_i(a)) \le \frac{1}{t}\tau(C_i(a)(a - P_ta))$$
(4.1)

for t > 0, since the right-hand side converges to $\tau(C_i(a)\mathcal{L}^{(p)}a)$ as $t \to 0$.

Since the approximating form

$$\mathscr{E}_t \colon L^2(\mathscr{M}, \tau) \longrightarrow [0, \infty), x \mapsto \frac{1}{t} \tau(x(x - P_t x))$$

is a quantum Dirichlet form, Equation (4.1) holds for $a \in L^2(\mathcal{M}, \tau)$ by Corollary 4.16.

To prove (4.1) for arbitrary $a \in L^p(\mathcal{M}, \tau)$, let (a_k) be a sequence in $L^2(\mathcal{M}, \tau) \cap L^p(\mathcal{M}, \tau)$ such that $a_k \to a$ in $L^p(\mathcal{M}, \tau)$. By [Tik87, Theorem 3.2] we have $C_i(a_k) \to C_i(a)$ with respect to $\|\cdot\|_p$ and $\|\cdot\|_q$ (resp. σ -weakly in the case p = 1). Using the continuity of P_t with respect to $\|\cdot\|_p$ and $\|\cdot\|_q$ (and additionally the bound $\|C_i(a_k)\|_{\mathcal{M}} \leq \|C_i\|_{\infty}$ in the case p = 1), we see that (4.1) continues to hold for arbitrary $a \in L^p(\mathcal{M}, \tau)$.

Finally, by Corollary 4.16 and the same approximation argument as above, we obtain

$$\frac{1}{t}\tau(C_1(a)(C_2(a) - P_tC_2(a))) \le \frac{1}{t}\tau(C_1(a)(a - P_ta)),$$

which gives

$$\mathscr{E}(C_1(a), C_2(a)) \le \tau(C_1(a)\mathscr{L}^{(p)}a)$$

in the limit $t \rightarrow 0$.

4.4 Fisher information

In this section we give a rigorous definition of the Fisher information in our setting and discuss some first connections between Fisher information, entropy and the transport metric W.

Lemma 4.18. Let (C_n) be a sequence of continuously differentiable, increasing Lipschitz functions on $[0,\infty)$ with $C_n(0) = 0$ and

$$\widetilde{C}_n(s,t) \nearrow \widetilde{\log}(s,t)$$

for all $s,t \ge 0$ (with the convention that the right-hand side equals ∞ whenever s = 0 or t = 0).

Then $\lim_{n\to\infty} \mathscr{E}(a, C_n(a))$ exists in $[0,\infty]$ for all $a \in D(\mathscr{E})_+$ and is independent from the choice of the sequence (C_n) .

Proof. We use the chain rule to get

$$\mathscr{E}(a, C_n(a)) = \langle \tilde{C}_n(L(a), R(a)) \partial a, \partial a \rangle_{\mathscr{H}}.$$

Denote by *e* the joint spectral measure of L(a) and R(a). Then

$$\begin{split} \langle \tilde{C}_n(L(a), R(a))\partial a, \partial a \rangle_{\mathscr{H}} &= \int_{[0,\infty)^2} \tilde{C}_n(s,t) d \langle e(s,t)\partial a, \partial a \rangle_{\mathscr{H}} \\ & \swarrow \int_{[0,\infty)^2} \widetilde{\log}(s,t) d \langle e(s,t)\partial a, \partial a \rangle_{\mathscr{H}} \end{split}$$

where the integrand is interpreted as ∞ whenever s = 0 or t = 0.

Definition 4.19 (Fisher information). The *Fisher information* of $a \in D(\mathcal{E})_+$ is defined as

$$\mathscr{I}(a) = \lim_{n \to \infty} \mathscr{E}(a, C_n(a)) \in [0, \infty]$$

for some (any) sequence (C_n) of continuously differentiable, increasing normal contractions with $\tilde{C}_n \nearrow \log$ pointwise.

An example of a sequence (C_n) that is admissible in the definition of the Fisher information is given by

$$C_n: [0,\infty) \longrightarrow [0,\infty), C_n(t) = \log(t+e^{-n})+n.$$

We will also need the following two different approximation results of the Fisher information:

Lemma 4.20. If $a \in D(\mathcal{E})_+$ with $\mathcal{I}(a) < \infty$, then

$$\mathscr{I}(a) = \lim_{n \to \infty} \mathscr{E}(a, ((\log \wedge n) \lor (-n) + n)(a)).$$

Proof. Let $f_n = (\log \wedge n) \vee (-n) + n$. By Corollary 4.16, the sequence $(\mathscr{E}(a, f_n(a)))_n$ is increasing, hence it suffices to show convergence along a subsequence. Let

$$C_k: [0,\infty) \longrightarrow [0,\infty), C_k(t) = \log(t+e^{-k}) + k$$

and $n_k \in \mathbb{N}$ such that $\mathscr{E}((C_k(a) \land n_k) \lor (-n_k)) \ge \mathscr{E}(C_k(a)) - \frac{1}{k}$. Then

$$\mathscr{E}(a, (C_k(a) \land n_k) \lor (-n_k)) \to \mathscr{I}(a), k \to \infty,$$

and

$$|(C_k(s) \land n_k) \lor (-n_k) - (C_k(t) \land n_k) \lor (-n_k)| \le |f_{n_k}(s) - f_{n_k}(t)| \le |\log s - \log t|.$$

An application of Corollary 4.16 yields

$$\mathscr{E}(a, f_{n_k}(a)) \to \mathscr{I}(a), k \to \infty.$$

Lemma 4.21. Let $a \in D(\mathcal{E})_+$. Then $\mathcal{I}(a) = \sup_n \mathcal{I}(a \wedge n)$.

Proof. By Corollary 4.16, the sequence $(\mathscr{I}(a \wedge n))_n$ is increasing and bounded from above by $\mathscr{I}(a)$. For the converse inequality let (C_m) be a sequence as in the definition of \mathscr{I} .

Since $C_m(a) = \lim_{n \to \infty} C_m(a \wedge n)$ in $L^2(\mathcal{M}, \tau)$ and $\mathscr{E}(C_m(a \wedge n)) \leq \mathscr{E}(C_m(a))$ by Corollary 4.16, we have $\mathscr{E}(C_m(a \wedge n)) \to \mathscr{E}(C_m(a))$ as $n \to \infty$ by the lower semicontinuity of \mathscr{E} . The same argument holds for $\mathscr{E}(a \wedge n)$ so that we get

$$\mathscr{I}(a) \ge \mathscr{I}(a \land n) \ge \mathscr{E}(a \land n, C_m(a \land n)) \to \mathscr{E}(a, C_m(a))$$

Taking the supremum over $m \in \mathbb{N}$, the assertion follows.

With the aid of the previous lemma, we can extend the Fisher information to $L^1_+(\mathcal{M},\tau)$ via $\mathscr{I}(\rho) = \sup_n \mathscr{I}(\rho \wedge n)$ if $\rho \wedge n \in D(\mathscr{E})_+$ for all $n \in \mathbb{N}$ and $\mathscr{I}(\rho) = \infty$ otherwise.

Lemma 4.22. The Fisher information is lower semicontinuous on $L^1_+(\mathcal{M},\tau)$.

Proof. By monotone approximation it suffices to show that maps of the form

$$L^{1}_{+}(\mathcal{M},\tau) \longrightarrow [0,\infty), \rho \mapsto \begin{cases} \mathscr{E}(\rho \wedge n, C(\rho \wedge n)) & \text{if } \rho \wedge n \in D(\mathscr{E}), \\ \infty & \text{otherwise} \end{cases}$$

are continuous for $n \in \mathbb{N}$ and $C \in C^1(\mathbb{R})$ with C' > 0.

Let (ρ_k) be a sequence in $L^1_+(\mathcal{M}, \tau)$ that converges to ρ in $L^1(\mathcal{M}, \tau)$ and satisfies $\sup_k \mathscr{E}(\rho_k \wedge n, C(\rho_k \wedge n)) < \infty$. By [Tik87, Theorem 3.2] we have $\rho_k \wedge n \to \rho \wedge n$ in $L^1(\mathcal{M}, \tau)$ and $L^2(\mathcal{M}, \tau)$. Moreover, since C' > 0, the sequence $(\mathscr{E}(\rho_k \wedge n))_k$ is bounded. Thus $\rho \wedge n \in D(\mathscr{E})$ and $\rho_k \wedge n \to \rho \wedge n$ weakly in $D(\mathscr{E})$.

By Lemma 2.13 we have $\tilde{C}(L(\rho_k \wedge n), R(\rho_k \wedge n)) \rightarrow \tilde{C}(L(\rho \wedge n), R(\rho \wedge n))$ strongly as $k \rightarrow \infty$. If we combine these convergences, we obtain

$$\begin{aligned} \mathscr{E}(\rho_k \wedge n, C(\rho_k \wedge n)) &= \langle \partial(\rho_k \wedge n), C(L(\rho_k \wedge n), R(\rho_k \wedge n)) \partial(\rho_k \wedge n) \rangle_{\mathscr{H}} \\ &\to \langle \partial(\rho \wedge n), \tilde{C}(L(\rho \wedge n), R(\rho \wedge n)) \partial(\rho \wedge n) \rangle_{\mathscr{H}} \\ &= \mathscr{E}(\rho \wedge n, C(\rho \wedge n)). \end{aligned}$$

Proposition 4.23. The Fisher information is convex and weakly lower semicontinuous on $L^1_+(\mathcal{M}, \tau)$.

Proof. For the convexity it suffices to show that \mathscr{I} is convex on $D(\mathscr{E})_+ \cap \mathscr{M}$. Indeed, if $\rho_0, \rho_1 \in L^1_+(\mathscr{M}, \tau)$ and $\lambda \in [0, 1]$, then

$$\mathscr{I}((1-\lambda)\rho_0 + \lambda\rho_1) \leq \liminf_{n \to \infty} \mathscr{I}((1-\lambda)(\rho_0 \wedge n) + \lambda(\rho_1 \wedge n))$$

by the lower semicontinuity of \mathcal{I} , and

$$(1-\lambda)\mathscr{I}(\rho_0 \wedge n) + \lambda\mathscr{I}(\rho_1 \wedge n) \leq (1-\lambda)\mathscr{I}(\rho_0) + \lambda\mathscr{I}(\rho_1)$$

by definition.

To prove convexity on $D(\mathscr{E})_+ \cap \mathscr{M}$ let

$$C_k: [0,\infty) \longrightarrow [0,\infty), t \mapsto \log(t+e^{-n})+n$$

and let $\mathscr{E}_{\varepsilon}$ be the quadratic form generated by $\mathscr{L}(1 + \varepsilon \mathscr{L})^{-1}$. Since

$$\mathcal{I}(a) = \lim_{k \to \infty} \lim_{\varepsilon \to 0} \mathcal{E}_{\varepsilon}(a, C_k(a))$$

4.4. FISHER INFORMATION

for $a \in D(\mathcal{E})_+ \cap \mathcal{M}$, it is sufficient to prove that $a \mapsto \mathcal{E}_{\varepsilon}(a, C_k(a))$ is convex for all $\varepsilon > 0$ and $k \in \mathbb{N}$.

Let $(\mathcal{H}_{\varepsilon}, \partial_{\varepsilon}, L_{\varepsilon}, R_{\varepsilon}, J_{\varepsilon})$ be the first-order differential calculus associated with $\mathscr{E}_{\varepsilon}$. By [CS03, Section 10.3] there exists $\eta_{\varepsilon} \in \mathcal{H}_{\varepsilon}$ such that $\partial_{\varepsilon}a = (L_{\varepsilon}(a) - R_{\varepsilon}(a))\eta_{\varepsilon}$ for all $a \in D(\mathscr{E})_{+} \cap \mathcal{M}$. Thus

$$\mathscr{E}_{\varepsilon}(a, C_k(a)) = \langle (L_{\varepsilon}(a) - R_{\varepsilon}(a))\eta_{\varepsilon}, (C_k(L_{\varepsilon}(a)) - C_k(R_{\varepsilon}(a)))\eta_{\varepsilon} \rangle_{\mathscr{H}_{\varepsilon}}.$$

For $\alpha > 0$ let

$$\Phi_{\alpha} \colon (0,\infty)^2 \longrightarrow \mathbb{R}, (s,t) \mapsto \frac{s^{\alpha+1}t^{-\alpha} + t - s^{\alpha}t^{1-\alpha} - s}{\alpha}$$

Note that $\Phi_{\alpha}(s,t) \rightarrow (s-t)(\log s - \log t)$ as $\alpha \searrow 0$. By dominated convergence we have

$$\Phi_{\alpha}(L_{\varepsilon}(a) + e^{-k}, R_{\varepsilon}(a) + e^{-k}) \to (L_{\varepsilon}(a) - R_{\varepsilon}(a))(C_{k}(L_{\varepsilon}(a)) - C_{k}(R_{\varepsilon}(a))).$$

as $\alpha \searrow 0$ in the weak operator topology. Hence it suffices to show that

$$D(\mathscr{E})_{+} \cap \mathscr{M} \longrightarrow \mathscr{L}(\mathscr{H}), a \mapsto \Phi_{\alpha}(L_{\varepsilon}(a) + e^{-k}, R_{\varepsilon}(a) + e^{-k})$$

is convex for all $k \in \mathbb{N}$ and $\alpha, \varepsilon > 0$.

Let $l(a) = L_{\varepsilon}(a) + e^{-k}$ and $r(a) = R_{\varepsilon}(a) + e^{-k}$. Since the images of L_{ε} and R_{ε} commute, we have

$$\Phi_{\alpha}(l(a), r(a)) = \frac{1}{\alpha}(l(a)(l(a)\#_{\alpha}r(a))^{-1}l(a) + r(a) - r(a)\#_{\alpha}l(a) - l(a)),$$

where $\#_{\alpha}$ is the operator mean with generating function $t \mapsto t^{\alpha}$. In particular, $\#_{\alpha}$ is jointly operator concave. Together with the joint operator convexity of the map $(x, y) \mapsto yx^{-1}y$ this implies the convexity of $a \mapsto l(a)(l(a)\#_{\alpha}r(a))^{-1}l(a)$. Hence $a \mapsto \Phi_{\alpha}(l(a), r(a))$ is convex as the sum of convex maps.

Finally, the weak lower semicontinuity follows from the convexity and the strong lower semicontinuity by the Hahn-Banach theorem. $\hfill \Box$

Now we turn to the connections of the Fisher information to quantities introduced in the previous section. Recall that we assume that is θ the logarithmic mean in this section.

Proposition 4.24. If $\rho \in \mathcal{D}(\mathcal{M}, \tau) \cap L^2(\mathcal{M}, \tau)$ and

$$\int_s^t \mathcal{I}(P_r\rho) dr < \infty$$

for all s, t > 0, then the curve $(P_t \rho)_{t>0}$ is admissible and

$$\|D(P_t\rho)\|_{P_t\rho}^2 \le \mathscr{I}(P_t\rho).$$

Proof. Let

$$C_n: (e^{-n}, \infty) \longrightarrow [0, \infty), t \mapsto \log(t + e^{-n}) + n.$$

Let $\rho_t = P_t \rho$ and $\xi_t^n = -\partial(C_n(\rho_t))$. Since $\rho \in L^2(\mathcal{M}, \tau)$, we have $\rho_t \in D(\mathcal{L})$. As C_n is continuously differentiable on a neighborhood of $\sigma(\rho_t)$, we have $\partial(C_n(\rho_t)) = \tilde{C}_n(L(\rho_t), R(\rho_t))\partial\rho_t$.

Denote by *e* the joint spectral measure of $L(\rho_t)$ and $R(\rho_t)$. An application of $0 \le \tilde{C}_n \cdot LM \le 1$ gives

$$\begin{split} \|\xi_t^n\|_{\rho_t}^2 &= \|(\mathbf{L}\mathbf{M}^{1/2}\tilde{C}_n)(L(\rho_t), R(\rho_t))\partial\rho_t\|_{\mathcal{H}}^2 \\ &= \int_{[0,\infty)^2} \mathbf{L}\mathbf{M}(s,t)\tilde{C}_n(s,t)^2 d\langle e(s,t)\partial\rho_t, \partial\rho_t\rangle_{\mathcal{H}} \\ &\leq \int_{[0,\infty)^2} \tilde{C}_n(s,t) d\langle e(s,t)\partial\rho_t, \partial\rho_t\rangle_{\mathcal{H}} \\ &= \mathcal{E}(\rho_t, C_n(\rho_t)) \\ &\leq \mathcal{I}(\rho_t). \end{split}$$

On the other hand, $\tilde{C}_n LM \nearrow 1$ implies

$$\begin{split} \langle \xi_t^n, \partial a \rangle_{\rho_t} &= -\int_{[0,\infty)^2} \tilde{C}_n(s,t) \mathrm{LM}(s,t) \, d \, \langle e(s,t) \partial \rho_t, \partial a \rangle_{\mathcal{H}} \\ &\to - \langle \partial \rho_t, \partial a \rangle_{\mathcal{H}} \\ &= \langle -\mathcal{L} \rho_t, a \rangle_{L^2(\mathcal{M},\tau)} \\ &= \tau(a \dot{\rho}_t) \end{split}$$

for all $a \in \mathcal{A}_{AM}$.

Let $\tilde{\xi}_t^n$ be the projection of ξ_t^n onto \mathscr{H}_{ρ_t} . From the computations above we conclude that $(\tilde{\xi}_t^n)_n$ converges weakly to some $\xi_t \in \mathscr{H}_{\rho_t}$ with $\|\xi_t\|_{\rho_t}^2 \leq \mathscr{I}(\rho_t)$ for a.e. t > 0 and

$$\langle \xi_t, \partial a \rangle_{\rho_t} = \tau(a\dot{\rho}_t)$$

for all $a \in \mathscr{A}_{AM}$.

Proposition 4.25 (Fisher information equals entropy dissipation). Assume that τ is finite. If $\rho \in \mathcal{D}(\mathcal{M}, \tau) \cap L^2(\mathcal{M}, \tau)$, then

$$\operatorname{Ent}(\rho) - \operatorname{Ent}(P_t \rho) = \int_0^t \mathscr{I}(P_s \rho) ds$$

for all $t \ge 0$. In particular, Ent is decreasing along $(P_t \rho)_{t \ge 0}$.

Proof. Let $C_n = (\log \wedge n) \lor (-n) + n$ and

$$f_n: [0,\infty) \longrightarrow \mathbb{R}, f_n(t) = -e^{-1} + \int_{e^{-1}}^t (C_n(r) + 1 - n) dr$$

Then $f_n \in C^1([0,\infty))$, $f_n(t) \nearrow t \log t$ for all $t \ge 0$, and $f'_n = C_n - n + 1$ is bounded and Lipschitz. Define furthermore

$$F_n: [0,\infty) \longrightarrow \mathbb{R}, s \mapsto \tau(f_n(P_s\rho)).$$

Since $s \mapsto P_s \rho$ is L^1 -differentiable, we can apply Lemma 4.5 to see that F_n is locally absolutely continuous and $F'_n(s) = -\tau(f'_n(P_s \rho) \mathscr{L} P_s \rho)$.

Thus

$$\begin{split} F_n(\rho) - F_n(P_t\rho) &= \int_0^t \tau(f'_n(P_s\rho) \mathscr{L} P_s\rho) s \\ &= \int_0^t \mathscr{E}(C_n(P_s\rho), P_s\rho) ds \\ &\to \int_0^t \mathscr{I}(P_s\rho) ds, n \to \infty. \end{split}$$

Here we used conservativeness for the fact that $\tau(\mathcal{L}\bar{\rho}) = 0$ for all $\bar{\rho} \in L^1(\mathcal{M}, \tau)$.

Since $\rho \in \mathcal{D}(\mathcal{M},\tau) \cap L^2(\mathcal{M},\tau) \subset D(\text{Ent})$, the monotone convergence theorem gives the convergence of the left-hand side to $\text{Ent}(\rho) - \text{Ent}(P_t\rho)$.

Corollary 4.26. Assume that τ is finite. If $\rho \in D(Ent)$, then

$$\int_0^\infty \mathscr{I}(P_r\rho) dr \leq \operatorname{Ent}(\rho),$$

 $(P_t\rho)_{t\geq 0}$ is an admissible curve, Ent is decreasing along $(P_t\rho)_{t\geq 0}$ and $\mathcal{W}(\rho, P_t\rho) \to 0$ as $t \to 0$.

Proof. Let $\rho_n = \frac{\rho \wedge n}{\tau(\rho \wedge n)}$. Since $\rho_n \to \rho$ in $L^1(\mathcal{M}, \tau)$, one has $P_t \rho_n \to P_t \rho$ in $L^1(\mathcal{M}, \tau)$ for all $t \ge 0$. Moreover,

$$\operatorname{Ent}(\rho_n) = \tau(\rho_n \log \rho_n) = \frac{1}{\tau(\rho \wedge n)} \tau((\rho \wedge n) \log(\rho \wedge n)) - \log \tau(\rho \wedge n) \to \operatorname{Ent}(\rho).$$

It follows from the lower semicontinuity of the entropy and Proposition 4.25 that

$$\operatorname{Ent}(P_t\rho) \leq \liminf_{n \to \infty} \operatorname{Ent}(P_t\rho_n) \leq \lim_{n \to \infty} \operatorname{Ent}(\rho_n) = \operatorname{Ent}(\rho)$$

for all $t \ge 0$. Thus Ent is decreasing along $(P_t \rho)_{t \ge 0}$.

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The lower semicontinuity of \mathscr{I} (Lemma 4.22) and Fatou's lemma imply

$$\int_0^\infty \mathscr{I}(P_r\rho)dr \leq \int_0^\infty \liminf_{n\to\infty} \mathscr{I}(P_r\rho_n)dr \leq \liminf_{n\to\infty} \int_0^\infty \mathscr{I}(P_r\rho_n)dr.$$

From Proposition 4.25 we deduce

$$\liminf_{n\to\infty}\int_0^\infty \mathscr{I}(P_r\rho_n)dr \leq \lim_{n\to\infty}\operatorname{Ent}(\rho_n) = \operatorname{Ent}(\rho).$$

Moreover,

$$\liminf_{n\to\infty}\int_0^\infty \|D(P_r\rho_n)\|_{P_r\rho_n}^2 dr \leq \liminf_{n\to\infty}\int_0^\infty \mathscr{I}(P_r\rho_n) dr$$

by Proposition 4.24. Thus $(P_t \rho)_{t \ge 0}$ is admissible by Theorem 3.30.

Finally, $\mathcal{W}(\rho, P_t \rho) \to 0$ as $t \to 0$ is a direct consequence of the admissibility of $(P_t \rho)_{t \ge 0}$.

CHAPTER 5

THE GRADIENT ESTIMATE $GE(K,\infty)$

In this chapter we introduce the gradient estimate

$$\|\partial P_t a\|_{\rho}^2 \le e^{-2Kt} \|\partial a\|_{P_t \rho}^2,$$

which is inspired by the classical Bakry–Émery estimate (see the original paper [BÉ85] or the monograph [BGL14])

$$\Gamma(P_t u) \le e^{-2Kt} P_t \Gamma(u).$$

In the case of the heat semigroup on a complete Riemannian manifold, the Bakry– Émery gradient estimate is equivalent to a lower bound on the Ricci curvature. Recently, it has been shown that this equivalence between gradient estimates and lower Ricci curvature bounds (in the sense of Lott–Villani–Sturm) extends to a large class of metric measure spaces [AGS14b, AGS15, EKS15]. Thus the gradient estimate from above can be interpreted as the noncommutative version of a lower Ricci curvature bound.

One of the reasons the gradient estimate is important for the gradient flow characterization in the next chapter is that it provides certain regularizing effects of the semigroup. In the first section we investigate some of these consequences of the gradient estimates, among them an L^{∞} -to- \mathscr{A}_{θ} -regularization property of the semigroup (Proposition 5.7) and an exponential contraction (or expansion) bound for the metric \mathscr{W} (Theorem 5.13). In the second section we discuss a method to obtain the gradient estimate from commutation relations (Proposition 5.18) and give some noncommutative examples.

Throughout this chapter let (\mathcal{M}, τ) be a tracial von Neumann algebra, \mathscr{E} a quantum Dirichlet form on $L^2(\mathcal{M}, \tau)$, $(\partial, \mathcal{H}, L, R, J)$ the associated first-order differential calculus and assume that τ is energy dominant. We further assume that

 θ can be represented by a symmetric operator mean. Denote by $(P_t)_{t\geq 0}$ the quantum Markov semigroup associated with \mathscr{E} and by $\mathscr{L} = \partial^* \partial$ its generator.

5.1 Gradient estimate, Feller property and contraction estimate

Definition 5.1 (GE(K, ∞)). Let $K \in \mathbb{R}$. The quantum Dirichlet form \mathscr{E} satisfies the gradient estimate GE(K, ∞) (for the mean θ) if

$$\|\partial P_t a\|_{\rho}^2 \le e^{-2Kt} \|\partial a\|_{P_t \rho}^2$$

for all $a \in D(\mathcal{E})$, $\rho \in \mathcal{D}(\mathcal{M}, \tau)$ and $t \ge 0$.

Remark 5.2. The gradient estimate $GE(K,\infty)$ is a modification of the classical Bakry-Émery gradient estimate. Indeed, if \mathscr{E} is a strongly local (commutative) Dirichlet form on $L^2(X,m)$, then the gradient estimate $GE(K,\infty)$ reads

$$\int_X \Gamma(P_t u) \rho \, dm \le e^{-2Kt} \int_X P_t \Gamma(u) \rho \, dm,$$

which is just a weak formulation of the Bakry-Émery gradient estimate

$$\Gamma(P_t u) \le e^{-2Kt} P_t \Gamma(u).$$

If \mathscr{E} is the standard Dirichlet energy on a complete Riemannian manifold (M,g), then \mathscr{E} satisfies $\operatorname{GE}(K,\infty)$ if and only if the Ricci curvature of (M,g) is bounded below by K.

Remark 5.3. In the classical Bakry-Émery gradient estimate there is an additional dimension parameter N, and $BE(K,\infty)$ corresponds to the case $N = \infty$. That is why we keep the parameter ∞ in our notation although we do not introduce any finite-dimensional variant of $GE(K,\infty)$.

Remark 5.4. For finite graphs, the gradient estimate $GE(K,\infty)$ was introduced in [EF18], where it was shown to be equivalent to *K*-convexity of the entropy along W-geodesics ([EF18, Theorem 3.1]). The latter was taken as definition for a lower Ricci curvature bound *K* of a graph in [EM14] (see also [Mie13]).

Some examples of quantum Dirichlet forms satisfying the gradient estimate will be discussed more systematically in the next section. Here we just give a simple (commutative) example. *Example* 5.5. Endow \mathbb{Z}^d with the natural graph structure given by

$$b(m,n) = \begin{cases} 1 & \text{if } |m-n| = 1, \\ 0 & \text{otherwise,} \end{cases}$$

and the uniform measure m = 1.

Since (\mathbb{Z}^d, b, m) has bounded degree, the Dirichlet forms $\mathscr{E}^{(D)}$ and $\mathscr{E}^{(N)}$ introduced in Example 1.25 coincide, and we simply denote them by \mathscr{E} . We will show that \mathscr{E} satisfies $GE(0,\infty)$ for the logarithmic mean. By a simple approximation argument it suffices to prove

$$\|\partial P_t u\|_{\rho}^2 \le \|\partial u\|_{P_t \rho}^2$$

for $u \in C_c(\mathbb{Z}^d)$ and $\rho \in C_c(\mathbb{Z}^d)_+$.

For this, we will approximate \mathbb{Z}^d by finite graphs and use known results for finite Markov chains. Let $K_j = \{-j, \dots, j\}^d$ and

$$L_j: \ell^2(K_j) \to \ell^2(K_j), L_j u(m) = \sum_{n \in K_j} b(m, n)(u(m) - u(n)).$$

This is the generator of the Dirichlet form \mathscr{E}_j associated with the weighted graph $(K_j, b|_{K_j \times K_j}, 1)$. Let (P_t^j) denote the associated semigroup. It follows from [FM16, Theorem 4.1] in combination with [EM14, Theorem 6.2] or [Mie13, Theorem 5.1] that \mathscr{E}_j satisfies GE(0, ∞) for the logarithmic mean.

We extend L_j to an operator on $\ell^2(\mathbb{Z}^d)$ by setting it zero on $\ell^2(\mathbb{Z}^d \setminus K_j)$. Clearly, if $u \in C_c(\mathbb{Z}^d)$ with $\operatorname{supp} u \subset K_j$, then $L_{j+1}u = Lu$, where L is the generator of \mathscr{E} . Since the sequence (L_j) is uniformly bounded, it follows that $L_j \to L$ strongly. Thus also $e^{-tL_j} \to e^{-tL}$ strongly.

Since \mathscr{E}_i satisfies $GE(0,\infty)$, we have

$$\frac{1}{2} \sum_{\substack{m,n \in K_j \\ m \sim n}} \hat{\rho}(m,n) (P_t^j u(m) - P_t^j u(n))^2 \le \frac{1}{2} \sum_{\substack{m,n \in K_j \\ m \sim n}} \widehat{P_t^j} \rho(m,n) (u(m) - u(n))^2$$

for all $u \in C_c(\mathbb{Z}^d)$, $\rho \in C_c(\mathbb{Z}^d)_+$ and $j \in \mathbb{N}$ such that $\operatorname{supp} u, \operatorname{supp} \rho \subset K_j$. By Fatou's lemma, the limes inferior as $j \to \infty$ of the left-hand side is bounded below by $\|\partial P_t u\|_{\rho}^2$, while the right-hand side converges to $\|\partial u\|_{P_t\rho}^2$ by the dominated convergence theorem. Hence

$$\left\|\partial P_t u\right\|_{\rho}^2 \le \left\|\partial u\right\|_{P_t \rho}^2$$

More generally, this method deducing a gradient estimate for a graph from gradient estimates for an exhaustion of finite subgraphs can be applied if the Laplacians of the subgraphs converge to the Laplacian of the original graph in the strong resolvent sense. This is the case for instance if the graph is locally finite and stochastically complete (in this case one can easily adapt the arguments from [KL12, Proposition 2.7]).

Remark 5.6. If θ is the arithmetic mean, then GE(K, ∞) reads

$$\Gamma(P_t a) \le e^{-2Kt} P_t \Gamma(a)$$

for $a \in D(\mathscr{E})$ self-adjoint. This noncommutative form of the Bakry–Émery gradient estimate was used for example in [JZ15] in the study of noncommutative Poincaré inequalities.

In general, the gradient estimate $GE(K,\infty)$ is not equivalent to the (noncommutative) Bakry-Émery gradient estimate in this form, even in the simplest (commutative) examples. For instance, if \mathscr{E} is the Dirichlet form associated with the weighted graph ($\{0,1\}, b, m$) with b(0,1) > 0, then one can show that the best possible constant K in $GE(K,\infty)$ for the logarithmic mean coincides with the best possible constant for the arithmetic mean if and only if m(0) = m(1).

Proposition 5.7 (Feller property). If \mathscr{E} satisfies $\operatorname{GE}(K,\infty)$ for some $K \in \mathbb{R}$, then P_t maps $L^2(\mathcal{M},\tau) \cap \mathcal{M}$ into \mathcal{A}_{θ} for t > 0.

Proof. Let $a \in L^2(\mathcal{M}, \tau) \cap \mathcal{M}_h$ and t > 0. Since P_t maps $L^2(\mathcal{M}, \tau)$ into $D(\mathcal{L})$, we can assume $a \in D(\mathcal{L}) \cap \mathcal{M}$. For $\rho \in D(\mathcal{L}) \cap L^1_+(\mathcal{M}, \tau) \cap \mathcal{M}$ define

$$\varphi\colon [0,t] \longrightarrow \mathbb{R}, \, \varphi(s) = \int_0^s \|\partial P_{t-r}a\|_{P_r\rho}^2 \, dr.$$

Note that $r \mapsto \widehat{P_r \rho}$ is strongly continuous by Lemma 2.13 and $r \mapsto \partial P_{t-r} a$ is continuous in \mathcal{H} , so that the integrand is continuous in r.

Since \mathscr{E} satisfies $\operatorname{GE}(K,\infty)$, the map $s \mapsto e^{-2Ks}\varphi'(s)$ is increasing. It follows from a comparison argument (see [AGS15, Lemma 2.2 and Equation (2.30)]) that

$$I_{2K}(t) \|\partial P_t a\|_{\rho}^2 = I_{2K}(t) \varphi'(0) \le \int_0^t \varphi'(s) \, ds = \int_0^t \|\partial P_{t-s} a\|_{P_s \rho}^2 \, ds, \tag{5.1}$$

where $I_{\kappa}(t) = \int_0^t e^{\kappa s} ds$.

By Lemma 2.23 and a direct calculation we have

$$\|\partial P_{t-s}a\|_{P_s\rho}^2 \leq \tau(\Gamma(P_{t-s}a)P_s\rho) = \frac{1}{2}\frac{d}{ds}\tau((P_{t-s}a)^2P_s\rho)$$

If we plug this into (5.1), we get

$$I_{2K}(t) \|\partial P_t a\|_{\rho}^2 \leq \frac{1}{2} \tau((P_t(a^2) - (P_t a)^2)\rho).$$

Thus

$$\|\partial P_t a\|_{\rho}^2 \le \frac{1}{2I_{2K}(t)} \|a\|_{\mathcal{M}}^2 \|\rho\|_1.$$

In the general case $\rho \in L^1_+(\mathcal{M}, \tau)$, one can use Lemma 2.3 and once more $\operatorname{GE}(K, \infty)$ to also get

$$\begin{split} \|\partial P_t a\|_{\rho}^2 &= \lim_{m \to \infty} \|\partial P_t a\|_{\rho \wedge m}^2 \\ &\leq \liminf_{m \to \infty} \liminf_{\delta \to 0} e^{-2K\delta} \|\partial P_{t-\delta} a\|_{P_{\delta}(\rho \wedge m)}^2 \\ &\leq \liminf_{m \to \infty} \liminf_{\delta \to 0} \frac{e^{-2K\delta}}{2I_{2K}(t-\delta)} \|a\|_{\mathcal{M}}^2 \|\rho \wedge m\|_1 \\ &= \frac{1}{2I_{2K}(t)} \|a\|_{\mathcal{M}}^2 \|\rho\|_1. \end{split}$$

Hence $P_t a \in \mathscr{A}_{\theta}$.

Remark 5.8. If \mathscr{E} is a strongly local (commutative) Dirichlet form, then Proposition 5.7 recovers the L^{∞} -to-Lipschitz Feller property of the heat flow on RCD spaces from [AGS14b, Theorem 6.8] (with essentially the same proof). If \mathscr{E} is not strongly local or not commutative, the correct analogue of the algebra of bounded Lipschitz functions seems to be \mathscr{A}_{AM} (see Example 2.8), so that Proposition 5.7 is in general weaker than (noncommutative) L^{∞} -to-Lipschitz regularization unless θ is the arithmetic mean.

Corollary 5.9. If \mathscr{E} satisfies $\operatorname{GE}(K,\infty)$, then $\mathscr{A}_{\theta} \cap \mathscr{M}_{1}$ is dense in $D(\mathscr{E}) \cap \mathscr{M}_{1}$ with respect to $\|\cdot\|_{\mathscr{E}}$ and strongly dense in \mathscr{M}_{1} .

Proof. The density of $\mathscr{A}_{\theta} \cap \mathscr{M}_1$ in $D(\mathscr{E}) \cap \mathscr{M}_1$ follows directly from Proposition 5.7. The strong density in \mathscr{M}_1 is then a consequence of Kaplansky's density theorem.

We now fulfill the promise made in Remark 3.9 and introduce a regularity property that ensures that the duality in the definition of admissible curves can be extended to \mathcal{A}_{θ} .

Definition 5.10 (Regular mean). The mean θ is called *regular* for \mathscr{E} if for all $a \in \mathscr{A}_{\theta}$ there exists a sequence (a_n) in \mathscr{A}_{AM} such that $a_n \to a \sigma$ -weakly, (a_n) is bounded in A_{θ} and $\partial a_n \to \partial a$ weakly in $\tilde{\mathscr{H}}_{\rho}$ for all $\rho \in \mathscr{D}(\mathscr{M}, \tau)$.

The next lemma then follows immediately from this definition.

Lemma 5.11. If the mean θ is regular for \mathcal{E} , then $\partial \mathcal{A}_{\theta} \subset \mathcal{H}_{\rho}$ for all $\rho \in \mathcal{D}(\mathcal{M}, \tau)$ and if $(\rho_t)_{t \in I}$ is an admissible curve in $\mathcal{D}(\mathcal{M}, \tau)$, then

$$\tau(a(\rho_t - \rho_s)) = \int_s^t \langle \partial a, D \rho_r \rangle_{\rho_r} dr$$

for all $a \in \mathcal{A}_{\theta}$ and $s, t \in I$.

Of course, the arithmetic mean is regular for every quantum Dirichlet form. For other means it may not be easy to check whether it is regular for a given quantum Dirichlet form. However, the gradient estimate $GE(K,\infty)$ yields a sufficient condition for regularity of means. More precisely, we have the following result.

Proposition 5.12. Let θ be a mean and $K \in \mathbb{R}$. If \mathscr{E} satisfies $GE(K,\infty)$ for θ and the arithmetic mean, then θ is regular for \mathcal{E} .

Proof. Let θ be a mean. For $a \in \mathcal{A}_{\theta}$ let $a_n = P_{t_n}a$ for some null sequence (t_n) . Since \mathscr{E} satisfies GE(K,∞) for AM, we have $a_n \in \mathscr{A}_{AM}$ by Proposition 5.7.

The σ -weak convergence of (a_n) to a is a consequence of the continuity of (P_t) . Moreover, $GE(K,\infty)$ for θ implies

$$\|\partial a_n\|_{\rho} \leq e^{-Kt_n} \|\partial a\|_{P_{t\rho}} \leq \max\{1, e^{-K\sup_n t_n}\} \|a\|_{\theta}$$

for all $\rho \in \mathcal{D}(\mathcal{M}, \tau)$, where the norms $\|\cdot\|_{\rho}$ and $\|\cdot\|_{P_t\rho}$ are to be understood with respect to the mean θ . Hence (a_n) is bounded in \mathscr{A}_{θ} .

Since $\|\partial a_n\|_{\rho} + \|\partial a_n\|_{\mathcal{H}}$ is bounded and $(D(\hat{\rho}^{1/2}), \langle \cdot, \cdot \rangle_{\mathcal{H}} + \langle \cdot, \cdot \rangle_{\rho})$ is complete, every subsequence of (∂a_n) has a subsequence that converges weakly in $D(\hat{\rho}^{1/2})$. Moreover, since $\partial a_n \to \partial a$ in \mathcal{H} , the weak limit is ∂a . Finally, since $D(\hat{\rho}^{1/2})$ is dense in \mathcal{H}_{ρ} and $\|\partial a_n\|_{\rho}$ is bounded, we also have $\partial a_n \to \partial a$ weakly in \mathcal{H}_{ρ} .

Theorem 5.13 (Contraction estimate). Assume that θ is regular for \mathcal{E} . If \mathcal{E} satisfies $\operatorname{GE}(K,\infty)$ for θ and $(\rho_t)_{t\in I}$ is an admissible curve in $\mathscr{D}(\mathcal{M},\tau)$, then $(P_T\rho_t)_{t\in I}$ is an admissible curve and $\|DP_T\rho_t\|_{P_T\rho_t} \leq e^{-KT} \|D\rho_t\|_{\rho_t}$ for a.e. $t \in I$. In particular, $\mathcal{W}(P_T\rho_0, P_T\rho_1) \leq e^{-KT} \mathcal{W}(\rho_0, \rho_1)$ for $\rho_0, \rho_1 \in \mathcal{D}(\mathcal{M}, \tau)$ and $T \geq 0$.

Proof. Let $(\rho_t)_{t \in I}$ be an admissible curve in $\mathcal{D}(\mathcal{M}, \tau)$. For all $s, t \in I$ and $a \in \mathcal{A}_{AM}$ we have

$$\begin{aligned} |\tau(a(P_T\rho_t - P_T\rho_s))| &= |\tau(P_Ta(\rho_t - \rho_s))| \\ &\leq \int_s^t \|\partial P_Ta\|_{\rho_r} \|D\rho_r\|_{\rho_r} dr \\ &\leq e^{-KT} \int_s^t \|\partial a\|_{P_T\rho_r} \|D\rho_r\|_{\rho_r} dr \end{aligned}$$

where we used Proposition 5.7 and Lemma 5.11 for the first and $GE(K,\infty)$ for the second inequality.

Thus, $(P_T \rho_r)_{r \in [0,1]}$ is an admissible curve with $||DP_T \rho_r||_{P_T \rho_r} \le e^{-KT} ||D\rho_r||_{\rho_r}$ for a.e. $r \in I$. Minimizing over all admissible curves connecting ρ_0 and ρ_1 yields the second claim.

Corollary 5.14. Assume that the logarithmic mean is regular for \mathscr{E} and \mathscr{E} satisfies $\operatorname{GE}(K,\infty)$ for the logarithmic mean. If $\rho \in \overline{D(\operatorname{Ent})}^{\mathscr{W}}$, then $\mathscr{W}(P_t\rho,\rho) \to 0$ as $t \to 0$.

Proof. In Corollary 4.26 we have already seen that this convergence holds for $\rho \in D(\text{Ent})$. If $\rho \in \overline{D(\text{Ent})}^{\mathcal{W}}$, let (ρ_k) be a sequence in D(Ent) such that $\mathcal{W}(\rho_k, \rho) \to 0$. By Theorem5.13 we have

$$\mathcal{W}(P_t\rho,\rho) \le (1+e^{-Kt})\mathcal{W}(\rho,\rho_k) + \mathcal{W}(P_t\rho_k,\rho_k).$$

Letting first $t \to 0$ and then $k \to \infty$ yields the claimed convergence.

5.2 Gradient estimate via intertwining relations

According to Remarks 5.2 and 5.4, examples of Dirichlet forms satisfying the gradient estimate GE include the Dirichlet energy on complete Riemannian manifolds with lower bounded Ricci curvature and the Dirichlet form associated with graphs satisfying the entropic curvature condition introduced by Erbar and Maas [EM12]. To obtain more examples and especially noncommutative ones, we adapt a technique used by Carlen and Maas [CM17a] in the finite-dimensional case.

Definition 5.15. Let $(\Omega, \mathcal{B}, \mu)$ be a measure space. We say that $(\partial, \mathcal{H}, L, R, J)$ decomposes as a direct integral over $(\Omega, \mathcal{B}, \mu)$ if $\mathcal{H} = \int_{\Omega}^{\oplus} L^2(\mathcal{M}, \tau) d\mu$, the left and right action decompose as

$$L(a)x(\omega) = ax(\omega)$$
$$R(a)x(\omega) = x(\omega)a$$

for $a \in \mathcal{M}$, $x \in \mathcal{H}$ and μ -a.e. $\omega \in \Omega$, and J acts as $J(x)(\omega) = -x(\omega)^*$ for $x \in \mathcal{H}$ and μ -a.e. $\omega \in \Omega$. In this case we write L_{ω} , R_{ω} and ∂_{ω} for the respective component functions.

In the special case when \mathscr{B} is the power set and μ the counting measure, we say that $(\partial, \mathcal{H}, L, R, J)$ decomposes as a direct sum over Ω .

Example 5.16 (Generators in Lindblad form). If $(v_j)_{j \in I}$ is a family of self-adjoint isometries in \mathcal{M} such that $\sum_{j \in I} v_j^2$ converges strongly, then

$$\mathscr{L}: L^{2}(\mathscr{M}, \tau) \longrightarrow L^{2}(\mathscr{M}, \tau), \, \mathscr{L}(a) = -\frac{1}{2} \sum_{j \in J} v_{j}^{2} a - 2v_{j} a v_{2} + a v_{j}^{2}$$

generates a bounded quantum Dirichlet form. This is a special case of a generator in Lindblad form.

The associated first-order differential calculus decomposes as a direct sum over ${\cal I}$ and

$$\partial_j(a) = [v_j, a] = v_j a - a v_j$$

Lemma 5.17. Let Φ and Ψ denote the representation of \mathcal{M} on $L^2(\mathcal{M}, \tau)$ by left and right multiplication, respectively. If $a \in \mathcal{M}_+$ and $t \ge 0$, then

$$P_t \theta(\Phi(a), \Psi(a)) P_t \leq \theta(\Phi(P_t a), \Psi(P_t a))$$

Proof. By the continuity property of operator means, it suffices to show the equality for invertible a. Moreover, by Löwner's theorem (see Proposition 2.20) it suffices to consider the case

$$\theta(r,s) = \frac{rs}{\lambda r + s}$$

with $\lambda \ge 0$.

For invertible a the desired inequality is obviously equivalent to

$$\theta(\Phi(P_t a), \Psi(P_t a))^{-1/2} P_t \theta(\Phi(a), \Psi(a)) P_t \theta(\Phi(P_t a), \Psi(P_t a))^{-1/2} \le 1.$$
(5.2)

Recall the elementary fact that for an element *x* of a C^* -algebra, $x^*x \le 1$ is equivalent to $xx^* \le 1$. It follows that (5.2) is equivalent to

$$P_t \theta(\Phi(P_t a), \Psi(P_t a))^{-1} P_t \le \theta(\Phi(a), \Psi(a))^{-1}.$$
(5.3)

Let $x \in L^2(\mathcal{M}, \tau)$. For θ of the form specified in (5.2) we have

$$\langle P_t \theta(\Phi(P_t a), \Psi(P_t a))^{-1} P_t x, x \rangle_2 = \tau(\lambda(P_t x)(P_t a)^{-1}(P_t x^*) + (P_t x^*)(P_t a)^{-1}(P_t a)).$$
(5.4)

Since P_t is completely positive, we can apply [LR74, Theorem 2] to get

$$(P_t x)(P_t a)^{-1}(P_t x^*) \le P_t (x a^{-1} x^*)$$
$$(P_t x^*)(P_t a)^{-1}(P_t x) \le P_t (x^* a^{-1} x).$$

Since P_t is trace-preserving, it follows that

$$\begin{aligned} \tau(\lambda(P_t x)(P_t a)^{-1}(P_t x^*) + (P_t x^*)(P_t a)^{-1}(P_t x)) &\leq \tau(\lambda x a^{-1} x^* + x^* a x) \\ &= \langle \theta(\Phi(a), \Psi(a))^{-1} x, x \rangle_2. \end{aligned}$$

In combination with (5.4) this yields

$$\langle P_t \theta(\Phi(P_t a), \Psi(P_t a))^{-1} P_t x, x \rangle_2 \le \langle \theta(\Phi(a), \Psi(a))^{-1} x, x \rangle_2$$

which completes the proof of (5.3).

Proposition 5.18. Assume that $(\partial, \mathcal{H}, L, R, J)$ decomposes as a direct integral over $(\Omega, \mathcal{B}, \mu)$. If there exists a measurable function $k : \Omega \longrightarrow \mathbb{R}$ such that

$$K = \mathop{\rm essinf}_{\omega\in\Omega} k(\omega) > -\infty$$

and for all $a \in D(\mathcal{E})$, t > 0 one has

$$\partial_{\omega} P_t a = e^{-k(\omega)t} P_t \partial_{\omega} a$$

for μ -a.e. $\omega \in \Omega$, then \mathscr{E} satisfies $\operatorname{GE}(K,\infty)$ for every symmetric operator mean. In particular, every operator mean is regular for \mathscr{E} .

Proof. Let $a \in D(\mathcal{E})$ and t > 0. By Corollary 2.25 it suffices to show

$$\|\partial P_t a\|_{\rho}^2 \le e^{-2Kt} \|\partial a\|_{P_t \rho}^2$$

for $\rho \in \mathcal{M}_+$.

Using the intertwining relation from the assumption, the self-adjointness of P_t and Lemma 5.17, we get

$$\langle \theta(L_{\omega}(\rho), R_{\omega}(\rho)) \partial_{\omega} P_{t} a, \partial_{\omega} P_{t} a \rangle_{a} \leq e^{-2k(\omega)t} \langle P_{t} \theta(L_{\omega}(\rho), R_{\omega}(\rho)) P_{t} \partial_{\omega} a, \partial_{\omega} a \rangle_{2}$$

$$\leq e^{-2Kt} \langle \theta(L_{\omega}(P_{t}\rho), R_{\omega}(P_{t}\rho)) \partial_{\omega} a, \partial_{\omega} a \rangle_{2}$$

for μ -a.e. $\omega \in \Omega$. Integration with respect to μ completes the proof of $GE(K,\infty)$.

The regularity of θ now follows from Lemma 5.12 (observe that $GE(K,\infty)$ holds for all symmetric operator means, so in particular for the arithmetic mean).

Example 5.19 (Flat Noncommutative Torus). The first-order differential calculus associated with the noncommutative heat semigroup on the noncommutative torus (see Example 1.26) decomposes as a direct sum over $\{1,2\}$. Moreover, P_t commutes with ∂_j for t > 0 and $j \in \{1,2\}$. Thus the associated quantum Dirichlet form satisfies $GE(0,\infty)$.

Example 5.20 (Free fermionic system at infinite temperature). Let \mathscr{E} be Gross' Dirichlet form for the free fermionic system (see Example 1.27). While $\mathscr{H} = \bigoplus_{j\geq 1} L^2(\mathbb{C}\ell(H),\tau)$ and L acts by componentwise left multiplication, the right action is given by

$$(R(a)x)_j = \gamma(a)x_j.$$

However, since $\gamma P_t = P_t \gamma$, the proof of Lemma 5.17 still goes through in this case and thus Proposition 5.18 can be applied in this example.

We claim that $a_j e^{-tN} \psi = e^{-t} e^{-tN} a_j \psi$ for $j \in \mathbb{N}$, t > 0 and $\psi \in D(a_j)$. By linearity it suffices to consider ψ of the form $\psi = e_{n_1} \wedge \cdots \wedge e_{n_k}$. One has

$$a_{j}e^{-tN}(e_{n_{1}}\wedge\cdots\wedge e_{n_{k}}) = a_{j}e^{-tk}(e_{n_{1}}\wedge\cdots\wedge e_{n_{k}})$$
$$= \frac{e^{-tk}}{\sqrt{k}}\sum_{l=1}^{k}(-1)^{l}\langle e_{j},e_{l}\rangle e_{n_{1}}\wedge\cdots\wedge \widehat{e_{n_{l}}}\wedge\cdots\wedge e_{n_{k}},$$

while

$$e^{-tN}a_{j}(e_{n_{1}}\wedge\cdots\wedge e_{n_{k}}) = \frac{1}{\sqrt{k}}\sum_{l=1}^{k}(-1)^{l}\langle e_{j},e_{l}\rangle e^{-tN}(e_{n_{1}}\wedge\cdots\wedge \widehat{e_{n_{l}}}\wedge\cdots\wedge e_{n_{k}})$$
$$= \frac{e^{-t(k-1)}}{\sqrt{k}}\sum_{l=1}^{k}(-1)^{l}\langle e_{j},e_{l}\rangle e_{n_{1}}\wedge\cdots\wedge \widehat{e_{n_{l}}}\wedge\cdots\wedge e_{n_{k}}.$$

Via the Chevalley-Segal isomorphism, this implies the intertwining relation

$$\partial_j P_t a = e^{-t} P_t \partial_j a.$$

Thus ${\mathscr E}$ satisfies $\operatorname{GE}(1,\infty).$

CHAPTER 6

GRADIENT FLOW OF THE ENTROPY

In this chapter we give the announced characterization of quantum Markov semigroup as metric gradient flow of the entropy. To be more precise, we will show that if (P_t) satisfies the gradient estimate $GE(K,\infty)$ and some technical conditions, then the evolution variational inequality

$$\frac{1}{2}\frac{d^{+}}{dt}\mathcal{W}(P_{t}\rho,\sigma)^{2} + \frac{K}{2}\mathcal{W}(P_{t}\rho,\sigma)^{2} + \operatorname{Ent}(P_{t}\rho) \leq \operatorname{Ent}(\sigma)$$

holds.

As the proof of the gradient flow characterization is fairly technical, we opted to first show it under the additional assumption of ultracontractivity (Theorem 6.6). The idea of the proof is the same as in the general case, but ultracontractivity makes several technical steps unnecessary that might obscure the outline of the proof.

A central difficulty in the proof of the gradient flow characterization, as already in the case of metric measure spaces, lies in the fact that we are working on L^1 , so that the heat flow curves may fail to be differentiable and Hilbert space methods are not directly applicable. To overcome this problem, Section 6.3 is devoted to a fine analysis of standard semigroup mollification techniques in our setting. In particular, we prove an entropy regularization estimate in Proposition 6.13.

In Section 6.4 we review the evolution variational inequality (EVI) formulation of gradient flows in metric spaces and complete the proof of the characterization of the Markovian quantum master equation as EVI gradient flow of the entropy (Theorem 6.15).

In part our proof strategy is a careful adaptation to the noncommutative setting of the paths taken by Ambrosio et al. (see [AGS15] in the case of infinitesimally Hilbertian metric measure spaces and [AES16] in the case of abstract local Dirichlet forms). However, both proofs rely strongly on duality (either the dual problem of the Monge–Kantorovich or the Benamou–Brenier formulation). Little is known on the dual formulation in the present setting, so we avoid it altogether. In this way, our approach gives a new proof variant even when restricted to the case of infinitesimally Hilbertian metric measure spaces (with finite measure).

As usual, let (\mathcal{M}, τ) be a tracial von Neumann algebra, \mathscr{E} a quantum Dirichlet form on $L^2(\mathcal{M}, \tau)$ such that τ is energy dominant, and $(\partial, \mathcal{H}, L, R, J)$ the associated first-order differential calculus. We further assume that τ is a state, $L^1(\mathcal{M}, \tau)$ is separable and θ is the logarithmic mean. We do not make any density assumptions on \mathscr{A}_{θ} – these follow automatically from the gradient estimate we introduce in the first section.

6.1 Gradient flows in metric spaces

In this section we shortly discuss several definitions and basic properties of gradient flows in metric spaces. An extensive overview over this topic can be found in [AGS08].

An extended metric space is a pair (X,d) consisting of a set X and a map $d: X \times X \longrightarrow [0,\infty]$ that satisfies all axioms of a metric, but may take the value ∞ . Let $S: X \longrightarrow (-\infty,\infty]$ be a proper lower semicontinuous functional and let D(S) denote its proper domain, that is,

$$D(S) = \{x \in X \mid S(x) < \infty\}.$$

The *descending* and *ascending slope* of S are defined by

$$|D^{+}S|(x) = \limsup_{y \to x} \frac{(S(y) - S(x))_{-}}{d(x, y)},$$
$$|D^{-}S|(x) = \limsup_{y \to x} \frac{(S(y) - S(x))_{+}}{d(x, y)},$$

if $x \in D(S)$ is not isolated. For isolated points $x \in D(S)$ one sets

 $|D^+S|(x) = |D^-S|(x) = 0,$

and furthermore $|D^+S| = |D^-S| = \infty$ on $X \setminus D(S)$.

As a further piece of notation we need the *upper right derivative* (or upper Dini derivative) $\frac{d^+}{dt}$ of a function f on a right-open interval I, which is defined by

$$\frac{d^+}{dt}f(t) = \limsup_{h \searrow 0} \frac{f(t+h) - f(t)}{h}$$

for $t \in I$.

Definition 6.1 (EDE and EVI gradient flow curves). Let (X,d) be an extended metric space and $S: X \longrightarrow (-\infty, \infty]$ a proper lower semicontinuous functional. A locally absolutely continuous curve $(\gamma_t)_{t\geq 0}$ in X is called *EDE gradient flow of* S if it satisfies the *energy dissipation equality*

$$S(\gamma_0) = S(\gamma_t) + \frac{1}{2} \int_0^t |\dot{\gamma}_s|^2 ds + \frac{1}{2} \int_0^t |D^- S|^2(\gamma_s) ds$$
(EDE)

for all $t \ge 0$.

Let $K \in \mathbb{R}$. The curve γ is called EVI_K gradient flow curve of S if it satisfies the evolution variational inequality

$$\frac{1}{2}\frac{d^+}{dt}d(\gamma_t, x)^2 + \frac{K}{2}d(\gamma_t, x)^2 + S(\gamma_t) \le S(x)$$
(EVI_K)

for all $t \ge 0$ and $x \in X$ with $d(x, \gamma_0) < \infty$.

A semigroup of continuous maps $T_t: D(S) \longrightarrow D(S), t \ge 0$, is called EVI_K gradient flow of S if

(F1) $d(T_t x, x) \rightarrow 0$ as $t \rightarrow 0$ for all $x \in X$,

(F2) *S* is decreasing along $(T_t x)_{t \ge 0}$ for all $t \ge 0$,

(F3) $(T_t x)_{t \ge 0}$ is an EVI_K gradient flow for all $x \in X$.

If \mathbb{R}^d is endowed with the Euclidean metric and $S \in C^1(\mathbb{R}^d)$, then a C^1 -curve γ is an EDE gradient flow curve of S if and only if it satisfies the classical gradient flow equality

$$\dot{\gamma}_t = -\nabla S(\gamma_t).$$

If moreover $S - \frac{K}{2} |\cdot|^2$ is convex, then the notion of EDE gradient flow curve, EVI_K gradient flow curve and classical gradient flow curve all coincide for C^1 -curves. Conversely, if S admits an EVI_K gradient flow, then $S - \frac{K}{2} |\cdot|^2$ is convex.

In general, if $(T_t)_{t\geq 0}$ is an EVI_K gradient flow of *S*, then $(T_tx)_{t\geq 0}$ is the unique EDE gradient flow curve starting in *x*.

While the existence of EVI_K gradient flow curves for a given functional is not guaranteed, the uniqueness is a consequence of the defining property (see e.g. [DS08, Proposition 3.1]):

Lemma 6.2. Let (X,d) be an extended metric space and $S: X \longrightarrow (-\infty,\infty]$ a proper lower semicontinuous functional. If γ , $\tilde{\gamma}$ are EVI_K gradient flow curves of S starting in γ_0 , $\tilde{\gamma}_0$ respectively, then

$$d(\gamma_t, \tilde{\gamma}_t) \le e^{-Kt} d(\gamma_0, \tilde{\gamma}_0)$$

for all $t \ge 0$.

In particular, there is at most one EVI_K gradient flow curve with a given starting point.

6.2 Proof of the gradient flow characterization in the ultracontractive case

In this section we give a proof of the gradient flow characterization for ultracontractive semigroups. While this case is included in the general theorem we will prove in Section 6.4 and the proof there is independent of the present section, we think it is instructive to discuss the ultracontractive case first because it eases several technical difficulties and thus makes the underlying structure of the proof more transparent.

The semigroup (P_t) is called *ultracontractive* if P_t maps $L^1(\mathcal{M}, \tau)$ into \mathcal{M} for all t > 0. Note that by the closed graph theorem, the map P_t is then automatically continuous from L^1 to \mathcal{M} . We denote the corresponding operator norm by $\|P_t\|_{1\to\infty}$.

The term "ultracontractive" was introduced by Davies and Simon [DS86], following a suggestion of Robinson. A review of the literature on ultracontractive semigroups is given in [DGS92]; a more up-to-date account can be found in the Notes and Historical Remarks to Section 6.6 in [Sim15]. Examples of ultracontractive semigroups include the heat semigroup on compact Riemannian manifolds and the noncommutative heat semigroup from Example 1.13.

For certain rate functions $||P_t||_{1\to\infty}$, ultracontractivity can be characterized in terms of Sobolev and Nash inequalities.

Proposition 6.3. Let d > 2 and $p = \frac{2d}{d-2}$. The following assertions are equivalent.

- (i) There exists C > 0 such that $||P_t a||_{\infty} \leq Ct^{-d/2} ||a||_1$ for all $a \in L^1(\mathcal{M}, \tau)$ and $t \in (0, 1)$.
- (ii) There exists C' > 0 such that $||a||_p^2 \le C' \mathscr{E}(a)$ for all $a \in D(\mathscr{E})$ with $\tau(a) = 0$.
- (iii) There exists C'' > 0 such that $||a||_2^{2+4/d} \le C'' \mathscr{E}(a) ||a||_1^{4/d}$ for all $a \in D(\mathscr{E})$ with $\tau(a) = 0$.

In the commutative case, this result is due to Varopoulos [Var85]. In the noncommutative case, this equivalence was proven by Junge and Mei [JM10, Theorem 1.1.1]. See also [Xio17, Theorem 1.1] for a quantitative result concerning a more general class of rate functions for $||P_t||_{1\to\infty}$.

In addition to "spatial" regularity, ultracontractivity also yields additional regularity in the time variable for the semigroup. To discuss this, we need some more definitions.

For $\alpha \in (0, \pi/2]$ let

$$\Sigma_{\alpha} = \{ z \in \mathbb{C} : |\arg(z)| < \alpha \}.$$

An analytic semigroup of angle α on a Banach space X is a family $(T_z)_{z \in \Sigma_{\alpha} \cup \{0\}}$ of bounded linear operators on X such that

- $T_0 = \text{id and } T_{z_1+z_2} = T_{z_1}T_{z_2} \text{ for } z_1, z_2 \in \Sigma_{\alpha},$
- the map $z \mapsto T_z$ is analytic on Σ_{α} ,
- the map $z \mapsto T_z$ is strongly continuous on $\Sigma_\beta \cup \{0\}$ for all $\beta \in (0, \alpha)$.

By a slight abuse of notation one also calls a strongly continuous semigroup analytic if it extends to an analytic semigroup. Every positive self-adjoint operator A on a Hilbert space generates an analytic semigroup given by $T_z = e^{-zA}$.

As discussed in Remark 1.7, this implies that the semigroup (P_t) on $L^2(\mathcal{M}, \tau)$ is analytic and thus, by an interpolation argument (see [Dav90, Theorem 1.4.2] in the commutative and [JLMX06, Proposition 5.4] in the noncommutative case), also the corresponding semigroup on $L^p(\mathcal{M}, \tau)$ for $p \in (1, \infty)$. However, the semigroup on $L^1(\mathcal{M}, \tau)$ may fail to be analytic, as is the case for instance for the Ornstein–Uhlenbeck semigroup (see for example [MPP02, Section 5]).

The following result shows that ultracontractivity is sufficient for analyticity on $L^1(\mathcal{M}, \tau)$. In fact, we can also give a simpler proof for analyticity on $L^p(\mathcal{M}, \tau)$ for all $p \in [1, \infty)$ in this case.

Proposition 6.4. If (P_t) is ultracontractive, then the semigroup $(P_t^{(p)})$ on $L^p(\mathcal{M}, \tau)$ is analytic with angle $\pi/2$.

Proof. By duality it suffices to check the claim for $p \in [1,2]$. Moreover, since the locally uniform limit of analytic functions is analytic, it is enough to show that there exists a locally bounded function $C: \Sigma_{\pi/2} \longrightarrow (0,\infty)$ such that

$$\|P_z a\|_p \le C(z) \|a\|_p$$

for all $a \in L^p(\mathcal{M}, \tau) \cap L^2(\mathcal{M}, \tau)$ and $z \in \Sigma_{\pi/2}$. By interpolation we can restrict to the case p = 1.

Let I be the inclusion $L^2(\mathcal{M},\tau) \hookrightarrow L^1(\mathcal{M},\tau)$. The semigroup property yields

$$\|P_{z}a\|_{1} \le \|I\|_{2 \to 1} \|P_{i \operatorname{Im} z}\|_{2 \to 2} \|P_{\operatorname{Re} z}\|_{1 \to 2} \|a\|_{1} \le \|P_{\operatorname{Re} z}\|_{1 \to 2} \|a\|_{1}.$$

By the semigroup property, $t \mapsto \|P_t\|_{1\to 2}$ is decreasing. Thus $t + is \mapsto \|P_t\|_{1\to 2}$ is bounded on $\{z \in \mathbb{C} \mid \text{Re} z \ge \delta\}$ for all $\delta > 0$.

Corollary 6.5. If (P_t) is ultracontractive, then the map

$$(0,\infty) \to L^1(\mathcal{M},\tau), a \mapsto P_t a$$

is differentiable for all $a \in L^1(\mathcal{M}, \tau)$.

Equivalently one can say that P_t maps $L^1(\mathcal{M},\tau)$ into $D(\mathcal{L}^{(1)})$ for all t > 0. Once again the Ornstein–Uhlenbeck semigroup shows that this is not the case in general.

Theorem 6.6. Assume that (P_t) is ultracontractive. If \mathscr{E} satisfies $GE(K,\infty)$, then (P_t) is an EVI_K gradient flow of Ent.

Proof. First note that bounded density operators lie dense in $(D(\text{Ent}), \mathcal{W})$ by Corollary 4.26 and the ultracontractivity of (P_t) . We tacitly assume $K \neq 0$, but all formulas can be easily adapted to the case K = 0.

Using the semigroup property of (P_t) and a standard approximation argument, it suffices to show that

$$\mathcal{W}(P_t\rho,\sigma)^2 \le \frac{1 - e^{-2Kt}}{2Kt} \mathcal{W}(\rho,\sigma)^2 + 2t(\operatorname{Ent}(\sigma) - \operatorname{Ent}(P_t\rho))$$
(6.1)

for all $\rho, \sigma \in D(\text{Ent}) \cap \mathcal{M}$ with $\mathcal{W}(\rho, \sigma) < \infty$, and t > 0.

Given an admissible curve $(\rho_s) \in C^1([0,1];L^1(\mathcal{M},\tau))$ let $\sigma_{s,t} = P_{st}\rho_s$. In order to establish (6.1), it suffices to show

$$\int_{0}^{1} \|D_{s}\sigma_{s,t}\|_{\sigma_{s,t}}^{2} ds \leq \frac{1 - e^{-2Kt}}{2Kt} \int_{0}^{1} \|D\rho_{s}\|_{\rho_{s}}^{2} ds + 2t(\operatorname{Ent}(\sigma) - \operatorname{Ent}(P_{t}\rho))$$
(6.2)

for every admissible curve (ρ_s) connecting σ and ρ .

Finally, let $\rho_s^{\varepsilon} = (1+\varepsilon)^{-1}(\rho_s+\varepsilon)$ and $\sigma_{s,t}^{\varepsilon} = P_{st}\rho_s^{\varepsilon}$. A direct calculation shows that $(\rho_s^{\varepsilon})_{s\in[0,1]}$ is admissible, continuously L^1 -differentiable and

$$\int_0^1 \|D\rho_s\|_{\rho_s}^2 ds = \lim_{\varepsilon \to 0} \int_0^1 \|D\rho_s^\varepsilon\|_{\rho_s^\varepsilon}^2 ds,$$

while the lower semicontinuity of the action functional (Theorem 3.30) implies

$$\int_0^1 \|D_s \sigma_{s,t}\|_{\sigma_{s,t}}^2 ds \leq \liminf_{\varepsilon \to 0} \int_0^1 \|D_s \sigma_{s,t}^\varepsilon\|_{\sigma_{s,t}^\varepsilon}^2 ds$$

Moreover, the lower semicontinuity gives $\operatorname{Ent}(P_t\rho) \leq \operatorname{liminf}_{\varepsilon \to 0} \operatorname{Ent}(P_t\rho^{\varepsilon})$ and a direct calculation show $\operatorname{Ent}(\sigma) = \operatorname{lim}_{\varepsilon \to 0} \operatorname{Ent}(\sigma^{\varepsilon})$.

Otherwise replacing ρ_s by ρ_s^{ε} , we can therefore assume that (ρ_s) , and therefore also $(\sigma_{s,t})$, is uniformly (for the latter in *s* and *t*) bounded away from zero. Also, by Lemma 3.22, we can assume that (ρ_s) has constant speed.

Since (P_t) is ultracontractive, we have $\sigma_{s,t} \in D(\mathscr{L}^{(2)}) \cap \mathscr{M}$ for all $s \in (0,1)$ and t > 0. Consequently, $(\sigma_{s,t})_s \in C^1((0,1); L^1(\mathscr{M}, \tau))$ and

$$\frac{d}{ds}\sigma_{s,t} = P_{st}\dot{\rho}_s - t\mathscr{L}^{(2)}\sigma_{s,t}.$$

Let $a \in \mathscr{A}_{AM}$. By $GE(K, \infty)$ and Lemma 3.10 we have

$$|\tau(aP_{st}\dot{\rho}_s)| = |\tau(\dot{\rho}_sP_{st}a)| \le e^{-Kst} \|D\rho_s\|_{\rho_s} \|\partial a\|_{\sigma_{s,t}}.$$

Thus there exists $\xi_{s,t} \in \mathcal{H}_{\sigma_{s,t}}$ with $\|\xi_{s,t}\|_{\sigma_{s,t}} \le e^{-Kst} \|D\rho_s\|_{\rho_s}$ such that $\tau(aP_{st}\dot{\rho}_s) = 0$ $\langle \partial a, \xi_{s,t} \rangle_{\sigma_{s,t}}$ for all $a \in \mathscr{A}_{AM}$.

On the other hand let $\eta_{s,t} = \partial \log(\sigma_{s,t})$. A direct calculation shows $\tau(a \mathscr{L}^{(2)} \sigma_{s,t}) =$ $\langle \partial a, \eta_{s,t} \rangle_{\sigma_{s,t}}$ for all $a \in \mathscr{A}_{AM}$. Hence $(\sigma_{s,t})$ is admissible with $D_s \sigma_{s,t} = \xi_{s,t} - t \eta_{s,t}$. Hence

$$\begin{split} \int_{0}^{1} \|D_{s}\sigma_{s,t}\|_{\sigma_{s,t}}^{2} ds &= \int_{0}^{1} \|\xi_{s,t} - t\eta_{s,t}\|_{\sigma_{s,t}}^{2} ds \\ &\leq \int_{0}^{1} (\|\xi_{s,t}\|_{\sigma_{s,t}}^{2} - 2t\langle\xi_{s,t} - t\eta_{s,t}, \eta_{s,t}\rangle_{\sigma_{s,t}}) ds \\ &\leq \int_{0}^{1} e^{-2Kst} \|D\rho_{s}\|_{\rho_{s}}^{2} ds - 2t \int_{0}^{1} \langle\xi_{s,t} - t\eta_{s,t}, \eta_{s,t}\rangle_{\sigma_{s,t}} ds \\ &= \frac{1 - e^{-2Kt}}{2Kt} \int_{0}^{1} \|D\rho_{s}\|_{\rho_{s}}^{2} ds - 2t \int_{0}^{1} \langle\xi_{s,t} - t\eta_{s,t}, \eta_{s,t}\rangle_{\sigma_{s,t}} ds. \end{split}$$

By Lemma 4.5 the map $s \mapsto \text{Ent}(\sigma_{s,t})$ is locally absolutely continuous and

$$\frac{d}{ds}\operatorname{Ent}(\sigma_{s,t}) = \tau(\log(\sigma_{s,t})(P_{st}\dot{\rho}_s - t\mathscr{L}^{(2)}\sigma_{s,t})).$$

Note that since $\sigma_{s,t} \in D(\mathscr{L}^{(2)})$ is bounded and bounded away from zero, we have $\log(\sigma_{s,t}) \in D(\mathcal{E}) \cap \mathcal{M}$. By Proposition 5.7 we can choose a uniformly bounded sequence (a_k) in \mathscr{A}_{AM} such that $a_k \to \log(\sigma_{s,t})$ with respect to $\|\cdot\|_{\mathscr{E}}$. Hence

$$\tau(\log(\sigma_{s,t})P_{st}\dot{\rho}_s) = \lim_{k \to \infty} \tau(a_k P_{st}\dot{\rho}_s) = \lim_{k \to \infty} \langle \partial a_k, \xi_{s,t} \rangle_{\sigma_{s,t}} = \langle \partial \log(\sigma_{s,t}), \xi_{s,t} \rangle_{\sigma_{s,t}},$$

where the last equality is justified since $\sigma_{s,t} \in \mathcal{M}$.

On the other hand,

$$\tau(\log(\sigma_{s,t})\mathscr{L}^{(2)}\sigma_{s,t}) = \lim_{k \to \infty} \tau(a_k \mathscr{L}^{(2)}\sigma_{s,t}) = \lim_{k \to \infty} \langle \partial a_k, \eta_{s,t} \rangle_{\sigma_{s,t}} = \langle \eta_{s,t}, \eta_{s,t} \rangle_{\sigma_{s,t}}$$

with the same justification for passing to the limit in the last equality.

Therefore

$$\operatorname{Ent}(P_t \rho) - \operatorname{Ent}(\sigma) = \int_0^1 \frac{d}{ds} \tau(\sigma_{s,t} \log \sigma_{s,t}) ds$$
$$= \int_0^1 \tau(\log(\sigma_{s,t})(P_{st}\dot{\rho}_s - t\mathscr{L}^{(2)}\sigma_{s,t}) ds$$
$$= \int_0^1 (\langle \xi_{s,t}, \eta_{s,t} \rangle_{\sigma_{s,t}} - t \| \eta_{s,t} \|_{\sigma_{s,t}}^2) ds.$$

This proves (6.2).

6.3 Mollification

As mentioned in the previous section, we need some more technical preparations before we can launch into the proof of the gradient flow characterization. These will be done in this section. Compared to the ultracontractive case, in general the trajectories of the heat flow miss both "spatial" and temporal regularity. In the following we will study how to approximate these trajectories by more regular curves while at the same time bounding several important quantities.

We first introduce a mollified version of (P_t) , which is a standard tool in the theory of operator semigroups. Let $\kappa \in C_c^{\infty}((0,\infty))$ be a positive function with support in (1,2) and $\int_0^{\infty} \kappa(r) dr = 1$. For $\varepsilon > 0$ and $p \in [1,\infty]$ define

$$\mathfrak{p}^{\varepsilon}: L^{p}(\mathcal{M}, \tau) \longrightarrow L^{p}(\mathcal{M}, \tau), \, \mathfrak{p}^{\varepsilon}a = \frac{1}{\varepsilon} \int_{0}^{\infty} \kappa\left(\frac{r}{\varepsilon}\right) P_{r}a \, dr,$$

where the integral is to be understood as Bochner integral if $p < \infty$ and as Pettis integral for the σ -weak topology if $p = \infty$. It is clear that $\mathfrak{p}^{\varepsilon}$ is positive and contractive on all L^p spaces.

The following Lemma is standard, see for example the proof of [EN00, Proposition 1.8].

Lemma 6.7. Let $p \in [1,\infty]$ and $a \in L^p(\mathcal{M},\tau)$. For all $\varepsilon > 0$ one has $\mathfrak{p}^{\varepsilon}a \in D(\mathscr{L}^{(p)})$ and

$$\mathscr{L}^{(p)}\mathfrak{p}^{\varepsilon}a = \frac{1}{\varepsilon^2}\int_0^{\infty}\kappa'\Big(\frac{r}{\varepsilon}\Big)P_ra\,dr.$$

If $p < \infty$, then $\mathfrak{p}^{\varepsilon} a \to a$ in $L^{p}(\mathcal{M}, \tau)$, and if $p = \infty$, then $\mathfrak{p}^{\varepsilon} a \to a \sigma$ -weakly as $\varepsilon \to 0$. If $a \in D(\mathscr{E})$, then $\mathfrak{p}^{\varepsilon} a \in D(\mathscr{E})$ and $\mathfrak{p}^{\varepsilon} a \to a$ with respect to $\|\cdot\|_{\mathscr{E}}$ as $\varepsilon \to 0$.

Lemma 6.8. Assume that \mathscr{E} satisfies $\operatorname{GE}(K,\infty)$ for some $K \in \mathbb{R}$. If $a \in \mathcal{M}$, then $\mathfrak{p}^{\varepsilon}a \in \mathscr{A}_{\mathrm{LM}}$ for $\varepsilon > 0$. Moreover, if $a \in \mathscr{A}_{\mathrm{AM}}$, then

$$\|\partial \mathfrak{p}^{\varepsilon} a\|_{\rho}^{2} \leq \|\partial a\|_{\rho}^{2} \sup_{r \in [0, 2\varepsilon]} e^{-2Kr}$$

and $\mathfrak{p}^{\varepsilon}a \to a$ in $\tilde{\mathscr{H}}_{\rho}$ for all $\rho \in \mathscr{D}(\mathcal{M}, \tau)$.

Proof. Let $\rho \in \mathcal{D}(\mathcal{M}, \tau) \cap \mathcal{M}$ be invertible. By $GE(K, \infty)$ we have

$$\|\partial P_r a\|_{\rho}^2 \le e^{-2K(r-\varepsilon)} \|\partial P_{\varepsilon} a\|_{P_{r-\varepsilon}\rho}^2$$

whenever $r \ge \varepsilon$. The right-hand side is bounded above by $e^{-2K(r-\varepsilon)} \|P_{\varepsilon}a\|_{LM}^2$, which is finite by Proposition 5.7. By Lemma 2.5 the map $a \mapsto \|\partial a\|_{\rho}^2$ is lower semicontinuous. Thus we can apply Jensen's inequality (compare the proof of Lemma 3.33)

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to see that

$$\|\partial \mathfrak{p}^{\varepsilon} \alpha\|_{\rho}^{2} \leq \frac{1}{\varepsilon} \int_{\varepsilon}^{2\varepsilon} \kappa\left(\frac{r}{\varepsilon}\right) \|\partial P_{r} \alpha\|_{\rho}^{2} dr \leq \frac{\|P_{\varepsilon} \alpha\|_{\mathrm{LM}}^{2}}{\varepsilon} \int_{0}^{\infty} e^{-2K(r-\varepsilon)} \kappa\left(\frac{r}{\varepsilon}\right) dr$$

The right-hand side is clearly bounded independently of ρ . Hence $\mathfrak{p}^{\varepsilon} a \in \mathscr{A}_{LM}$.

Now let $\rho \in \mathcal{D}(\mathcal{M}, \tau)$ be arbitrary and assume that $a \in \mathscr{A}_{AM}$. By $GE(K, \infty)$ we have

$$\|\partial \mathfrak{p}^{\varepsilon} a\|_{\rho}^{2} \leq \frac{1}{\varepsilon} \int_{0}^{\infty} \kappa\left(\frac{r}{\varepsilon}\right) \|\partial P_{r} a\|_{\rho}^{2} dr \leq \frac{1}{\varepsilon} \int_{0}^{\infty} \kappa\left(\frac{r}{\varepsilon}\right) e^{-2Kr} \|\partial a\|_{P_{r}\rho}^{2} dr$$

It follows from the upper semicontinuity and concavity of $\rho \mapsto \|\partial a\|_{\rho}^2$ by an application of Jensen's inequality that

$$\|\partial \mathfrak{p}^{\varepsilon} a\|_{\rho}^{2} \leq \left(\sup_{r \in [0, 2\varepsilon]} e^{-2Kr}\right) \frac{1}{\varepsilon} \int_{0}^{\infty} \kappa\left(\frac{r}{\varepsilon}\right) \|\partial a\|_{P_{r}\rho}^{2} dr \leq \|\partial a\|_{\mathfrak{p}^{\varepsilon}\rho}^{2} \sup_{r \in [0, 2\varepsilon]} e^{-2Kr}.$$

Hence

$$\limsup_{\varepsilon \to 0} \|\partial \mathfrak{p}^{\varepsilon} a\|_{\rho}^{2} \le \limsup_{\varepsilon \to 0} \|\partial a\|_{\mathfrak{p}^{\varepsilon} \rho}^{2} \le \|\partial a\|_{\rho}^{2}$$
(6.3)

by Theorem 2.14.

Thus $(\partial \mathfrak{p}^{\varepsilon} a)_{\varepsilon>0}$ is a bounded net in the Hilbert space $D(\hat{
ho}^{1/2})$ with inner product

$$\langle \cdot, \cdot \rangle_{\mathcal{H}} + \langle \hat{\rho}^{1/2} \cdot, \hat{\rho}^{1/2} \cdot \rangle_{\mathcal{H}}$$

On the other hand, since $\partial \mathfrak{p}^{\varepsilon} a \to \partial a$ in \mathscr{H} , every weak limit point of $(\mathfrak{p}^{\varepsilon} a)_{\varepsilon>0}$ in $D(\hat{\rho}^{1/2})$ coincides with ∂a . Thus $\partial \mathfrak{p}^{\varepsilon} a \to \partial a$ also weakly in $\tilde{\mathscr{H}}_{\rho}$. Finally, (6.3) implies that the convergence is indeed strong.

Lemma 6.9. Let $\rho \in \mathcal{D}(\mathcal{M}, \tau)$. For all $\varepsilon > 0$ one has $\operatorname{Ent}(\mathfrak{p}^{\varepsilon}(\rho)) \leq \operatorname{Ent}(P_{\varepsilon}\rho)$. If $\rho \in D(\operatorname{Ent})$, then $\mathfrak{p}^{\varepsilon}(\rho) \in D(\operatorname{Ent})$ and $\mathcal{W}(\rho, \mathfrak{p}^{\varepsilon}(\rho)) \to 0$ as $\varepsilon \to 0$.

Proof. Since the entropy is a convex lower semicontinuous functional and decreasing along heat flow trajectories, Jensen's inequality implies

$$\operatorname{Ent}(\mathfrak{p}^{\varepsilon}(\rho)) \leq \frac{1}{\varepsilon} \int_{\varepsilon}^{2\varepsilon} \kappa\left(\frac{r}{\varepsilon}\right) \operatorname{Ent}(P_{r}\rho) dr \leq \operatorname{Ent}(P_{\varepsilon}\rho).$$

If $\rho \in D(\text{Ent})$, then $(P_t \rho)_{t \ge 0}$ is admissible by Corollary 4.26. Let

$$\sigma \colon [0,1] \longrightarrow \mathcal{D}(\mathcal{M},\tau), \, \sigma_t = \frac{1}{\varepsilon} \int_0^\infty \kappa \left(\frac{r}{\varepsilon}\right) P_{rt} \rho \, dr$$

and

$$\sigma^{n}: [0,1] \longrightarrow \mathscr{D}(\mathscr{M},\tau), \sigma^{n}_{t} = \sum_{k=1}^{2n} P_{\frac{k-1}{n}\varepsilon t} \rho \cdot \int_{\frac{k-1}{n}}^{\frac{k}{n}} \kappa(r) dr$$

Since $(P_{rt}\rho)_{r\geq 0}$ is L^1 continuous, we have $\sigma_t^n \to \sigma_t$ in L^1 for all $t \in [0, 1]$. As σ^n is a convex combination of admissible curves, it is itself admissible and

$$\|D_t\sigma_t^n\|_{\sigma_t^n}^2 \leq \sum_{k=1}^{2n} \|D_tP_{\frac{k-1}{n}\varepsilon t}\rho\|^2 \cdot \int_{\frac{k-1}{n}}^{\frac{k}{n}} \kappa(r) dr$$

by Lemma 3.24.

It follows from Theorem 3.30 and Corollary 4.26 that σ is an admissible curve connecting ρ and $\mathfrak{p}^{\varepsilon}(\rho)$ with

$$\begin{split} \int_0^1 \|D\sigma_t\|_{\sigma_t}^2 dt &\leq \liminf_{n \to \infty} \sum_{k=1}^{2n} \int_0^1 \|D_t P_{\frac{k-1}{n}\varepsilon t}\|^2 dt \cdot \int_{\frac{k-1}{n}}^{\frac{k}{n}} \kappa(r) dr \\ &\leq 2\varepsilon \int_0^{2\varepsilon} \|DP_t \rho\|_{P_t \rho}^2 dt \cdot \int_0^2 \kappa(r) dr \\ &\to 0 \end{split}$$

as $\varepsilon \to 0$.

Corollary 6.10. The space $D(\mathcal{L}^{(1)}) \cap D(\text{Ent})$ is dense in $(D(\text{Ent}), \mathcal{W})$.

Lemma 6.11. Assume that the logarithmic mean is regular for \mathscr{E} and \mathscr{E} satisfies $\operatorname{GE}(K,\infty)$. If $(\rho_t)_{t\in[0,1]}$ is an admissible curve in $\mathscr{D}(\mathcal{M},\tau)$, then $(\mathfrak{p}^{\varepsilon}\rho_t)_{t\in[0,1]}$ is admissible for all $\varepsilon > 0$ and

$$\begin{split} \limsup_{\varepsilon \to 0} &\int_0^1 \|D_t \mathfrak{p}^{\varepsilon}(\rho_t)\|_{\mathfrak{p}^{\varepsilon}(\rho_t)}^2 dr \leq \int_0^1 \|D\rho_t\|_{\rho_t}^2 dr,\\ \limsup_{\varepsilon \to 0} &\sup_{t \in [0,1]} \|D_t \mathfrak{p}^{\varepsilon} \rho_t\|_{\mathfrak{p}_{\varepsilon} \rho_t}^2 \leq \underset{t \in [0,1]}{\mathrm{ess}} \|D\rho_t\|_{\rho_t}. \end{split}$$

If additionally $(\rho_t) \in C^1([0,1]; L^1(\mathcal{M}, \tau))$, then $(\mathfrak{p}^{\varepsilon} \rho_t)_t \in C^1([0,1]; L^1(\mathcal{M}, \tau))$ and $\frac{d}{dt} \mathfrak{p}^{\varepsilon} \rho_t = \mathfrak{p}^{\varepsilon} \dot{\rho}_t$.

Proof. Let $\rho_s^{\varepsilon} = \mathfrak{p}^{\varepsilon} \rho_s$. For $a \in \mathscr{A}_{AM}$ and $s, t \in [0, 1]$ we have

$$\begin{split} |\tau(a(\rho_t^{\varepsilon} - \rho_s^{\varepsilon}))| &\leq \frac{1}{\varepsilon} \int_0^{\infty} \kappa \left(\frac{r}{\varepsilon}\right) |\tau(P_r a(\rho_t - \rho_s))| \, dr \\ &\leq \frac{1}{\varepsilon} \int_0^{2\varepsilon} \kappa \left(\frac{r}{\varepsilon}\right) \int_s^t \|\partial P_r a\|_{\rho_u} \|D\rho_u\|_{\rho_u} \, du \, dr \\ &\leq \int_s^t \|D\rho_u\|_{\rho_u} \frac{1}{2\varepsilon} \int_0^{\varepsilon} e^{-Kr} \kappa \left(\frac{r}{\varepsilon}\right) \|\partial a\|_{P_r \rho_u} \, dr \, du, \end{split}$$

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where we used Proposition 5.7 and Lemma 5.11 in the second and $\operatorname{GE}(K,\infty)$ in the third inequality. Let $C(\varepsilon) = \sup_{r \in [0,2\varepsilon]} e^{-Kr}$ and note that $C(\varepsilon) \to 1$ as $\varepsilon \to 0$. An application of Jensen's inequality yields

$$\frac{1}{\varepsilon}\int_0^\infty \kappa\left(\frac{r}{\varepsilon}\right)\|\partial a\|_{P_r\rho_u}\,dr \leq \left(\frac{1}{\varepsilon}\int_0^\infty \kappa\left(\frac{r}{\varepsilon}\right)\|\partial a\|_{P_r\rho_u}^2\,dr\right)^{1/2} \leq \|\partial a\|_{\rho_u^\varepsilon}^\varepsilon.$$

Hence

$$|\tau(a(\rho_t^{\varepsilon}-\rho_s^{\varepsilon}))| \leq C(\varepsilon) \int_s^t \|D\rho_u\|_{\rho_u} \|\partial a\|_{\rho_u^{\varepsilon}} \, du.$$

Thus $(\rho_t^{\varepsilon})_{t \in [0,1]}$ is admissible with $\|D_t \rho_t^{\varepsilon}\|_{\rho_t^{\varepsilon}} \le C(\varepsilon) \|D\rho_t\|_{\rho_t}$ for a.e. $t \in [0,1]$. This settles both of the claimed inequalities.

Finally, the claim concerning the differentiability follows easily from an application of the dominated convergence theorem. $\hfill\square$

Lemma 6.12. Assume that the logarithmic mean is regular for \mathscr{E} and \mathscr{E} satisfies $\operatorname{GE}(K,\infty)$ for some $K \in \mathbb{R}$. For every admissible curve $(\rho_s)_{s \in [0,1]} \in C^1([0,1];L^1(\mathcal{M},\tau))$ there exists a sequence $\varepsilon_n \searrow 0$ such that the curves $(\rho_s^n)_{s \in [0,1]}$ defined by $\rho_s^n = (1 + 1/n)^{-1} \mathfrak{p}^{\varepsilon_n}(\rho_s + 1/n)$ satisfy

- (a) $(\rho_s^n)_{s \in [0,1]} \in C^1([0,1]; L^1(\mathcal{M}, \tau))$ for $n \in \mathbb{N}$,
- (b) $\rho_s^n \in D(\mathcal{L}^{(1)})$ for $s \in [0, 1]$, $n \in \mathbb{N}$,
- (c) $\rho_s^n \ge \frac{1}{2n}$ for $s \in [0, 1], n \in \mathbb{N}$,
- (d) $\rho_s^n \to \rho_s$ in $L^1(\mathcal{M}, \tau)$ for $s \in [0, 1]$,
- (e) $\operatorname{Ent}(\rho_0^n) \leq \operatorname{Ent}(\rho_0)$, $\operatorname{Ent}(\rho_1^n) \leq \operatorname{Ent}(\rho_1)$ for $n \in \mathbb{N}$,
- (f) $\limsup_{n \to \infty} \int_0^1 \|D\rho_s^n\|_{\rho_s^n}^2 ds \le \int_0^1 \|D\rho_s\|_{\rho_s}^2 ds, \\ \limsup_{n \to \infty} \operatorname{ess\,sup}_{s \in [0,1]} \|D\rho_s^n\|_{\rho_s^n}^2 \le \operatorname{ess\,sup}_{s \in [0,1]} \|D\rho_s\|_{\rho_s}^2.$

Proof. Let $\tilde{\rho}_s^n = (1+1/n)^{-1}(\rho_s+1/n)$. Clearly the curves $(\tilde{\rho}_s^n)_s$ satisfy (a), (c) and (d). Property (e) follows from the convexity of Ent. Moreover,

$$\tau(a(\tilde{\rho}_t^n - \tilde{\rho}_s^n)) = (1 + 1/n)^{-1} \tau(a(\rho_t - \rho_s))$$

implies $\|D\tilde{\rho}_{s}^{n}\|_{\tilde{\rho}_{s}^{n}} = (1+1/n)^{-1} \|D\rho_{s}\|_{\rho_{s}}.$

Now let $\rho_s^n = \mathfrak{p}^{\varepsilon_n} \tilde{\rho}_s^n$ for a strictly positive null sequence (ε_n) . The curve (ρ_s^n) satisfies (a) by Lemma 6.11, (b) by Lemma 6.7 and (c) as a direct consequence of the positivity of (P_t) . Moreover,

$$\|\rho_s^n - \rho_s\|_1 \le \|\mathfrak{p}^{\varepsilon_n}\tilde{\rho}_s^n - \mathfrak{p}^{\varepsilon_n}\rho_s\|_1 + \|\mathfrak{p}^{\varepsilon_n}\rho_s - \rho_s\|_1 \le \|\tilde{\rho}_s^n - \rho_s\|_1 + \|\mathfrak{p}^{\varepsilon_n}\rho_s - \rho_s\|_1 \to 0.$$

Thus (d) is satisfied. Property (e) follows from Lemma 6.9. Finally, by Lemma 6.11 we can achieve (f) if we choose (ε_n) appropriately.

Lemma 6.12 gives entropy estimates at the endpoints of the connecting curves, but we will need entropy estimates for the entire curve. In [AGS15] these are established via a logarithmic Harnack inequality. Since the proof relies on the second-order chain rule for the Laplacian, there seems to be little hope to generalize it beyond the local setting. Indeed, obtaining Harnack inequalities from Bakry–Émery-type Ricci curvature bounds has turned out to be exceptionally challenging in the non-local case. For the gradient estimate used here, there seem to be no results in this direction even in the case of finite graphs (see however [CLY14, BHL⁺15, DKZ17, Mü18] for Harnack inequalities on graphs under related assumptions).

Instead we adopt a different approach. The kind of entropy estimate we need is a consequence of the EVI gradient flow characterization (see [DS08, Theorem 3.1]) and it turns out that one can run the portion of the proof needed to show only this consequence with the weaker regularity estimates already established in Lemma 6.12. This is done in the next proposition.

Proposition 6.13 (Entropy regularization). Assume that \mathscr{E} satisfies $GE(K,\infty)$. If $\rho_0, \rho_1 \in \mathscr{D}(\mathcal{M}, \tau)$, then

$$\operatorname{Ent}(P_t\rho_1) \le \operatorname{Ent}(\rho_0) + \frac{1}{2t} \left(\int_0^1 e^{-2Kst} \, ds \right) \mathcal{W}^2(\rho_0, \rho_1)$$

for t > 0*.*

Proof. Let

$$C(K,t) = \int_0^1 e^{-2Kst} \, ds.$$

We can assume that $\operatorname{Ent}(\rho_0) < \infty$ and $\mathcal{W}(\rho_0, \rho_1) < \infty$. By Lemmas 3.22 and 3.33, for every $\varepsilon > 0$ there exists an admissible curve $(\rho_s) \in C^1([0,1]; L^1(\mathcal{M}, \tau))$ such that

$$\operatorname{ess\,sup}_{s\in[0,1]} \|D\rho_s\|_{\rho_s}^2 \le \mathcal{W}(\rho_0,\rho_1)^2 + \varepsilon$$

Let $(\rho_s^n)_{s \in [0,1]}$, $n \in \mathbb{N}$, be curves defined in Lemma 6.12. If we can show

$$\operatorname{Ent}(P_t \rho_1^n) \le \operatorname{Ent}(\rho_0^n) + \frac{C(K, t)}{2t} \operatorname{ess\,sup}_{s \in [0, 1]} \|D\rho_s^n\|_{\rho_s^n}^2,$$
(6.4)

then the claim of the proposition follows by taking the limit $n \to \infty$ and then the limit $\varepsilon \to 0$.

Let (C_k) be an increasing sequence in $C^1((0,\infty))$ such that each C_k is increasing, 1-Lipschitz, $C_k(s) = s$ if $s \le k - 1$ and $C_k(s) = k$ if $s \ge n$. Let $f_k = C_k \circ \log$ and

$$F_k: (0,\infty) \to \mathbb{R}, t \mapsto \int_0^t (f_k(s)+1) ds$$

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Note that $f_k(s) \nearrow \log s$ and by monotone convergence also $F_k(t) \nearrow t \log t$.

Thus, in order to prove (6.4), it suffices to show

$$\tau(F_k(P_t\rho_1)) \le \tau(F_k(\rho_0)) + \frac{C(K,t)}{2t} \int_0^1 \|D\rho_s^n\|_{\rho_s^n}^2 \, ds.$$
(6.5)

Let $\sigma_s = P_{st}\rho_s^n$. Since $\rho_s^n \in D(\mathscr{L}^{(1)})$ for all $s \in [0,1]$, the curve (σ_s) is L^1 -differentiable with derivative

$$\dot{\sigma}_s = P_{st}\dot{\rho}_s^n - t\mathscr{L}^{(1)}\sigma_s.$$

Hence, by Lemma 4.5,

$$\tau(F_k(P_t\rho_1) - F_k(\rho_0)) = \int_0^1 \tau(f_k(\sigma_s)(P_{st}\dot{\rho}_s^n - t\mathcal{L}^{(1)}\sigma_s)) ds.$$
(6.6)

Since (P_{st}) maps \mathcal{M} into \mathcal{A}_{LM} by Proposition 5.7, we have

$$\begin{aligned} |\tau(f_{k}(\sigma_{s})P_{st}\dot{\rho}_{s}^{n})| &\leq \|\partial P_{st}f_{k}(\sigma_{s})\|_{\rho_{s}^{n}}\|D\rho_{s}^{n}\|_{\rho_{s}^{n}} \\ &\leq e^{-Kst}\|\partial f_{k}(\sigma_{s})\|_{\sigma_{s}}\|D\rho_{s}^{n}\|_{\rho_{s}^{n}} \\ &\leq \frac{e^{-2Kst}}{2t}\|D\rho_{s}^{n}\|_{\rho_{s}^{n}}^{2} + \frac{t}{2}\|\partial f_{k}(\sigma_{s})\|_{\sigma_{s}}^{2}, \end{aligned}$$
(6.7)

where we used the admissibility of $(\rho_s^n)_s$ and Lemma 5.11 for the first inequality, $GE(K,\infty)$ for the second and Young's inequality for the third.

We are now going to estimate the second summand. Note that by definition $0 \le f'_k(s) \le 1/s$ and for each fixed $k \in \mathbb{N}$ there exists $l \in \mathbb{N}$ such that $f_k(s) = f_k(s \land l)$ for all s > 0.

Since $\sigma_s \in D(\mathscr{L}^{(1)})$, we have $\sigma_s \wedge m \in D(\mathscr{E})$ for all $m \in \mathbb{N}$ by Lemma 4.17. Thus, writing *e* for the joint spectral measure of $L(\sigma_s \wedge m)$ and $R(\sigma_s \wedge m)$,

$$\begin{split} \|\partial f_k(\sigma_s)\|_{\sigma_s \wedge m}^2 &= \|\partial f_k(\sigma_s \wedge m)\|_{\sigma_s \wedge m}^2 \\ &= \int_{(0,\infty)^2} \tilde{f}_k(s,t)^2 \widehat{\log}(s,t) d \langle e(s,t) \partial (\sigma_s \wedge m), \partial (\sigma_s \wedge m) \rangle_{\mathcal{H}} \\ &\leq \langle \tilde{f}_k(L(\sigma_s \wedge m), R(\sigma_s \wedge m)) \partial (\sigma_s \wedge m), \partial (\sigma_s \wedge m) \rangle_{\mathcal{H}} \\ &= \langle \partial f_k(\sigma_s), \partial (\sigma_s \wedge m) \rangle_{\mathcal{H}} \\ &\leq \tau(f_k(\sigma_s) \mathcal{L}^{(1)} \sigma_s), \end{split}$$

where we used $\tilde{f}_k \leq \log$ and Lemma 4.17. Now we can let *m* go to infinity to obtain

$$\|\partial f_k(\sigma_s)\|_{\sigma_s}^2 \leq \tau(f_k(\sigma_s)\mathcal{L}^{(1)}\sigma_s).$$

If we plug this inequality into (6.7), we get

$$|\tau(f_k(\sigma_s)P_{st}\dot{\rho}_s^n)| \leq \frac{e^{-2Kst}}{2t} \|D\rho_s^n\|_{\rho_s^n}^2 + \frac{t}{2}\tau(f_k(\sigma_s)\mathcal{L}^{(1)}\sigma_s),$$

which we can then apply to (6.6) to obtain

$$\tau(F_{k}(P_{t}\rho_{1}) - F_{k}(\rho_{0})) \leq \int_{0}^{1} \frac{e^{-2Kst}}{2t} \|D\rho_{s}^{n}\|_{\rho_{s}^{n}}^{2} ds$$

$$\leq \frac{C(K,t)}{2t} \operatorname{ess\,sup}_{s \in [0,1]} \|D\rho_{s}^{n}\|_{\rho_{s}^{n}}^{2}.$$
(6.8)

This settles (6.5).

Corollary 6.14. Assume that & satisfies $\operatorname{GE}(K,\infty)$ for some $K \in \mathbb{R}$. For every admissible curve $(\rho_s)_{s \in [0,1]} \in C^1([0,1];L^1(\mathcal{M},\tau))$ with $\operatorname{Ent}(\rho_0) < \infty$ the curves $(\rho_s^n)_{s \in [0,1]}$ defined in Lemma 6.12 satisfy

- (g) $\sup_{s \in [0,1]} \operatorname{Ent}(\rho_s^n) < \infty$ for $n \in \mathbb{N}$,
- (h) $\sup_{t\geq 0} \sup_{s\in[0,1]} \mathscr{I}(P_t\rho_s^n) < \infty$ for $n \in \mathbb{N}$.

Proof. As in the proof of Lemma 6.12 let $\tilde{\rho}_s^n = (1 + 1/n)^{-1}(\rho_s + 1/n)$ and $\rho_s^n = \mathfrak{p}^{\varepsilon_n} \tilde{\rho}_s^n$ for a suitably chosen strictly positive null sequence (ε_n) . By Lemma 6.9 we have $\operatorname{Ent}(\rho_s^n) \leq \operatorname{Ent}(P_{\varepsilon_n} \tilde{\rho}_s^n)$. We can apply Theorem 6.13 to the right-hand side to get

$$\operatorname{Ent}(P_{\varepsilon_n}\tilde{\rho}_s^n) \leq \operatorname{Ent}(\tilde{\rho}_0^n) + C(K,\varepsilon_n) \mathcal{W}(\tilde{\rho}_0^n,\tilde{\rho}_s^n)^2 \\ \leq \frac{n}{n+1} \left(\operatorname{Ent}(\rho_0) + C(K,\varepsilon_n) \int_0^1 \|D\rho_r\|_{\rho_r}^2 dr \right)^2$$

The latter is clearly bounded independently of $s \in [0, 1]$. This proves (g).

To establish (h), we use Jensen's inequality (which is applicable according to Lemma 4.22 and Proposition 4.23) to see that

$$\mathscr{I}(P_t\rho_s^n) \leq \frac{1}{\varepsilon_n} \int_{\varepsilon_n}^{\infty} \kappa\left(\frac{r}{\varepsilon_n}\right) \mathscr{I}(P_{t+r}\tilde{\rho}_s^n) dr \leq \frac{\|\kappa\|_{\infty}}{\varepsilon_n} \int_{\varepsilon_n}^{\infty} \mathscr{I}(P_rP_t\tilde{\rho}_s^n) dr$$

By Corollary 4.26, we have

$$\int_{\varepsilon_n}^{\infty} \mathscr{I}(P_r P_t \tilde{\rho}_s^n) dr \leq \operatorname{Ent}(P_{t+\varepsilon_n} \tilde{\rho}_s^n) \leq \operatorname{Ent}(P_{\varepsilon_n} \tilde{\rho}_s^n).$$

We have already seen in the first part that the right-hand side is bounded independently of $s \in [0, 1]$.

6.4 Proof of the gradient flow characterization: the general case

With preparations done in the previous section, we can immediately launch the proof of the gradient flow characterization. With the exception of some technical difficulties, we follow the general outline of Section 6.2.

Theorem 6.15. Assume that τ is finite, $L^1(\mathcal{M}, \tau)$ is separable and the logarithmic mean is regular with respect to \mathcal{E} . If \mathcal{E} satisfies $\operatorname{GE}(K, \infty)$, then (P_t) is an EVI_K gradient flow of Ent.

Proof. The continuity of (P_t) with respect to \mathcal{W} is a consequence of Theorem 5.13. Moreover, it was proven in Corollary 4.26 that $(P_t)_{t\geq 0}$ is strongly continuous with respect to \mathcal{W} and that Ent is decreasing along $(P_t\rho)$. It remains to show that

$$\frac{1}{2}\frac{d^{+}}{dt}\mathcal{W}(P_{t}\rho_{1},\rho_{0})^{2} + \frac{K}{2}\mathcal{W}(\rho_{0},\rho_{1})^{2} + \operatorname{Ent}(P_{t}\rho_{1}) \leq \operatorname{Ent}(\rho_{0})$$
(6.9)

for $\rho_0, \rho_1 \in D(\text{Ent})$ with $\mathcal{W}(\rho_0, \rho_1) < \infty$ and $t \ge 0$. Since (P_t) is a semigroup, it suffices to check (6.9) at t = 0.

If we can prove

$$\mathcal{W}(P_t\rho_1,\rho_0)^2 \le \left(\int_0^1 e^{-2Kst}\right) \mathcal{W}(\rho_0,\rho_1)^2 - 2t(\operatorname{Ent}(P_t\rho_1) - \operatorname{Ent}(\rho_0)), \tag{6.10}$$

then

$$\frac{\mathscr{W}(P_t\rho_1)^2 - \mathscr{W}(\rho_0,\rho_1)^2}{2t} \le \operatorname{Ent}(\rho_0) - \operatorname{Ent}(P_t\rho_1) + \frac{\int_0^1 e^{-2Kst} ds - 1}{2t} \mathscr{W}(\rho_0,\rho_1)^2,$$

from which (6.9) at t = 0 follows in the limit $t \rightarrow 0$.

In order to prove (6.10), let $\varepsilon > 0$ and let $(\rho_s) \in C^1([0,1]; L^1(\mathcal{M}, \tau))$ be an admissible curve with

$$\operatorname{ess\,sup}_{s\in[0,1]} \|D\rho_s\|_{\rho_s} \leq \mathcal{W}(\rho_0,\rho_1) + \varepsilon.$$

Let $(\rho_s^n)_{s \in [0,1]}$ be the curves defined in Lemma 6.12 and let $\sigma_{s,t} = P_{st}\rho_s^n$. Since $\rho_s^n \in D(\mathscr{L}^{(1)})$, for each $t \ge 0$ the curve $(\sigma_{s,t})_{s \in [0,1]}$ is L^1 -differentiable with derivative

$$\frac{d}{ds}\sigma_{s,t} = P_{st}\dot{\rho}_s^n - t\mathscr{L}^{(1)}\sigma_{s,t}.$$
(6.11)

We will now show that the curve $(\sigma_{s,t})_{s \in [0,1]}$ is admissible by evaluating both summands separately.

Since \mathscr{E} satisfies $GE(K,\infty)$, the logarithmic mean is regular for \mathscr{E} and (ρ_s^n) is admissible, Proposition 5.7 and Lemma 5.11 imply

$$|\tau(aP_{st}\dot{\rho}_{s}^{n})| = |\tau(\dot{\rho}_{s}^{n}P_{st}a)| \le \|\partial P_{st}a\|_{\rho_{s}^{n}}\|D\rho_{s}^{n}\|_{\rho_{s}^{n}} \le e^{-Kst}\|\partial a\|_{\sigma_{s,t}}\|D\rho_{s}^{n}\|_{\rho_{s}^{n}}$$

for all $a \in D(\mathscr{E}) \cap \mathscr{M}$ with $\partial a \in D(\hat{\sigma}_{s,t}^{1/2})$. Thus there exists a unique ξ_s in $\tilde{\mathscr{H}}_{\sigma_{s,t}}$ such that

$$\tau(aP_{st}\dot{\rho}_s^n) = \langle \partial a, \xi_s \rangle_{\sigma_{s,t}} \tag{6.12}$$

for all $a \in D(\mathscr{E}) \cap \mathscr{M}$ with $\partial a \in D(\hat{\sigma}_{s,t}^{1/2})$. Moreover, $\|\xi_s\|_{\sigma_s} \leq e^{-Kst} \|D\rho_s^n\|_{\rho_s^n}$. Some more work is necessary for the second summand in (6.11). If $\sigma_{s,t} \in$ $D(\mathcal{L}^{(2)})$, then

$$\tau(a\mathscr{L}^{(1)}\sigma_{s,t}) = \langle \partial a, \partial \sigma_{s,t} \rangle_{\mathscr{H}} = \langle \partial a, \partial \log \sigma_{s,t} \rangle_{\sigma_{s,t}}.$$

To show the equality of the left- and right-hand side in the general case (the middle is of course not well-defined), we argue by approximation.

Let $\tilde{\rho}_s^n = (1 + 1/n)^{-1}(\rho_s + 1/n)$ and recall that $\rho_s^n = \mathfrak{p}^{\varepsilon_n} \tilde{\rho}_s^n$. Moreover, let $\sigma_{s,t}^N =$ $P_{st}\mathfrak{p}^{\varepsilon_n}(\tilde{\rho}^n_s \wedge N)$. If $a \in D(\mathcal{E}) \cap \mathcal{M}$ with $\partial a \in D(\hat{\sigma}^{1/2}_{s,t})$, then

$$\tau(a\mathscr{L}^{(1)}\sigma_{s,t}) = \lim_{N \to \infty} \tau((\mathscr{L}^{(2)}\mathfrak{p}^{\varepsilon_n}a)P_{st}(\tilde{\rho}^n_s \wedge N))$$
$$= \lim_{N \to \infty} \langle \partial \mathfrak{p}^{\varepsilon_n}a, \partial P_{st}(\tilde{\rho}^n_s \wedge N) \rangle_{\mathscr{H}}$$
$$= \lim_{N \to \infty} \langle \partial a, \partial \log \sigma^N_{s,t} \rangle_{\sigma^N_{s,t}}.$$
(6.13)

Since $\sigma_{s,t}^N \leq \sigma_{s,t}$ and $\sigma_{s,t}^N \to \sigma_{s,t}$ in $L^1(\mathcal{M}, \tau)$ as $N \to \infty$, we have

$$\widehat{\sigma_{s,t}^{N}}^{1/2} \partial a \to \widehat{\sigma}_{s,t}^{1/2} \partial a \tag{6.14}$$

strongly in \mathcal{H} as $N \to \infty$ by Lemma 2.25.

We will now show that $\widehat{\sigma_{s,t}^{N}}^{1/2} \partial \log \sigma_{s,t}^{N} \rightarrow \widehat{\sigma}_{s,t}^{1/2} \partial \log \sigma_{s,t}$ weakly in \mathcal{H} . By Jensen's inequality and Corollary 4.26,

$$\begin{aligned} \mathscr{I}\left(\frac{\sigma_{s,t}^{N}}{\tau(\tilde{\rho}_{s}^{n}\wedge N)}\right) &\leq \frac{\|\kappa\|_{\infty}}{\varepsilon_{n}} \int_{\varepsilon_{n}}^{\infty} \mathscr{I}\left(P_{r}P_{st}\frac{\tilde{\rho}_{s}^{n}\wedge N}{\tau(\tilde{\rho}_{s}^{n}\wedge N)}\right))dr \\ &\leq \frac{\|\kappa\|_{\infty}}{\varepsilon_{n}} \operatorname{Ent}\left(P_{\varepsilon_{n}}\frac{\tilde{\rho}_{s}^{n}\wedge N}{\tau(\tilde{\rho}_{s}^{n}\wedge N)}\right) \\ &\leq \frac{\|\kappa\|_{\infty}}{\varepsilon_{n}} \tau((P_{\varepsilon_{n}}(\tilde{\rho}_{s}^{n}\wedge N)\log P_{\varepsilon_{n}}(\tilde{\rho}_{s}^{n}\wedge N))_{+}) \\ &\quad -\frac{\|\kappa\|_{\infty}}{\varepsilon_{n}}\log\tau(\tilde{\rho}_{s}^{n}\wedge N). \end{aligned}$$
(6.15)

6.4. PROOF OF THE GENERAL CASE

For the first summand observe that $t \mapsto (t \log t)_+$ is increasing, which implies by Proposition 4.1 that

$$\tau((P_{\varepsilon_n}(\tilde{\rho}_s^n \wedge N)\log P_{\varepsilon_n}(\tilde{\rho}_s^n \wedge N))_+) \le \tau((P_{\varepsilon_n}\tilde{\rho}_s^n \log P_{\varepsilon_n}\tilde{\rho}_s^n)_+)$$

The right-hand side is finite by Proposition 6.13. Since $\tau(\tilde{\rho}_s^n) \to 1$, we infer from (6.15) that $\sup_N \mathscr{I}(\sigma_{s,t}^N) < \infty$. The lower bound $\sigma_{s,t}^N \ge 1/n$ then implies

$$\sup_{N} \mathscr{E}(\log \sigma_{s,t}^{N}) \le n \sup_{N} \mathscr{I}(\sigma_{s,t}^{N}) < \infty.$$

From $\sigma_{s,t}^N \to \sigma_{s,t}$ in $L^1(\mathcal{M}, \tau)$ we infer $\log \sigma_{s,t}^N \to \log \sigma_{s,t}$ in $L^2(\mathcal{M}, \tau)$ by [Tik87, Theorem 3.2]. Together with the bound on the energy this implies $\log \sigma_{s,t}^N \to \log \sigma_{s,t}$ weakly in $(D(\mathcal{E}), \langle \cdot, \cdot \rangle_{\mathcal{E}})$.

If $\xi \in D(\hat{\sigma}_{s,t}^{1/2})$, then

$$\langle \widehat{\sigma_{s,t}^{N}}^{1/2} \partial \log \sigma_{s,t}^{N}, \xi \rangle_{\mathcal{H}} = \langle \partial \log \sigma_{s,t}^{N}, \widehat{\sigma_{s,t}^{N}}^{1/2} \xi \rangle_{\mathcal{H}} \to \langle \partial \log \sigma_{s,t}, \hat{\sigma}_{s,t}^{1/2} \xi \rangle_{\mathcal{H}}$$

as $N \to \infty$ by Lemma 2.25. Since $D(\hat{\sigma}_{s,t}^{1/2})$ is dense in \mathscr{H} and $\sup_N \mathscr{I}(\sigma_{s,t}^N) < \infty$, this implies

$$\widehat{\sigma_{s,t}^{N}}^{1/2} \partial \log \sigma_{s,t}^{N} \to \widehat{\sigma}_{s,t}^{1/2} \partial \log \sigma_{s,t}$$

weakly in \mathcal{H} as $N \to \infty$.

If we combine this convergence with (6.14), then we can deduce from (6.13) that

$$\tau(a\mathscr{L}^{(1)}\sigma_{s,t}) = \langle \partial a, \partial \log \sigma_{s,t} \rangle_{\sigma_{s,t}}$$
(6.16)

for all $a \in D(\mathcal{E}) \cap \mathcal{M}$ with $\partial a \in D(\hat{\sigma}_{s,t}^{1/2})$.

Let $\eta_{s,t} = \partial \log \sigma_{s,t}$. If we combine the results (6.12) and (6.16), we see that $(\sigma_{s,t})_{s \in [0,1]}$ is admissible and

$$\|D_s\sigma_{s,t}\|_{\sigma_{s,t}}^2 \le \|\xi_{s,t} - t\eta_{s,t}\|_{\sigma_{s,t}}^2.$$

Thus

$$\begin{split} \int_{0}^{1} \|D_{s}\sigma_{s,t}\|_{\sigma_{s,t}}^{2} ds &\leq \int_{0}^{1} \|\xi_{s,t} - t\eta_{s,t}\|_{\sigma_{s,t}}^{2} ds \\ &= \int_{0}^{1} (\|\xi_{s,t}\|_{\sigma_{s,t}}^{2} - 2t\langle\eta_{s,t},\xi_{s,t} - t\eta_{s,t}\rangle_{\sigma_{s,t}} - t^{2} \|\eta_{s,t}\|_{\sigma_{s,t}}^{2}) ds \\ &\leq \int_{0}^{1} (\|\xi_{s,t}\|_{\sigma_{s,t}}^{2} - 2t\langle\eta_{s,t},\xi_{s,t} - t\eta_{s,t}\rangle_{\sigma_{s,t}}) ds \\ &\leq \left(\int_{0}^{1} e^{-2Kst} ds\right) \operatorname{ess\,sup}_{s\in[0,1]} \|D\rho_{s}^{n}\|_{\rho_{s}^{n}}^{2} \\ &- 2t \int_{0}^{1} \langle\eta_{s,t},\xi_{s,t} - t\eta_{s,t}\rangle_{\sigma_{s,t}} ds. \end{split}$$
(6.17)

Let (C_k) be an increasing sequence in $C^1((0,\infty))$ such that each C_k is increasing, 1-Lipschitz, $C_k(s) = s$ if $s \le k - 1$ and $C_k(s) = k$ if $s \ge n$. Let $f_k = C_k \circ \log$ and

$$F_k: (0,\infty) \to \mathbb{R}, t \mapsto \int_0^t (f_k(s)+1) ds.$$

As in the proof of Proposition 6.13 one can show

$$\tau(F_k(P_t\rho_1^n) - F_k(\rho_0^n)) = \int_0^1 \tau(f_k(\sigma_{s,t})(P_{s,t}\rho_s^n - t\mathcal{L}^{(1)}\sigma_{s,t})) ds$$

Since $f_k(\sigma_{s,t}) \in D(\mathcal{E}) \cap \mathcal{M}$ by Lemma 4.17 and $\|\partial f_k(\sigma_{s,t})\|_{\sigma_{s,t}}^2 \leq \mathcal{I}(\sigma_{s,t})$, we can apply (6.12) and (6.16) to get

$$\tau(F_k(P_t\rho_1^n) - F_k(\rho_0^n)) = \int_0^1 \langle \partial f_k(\sigma_{s,t}), \xi_{s,t} - t\eta_{s,t} \rangle_{\sigma_{s,t}} \, ds \tag{6.18}$$

Since $f_k(\sigma_{s,t}) \to \log \sigma_{s,t}$ in $L^2(\mathcal{M}, \tau)$ as $k \to \infty$ and $\|\partial f_k(\sigma_{s,t})\|_{\sigma_{s,t}}^2 \leq \mathscr{I}(\sigma_{s,t})$, we have $\partial f_k(\sigma_{s,t}) \to \partial \log \sigma_{s,t} = \eta_{s,t}$ weakly in $\tilde{\mathscr{H}}_{\sigma_{s,t}}$ and the integrand on the right-hand side of (6.18) is pointwise bounded by $\mathscr{I}(\sigma_{s,t})^{1/2} \|\xi_{s,t} - t\eta_{s,t}\|_{\sigma_{s,t}}$.

By the dominated convergence theorem,

$$\lim_{k\to\infty}\int_0^1\langle\partial f_k(\sigma_{s,t}),\xi_{s,t}-t\eta_{s,t}\rangle_{\sigma_{s,t}}\,ds=\int_0^1\langle\eta_{s,t},\xi_{s,t}-t\eta_{s,t}\rangle_{\sigma_{s,t}}\,ds.$$

On the other hand, the left-hand side of (6.18) converges to $\text{Ent}(P_t\rho_1) - \text{Ent}(\rho_0)$ by the monotone convergence theorem.

Then (6.17) becomes

$$\int_{0}^{1} \|D_{s}\sigma_{s,t}\|_{\sigma_{s,t}}^{2} ds \leq \left(\int_{0}^{1} e^{-2Kst} ds\right) \underset{s \in [0,1]}{\operatorname{ess\,sup}} \|D\rho_{s}^{n}\|_{\rho_{s}^{n}}^{2} -2t(\operatorname{Ent}(P_{t}\rho_{1}^{n}) - \operatorname{Ent}(\rho_{0}^{n})).$$
(6.19)

Since $\sigma_{s,t} = P_{st}\rho_s^n \to P_{st}\rho_s$ in $L^1(\mathcal{M},\tau)$ as $n \to \infty$, Theorem 3.30 can be used to see that the curve $(P_{st}\rho_s)_s$ is admissible and

$$\mathcal{W}(\rho_0, P_t \rho_1)^2 \leq \int_0^1 \|D_s(P_{st} \rho_s)\|_{P_{st\rho_s}}^2 \leq \liminf_{n \to \infty} \int_0^1 \|D_s(P_{st} \rho_s^n)\|_{P_{st} \rho_s^n}^2 ds.$$

By Lemma 6.12 we have

Furthermore, using the lower semicontinuity of the entropy and Lemma 6.12, we obtain $\operatorname{Ent}(P_t\rho_1^n) \to \operatorname{Ent}(P_t\rho_1)$, $\operatorname{Ent}(\rho_0^n) \to \operatorname{Ent}(\rho_0)$.

These inequalities allow to pass to the limit $n \to \infty$ in (6.19) to get

$$\mathcal{W}(\rho_0, P_t \rho_1)^2 \leq \left(\int_0^1 e^{-2Kst} \, ds\right) (\mathcal{W}(\rho_0, \rho_1) + \varepsilon)^2 - 2t (\operatorname{Ent}(P_t \rho_1) - \operatorname{Ent}(\rho_0)),$$

which yields (6.10) as $\varepsilon \searrow 0$.

As a consequence of the uniqueness of EVI_K gradient flow curves (Lemma 6.2) we note the following corollary.

Corollary 6.16. A curve $(\rho_t)_{t\geq 0}$ with $\rho_0 \in D(\text{Ent})$ is an EVI_K gradient flow curve of Ent if and only if $\rho_t = P_t \rho_0$ for all $t \geq 0$.

CHAPTER 7

GEODESIC CONVEXITY AND FUNCTIONAL INEQUALITIES

In this chapter we will study some important consequences of the gradient flow characterization, namely functional inequalities for \mathscr{E} and the (semi-) convexity of the entropy along geodesics in $(\mathscr{D}(\mathcal{M}, \tau), \mathcal{W})$.

Functional inequalities like the ones discussed in Section 7.2 are a classical topic in the study of Markov semigroups, both commutative and noncommutative. Among other things, some of the early interest in the entropic gradient flow characterization of the heat flow stemmed from the possibility to obtain new proofs and improved versions of classical functional inequalities as in [OV00]. Also one of the striking applications of the noncommutative analog developed in [CM17a] was a new sharp estimate for the entropy decay along the Bosonic Ornstein–Uhlenbeck semigroup. In this thesis we restrict our attention to some relatively simple functional inequalities for illustrative purposes, but we think that this framework could be the starting point for much deeper investigations.

Semi-convexity of the entropy along Wasserstein geodesics was taken as basis for the study of synthetic Ricci curvature bounds by Lott–Villani [LV09] and Sturm [Stu06a, Stu06b] and could therefore also be an entrance gate to the study of Ricci curvature in noncommutative geometry. In fact, it was proposed as a definition for Ricci curvature in [Hor18].

As mentioned before, even the existence of \mathcal{W} -geodesics is not clear in general. The situation is much better if (P_t) satisfies the gradient estimate $\operatorname{GE}(K,\infty)$ and we restrict our attention to the domain of the entropy (Theorem 7.15). This is due to two ingredients, which we will study next: First, the sublevel sets of the entropy are compact in the weak L^1 -topology (Lemma 7.1). Together with the lower semicontinuity of the the action functional with respect to pointwise weak convergence in L^1 , this can be employed for the standard existence proof of minimizers for a variational problem, provided one can always find a minimizing sequence with uniformly bounded entropy. As we will see, the latter is essentially a consequence of the evolution variational inequality (Proposition 7.2).

Once the existence of geodesics is proven, the semi-convexity of the entropy along them follows from abstract results on gradient flows (Theorem 7.19). Finally, we summarize the relations between the gradient estimate $GE(K,\infty)$, the evolution variational inequality EVI_K and K-convexity of the entropy in Theorem 7.22.

As usual, let (\mathcal{M}, τ) be a tracial von Neumann algebra, \mathscr{E} a quantum Dirichlet form on $L^2(\mathcal{M}, \tau)$ such that τ is energy dominant, and $(\partial, \mathcal{H}, L, R, J)$ the associated first-order differential calculus. We further assume that τ is a state, $L^1(\mathcal{M}, \tau)$ is separable and θ is the logarithmic mean.

7.1 Admissibility of absolutely continuous curves

In this section we will show that if the quantum Dirichlet form \mathscr{E} satisfies the gradient estimate $\operatorname{GE}(K,\infty)$ for some $K \in \mathbb{R}$, then the distance between density operators with finite density is realized by curves with uniformly bounded entropy (Proposition 7.2) and 2-locally absolutely continuous curves in $(\mathscr{D}(\mathcal{M},\tau),\mathcal{W})$ with uniformly bounded entropy are admissible (Proposition 7.4).

On important ingredient is that an uniform bound on the entropy yields weak compactness, as the following lemma shows.

Lemma 7.1. The sublevel sets of Ent are compact in the weak L^1 -topology.

Proof. The sublevel sets are closed since F is lower semicontinuous by Lemma 4.2. Moreover, they are precompact in the weak l^1 topology by Proposition B.3.

One important technical step in the proof of the gradient flow characterization in the last chapter was the existence of a family of admissible curves with control on the entropy of the endpoints. We will now refine this result and show that one can even get entropy control along the entire curve as long as the endpoints have finite entropy.

Proposition 7.2. For all $K, \alpha, D > 0$ there exists a constant $C(K, \alpha, D) > 0$ such that the following folds:

If the form & satisfies $GE(K,\infty)$, $\rho_0, \rho_1 \in D(Ent)$ with $Ent(\rho_0), Ent(\rho_1) \leq \alpha$, and $\mathcal{W}(\rho_0, \rho_1) \leq D$, then there is a sequence of admissible curves $(\rho_t^n)_{t \in [0,1]}$ connecting

 ρ_0 and ρ_1 such that

$$\sup_{n \in \mathbb{N}} \sup_{t \in [0,1]} \operatorname{Ent}(\rho_t^n) \le C(K, \alpha, D)$$

and

$$\int_0^1 \|D\rho_t^n\|_{\rho_t^n}^2 dt \to \mathcal{W}(\rho_0,\rho_1)^2$$

Proof. For $n \in \mathbb{N}$ let $(\sigma_t^n)_{t \in [0,1]}$ be an admissible L_n -Lipschitz curve in $(\mathcal{D}(\mathcal{M},\tau),\mathcal{W})$ connecting ρ_0 and ρ_1 such that $L_n^2 \leq \mathcal{W}(\rho_0,\rho_1)^2 + \frac{1}{n^2}$.

Let $\tilde{\sigma}_t^n = P_{1/n} \sigma_t^n$. Since (P_t) is an EVI_K gradient flow of Ent by Theorem 6.15, Theorem 3.2 of [DS08] asserts

$$\operatorname{Ent}(\tilde{\sigma}_{t}^{n}) \leq (1-t)\operatorname{Ent}(\rho_{0}) + t\operatorname{Ent}(\rho_{1}) - \frac{K}{2}t(1-t)\mathcal{W}(\rho_{0},\rho_{1})^{2} + \frac{1}{2n^{2}I_{K}(1/n)}$$

where $I_K(t) = \int_0^t e^{Kr} dr$.

As $n^2 I_K(1/n) \to \infty$ as $n \to \infty$, the supremum

$$c(K) = \sup_{n \in \mathbb{N}} \frac{1}{2n^2 I_K(1/n)}$$

is finite. Thus

$$\sup_{n \in \mathbb{N}} \sup_{t \in [0,1]} \operatorname{Ent}(\tilde{\sigma}_t^n) \le \alpha + \frac{|K|}{2} D^2 + c(K).$$

Furthermore, Theorem 5.13 implies $\|D\tilde{\sigma}_t^n\|_{\tilde{\sigma}_t^n} \le e^{-K/n} \|D\sigma_t^n\|_{\sigma_t^n}$ for a.e. $t \in [0, 1]$.

Moreover, $\operatorname{Ent}(P_s\rho_0) \leq \operatorname{Ent}(\rho_0) \leq \alpha$ and $(P_s\rho_0)_{s\geq 0}$ is admissible by Corollary 4.26, hence

$$\int_0^{1/n} \|D_s P_s \rho_0\|_{P_s \rho_0}^2 ds \to 0$$

as $n \to \infty$. Of course, the same holds for ρ_0 replaced by ρ_1 .

Hence one can concatenate $(P_t \rho_0)_{t \in [0, 1/n]}$, $(\tilde{\sigma}_t^n)_{t \in [0, 1]}$ and $(P_{\frac{1}{n} - t} \rho_1)_{t \in [0, 1/n]}$ to get a curve (ρ_t^n) with the desired properties.

Definition 7.3. We say that the entropy has *regular sublevel sets* if every curve $(\rho_t) \in \operatorname{AC}^2_{\operatorname{loc}}(I; (\mathcal{D}(\mathcal{M}, \tau), \mathcal{W}))$ with uniformly bounded entropy is admissible and $\|D\rho_t\|_{\rho_t} = |\dot{\rho}_t|_{\mathcal{W}}$ for a.e. $t \in I$.

Proposition 7.4. If \mathscr{E} satisfies $\operatorname{GE}(K,\infty)$, then the entropy has regular sublevel sets.

Proof. First assume that $(\rho_t) \in AC^2([0,1]; (\mathcal{D}(\mathcal{M},\tau), \mathcal{W}))$. Since (ρ_t) is continuous on a compact interval, it is uniformly continuous. Thus, for every $\varepsilon > 0$ there exists a partition $0 = t_0 < t_1 < \cdots < t_n = 1$ of [0,1] such that $\mathcal{W}(\rho_{t_{k-1}}, \rho_t) < \varepsilon$ for all $t \in [t_{k-1}, t_k], 1 \le k \le n$.

For $k \in \{1, ..., n\}$ let $\sigma^{k, \varepsilon} \colon [t_{k-1}, t_k] \longrightarrow \mathscr{D}(\mathscr{M}, \tau)$ be an admissible curve with $\sigma_{t_{k-1}}^{k, \varepsilon} = \rho_{t_{k-1}}, \sigma_{t_k}^{k, \varepsilon} = \rho_{t_k}$ and

$$\int_{t_{k-1}}^{t_k} \|D\sigma_r^{k,\varepsilon}\|_{\sigma_r^{k,\varepsilon}}^2 dr \leq \frac{\mathcal{W}(\rho_{t_{k-1}},\rho_{t_k})^2}{t_k - t_{k-1}} + \frac{\varepsilon}{n}.$$

Moreover, by Proposition 7.2, the curves $\sigma^{k,\varepsilon}$ can be chosen such that

$$\sup_{\varepsilon \in (0,1)} \sup_{k \in \mathbb{N}} \sup_{t \in [t_{k-1}, t_k]} \operatorname{Ent}(\sigma_t^{k, \varepsilon}) < \infty.$$
(7.1)

Denote by ρ^{ε} the concatenation of $\sigma^{1,\varepsilon}, \ldots, \sigma^{n,\varepsilon}$. Then

$$\begin{split} \int_0^1 \|D\rho_r^{\varepsilon}\|_{\rho_r^{\varepsilon}}^2 dr &= \sum_{k=1}^n \int_{t_{k-1}}^{t_k} \|D\sigma_r^{k,\varepsilon}\|_{\sigma_r^{k,\varepsilon}}^2 dr \\ &\leq \varepsilon + \sum_{k=1}^n \frac{\mathcal{W}(\rho_{t_{k-1}},\rho_{t_k})^2}{t_k - t_{k-1}} \\ &\leq \varepsilon + \sum_{k=1}^n \int_{t_{k-1}}^{t_k} |\dot{\rho}_r|_{\mathcal{W}}^2 dr \\ &= \varepsilon + \int_0^1 |\dot{\rho}_r|_{\mathcal{W}}^2 dr. \end{split}$$

Moreover, for every $t \in [0,1]$ there is a $k \in \{1,...,n\}$ such that $\mathcal{W}(\rho_{t_k},\rho_t) < \varepsilon$, hence

$$\mathcal{W}(\rho_t^{\varepsilon}, \rho_t) \leq \mathcal{W}(\rho_t^{\varepsilon}, \rho_{t_k}^{\varepsilon}) + \mathcal{W}(\rho_{t_k}^{\varepsilon}, \rho_{t_k}) + \mathcal{W}(\rho_{t_k}, \rho_t) < 3\varepsilon.$$

Thus, $\mathcal{W}(\rho_t^{\varepsilon}, \rho_t) \to 0$ as $\varepsilon \searrow 0$.

By Lemma 7.1 and the uniform bound on the entropy (7.1), for every $t \in [0,1]$ and every sequence (ε_n) converging to 0 there is a subsequence $(\varepsilon_{n(k)})$ and $\tilde{\rho}_t \in \mathcal{D}(\mathcal{M},\tau)$ such that $\rho_t^{\varepsilon_{n(k)}} \to \tilde{\rho}_t$ weakly in L^1 as $k \to \infty$. In particular, $\tau(\rho_t^{\varepsilon_{n(k)}}a) \to \tau(\tilde{\rho}_t a)$ for all $a \in \mathscr{A}_{AM}$.

On the other hand, $\mathcal{W}(\rho_t^{\varepsilon_{n(k)}}, \rho_t) \to 0$ implies $\tau(\rho_t^{\varepsilon_{n(k)}}a) \to \tau(\rho_t a)$ for all $a \in \mathscr{A}_{AM}$ by Proposition 3.20. Since $\mathscr{A}_{AM} \subset \mathscr{M}$ is σ -weakly dense by Corollary 5.9 and the regularity of the logarithmic mean, it follows that $\tilde{\rho}_t = \rho_t$ for all $t \in [0, 1]$. Therefore, $\rho_t^{\varepsilon} \to \rho_t$ weakly in L^1 as $\varepsilon \searrow 0$ for all $t \in [0, 1]$.

By Theorem 3.30, the curve (ρ_t) is admissible and

$$\int_0^1 \|D\rho_r\|_{\rho_r}^2 dr \leq \liminf_{\varepsilon \searrow 0} \int_0^1 \|D\rho_r^\varepsilon\|_{\pi_r^\varepsilon}^2 dr \leq \int_0^1 |\dot{\rho}_r|_{\mathscr{W}}^2 dr.$$

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As the reverse inequality is obvious, we conclude $||D\rho_r||_{\rho_r} = |\dot{\rho}_r|_{\mathcal{W}}$ for a.e. $r \in [0, 1]$.

In the general case $(\rho_t) \in \mathrm{AC}^2_{\mathrm{loc}}(I; (\mathcal{D}(\mathcal{M}, \tau), \mathcal{W}))$ one can simply partition I into countably many compact intervals to obtain the same result.

7.2 Transport inequalities

In this section we discuss functional inequalities that are implied by the gradient estimate $GE(K,\infty)$. Up to technicalities, the proofs are very similar to the ones in [CM17a, CM18] in the finite-dimensional case, which in turn closely follow the original arguments by [OV00].

Definition 7.5. Let C > 0. The Dirichlet form \mathscr{E} satisfies

• the modified logarithmic Sobolev inequality with constant C if

$$C\mathrm{Ent}(\rho) \leq \frac{1}{2}\mathcal{I}(\rho)$$

for all $\rho \in \mathcal{D}(\mathcal{M}, \tau)$,

• the *Talagrand inequality* with constant *C* if

$$\mathcal{W}(\rho, 1)^2 \leq C \operatorname{Ent}(\rho)$$

for all $\rho \in \mathcal{D}(\mathcal{M}, \tau)$,

• the *Poincaré inequality* with constant *C* if

$$\|a - \tau(a)\|_2^2 \le C^2 \mathscr{E}(a)$$

for all $a \in L^2(\mathcal{M}, \tau)$.

Note that the Poincaré inequality with constant C holds if and only if the spectrum of the generator of \mathscr{E} restricted to the orthogonal complement of 1 is contained in $[C^{-2},\infty)$.

We will need the following refined version of the Arzelà-Ascoli theorem (see [AGS08, Proposition 3.3.1]). Note that in the cited reference there is the additional global assumption of completeness on d, but this follows from the lower semicontinuity property of d in this case.

Proposition 7.6. Let (K, \mathcal{T}) be a sequentially compact Hausdorff space and d a metric on K such that $x_n \to x$, $y_n \to y$ with respect to \mathcal{T} implies

$$d(x,y) \leq \liminf_{n \to \infty} d(x_n, y_n).$$

If (γ^n) is a sequence of curves from [0,1] to K that is equicontinuous with respect to d, then there exists a subsequence (γ^{n_k}) and a d-continuous curve γ from [0,1] to K such that $\gamma_t^{n_k} \to \gamma_t$ with respect to \mathcal{T} for all $t \in [0,1]$.

Lemma 7.7. For $\alpha > 0$ let $S_{\alpha} = \{\rho \in \mathcal{D}(\mathcal{M}, \tau) \mid \text{Ent}(\rho) \leq \alpha\}$. If L > 0 and $((\rho_t^n)_{t \in [0,1]})_n$ is a sequence of admissible curves in S_{α} such that

$$\int_s^t \|D\rho_r^n\|_{\rho_r^n}^2 dr \le L^2 |t-s|$$

for all $s,t \in [0,1]$ and $n \in \mathbb{N}$, then there exists an admissible curve (ρ_t) in S_{α} and a subsequence $(\rho^{n_k})_k$ of (ρ^n) such that

$$\rho_t^{n_k} \to \rho_t$$

weakly in L^1 for all $t \in [0, 1]$, and

$$\int_0^1 \|D\rho_t\|_{\rho_t}^2 \leq \liminf_{n \to \infty} \int_0^1 \|D\rho_t^n\|_{\rho_t^n}^2 dt.$$

Proof. Otherwise passing to a subsequence, we can assume that $\int_0^1 ||D\rho_t^n||_{\rho_t^n}^2 dt$ converges. If $a \in \mathscr{A}_{AM}$, then

$$|\tau((\rho_t^n - \rho_s^n)a)| \le \int_s^t \|\partial a\|_{\rho_r^n} \|D\rho_r^n\|_{\rho_r^n} \, dr \le L \|a\|_{\mathrm{AM}} |t-s|$$

for all $s, t \in [0, 1]$ and $n \in \mathbb{N}$. Thus (ρ^n) is uniformly equicontinuous with respect to the metric

$$d: \mathcal{D}(\mathcal{M}, \tau) \times \mathcal{D}(\mathcal{M}, \tau) \longrightarrow [0, \infty), d(\rho, \sigma) = \sup_{\|a\|_{AM} \le 1} |\tau(a(\rho - \sigma))|$$

By Lemma 7.1, the set S_{α} is sequentially compact with respect to the weak topology on L^1 . Moreover, d clearly satisfies the lower semicontinuity property from Proposition 7.6 with respect to the weak L^1 -topology. Hence we get a subsequence (ρ^{n_k}) and a curve (ρ_t) in S_{α} such that $\rho_t^{n_k} \to \rho_t$ weakly in L^1 for all $t \in [0, 1]$. The remaining assertions follow from Theorem 3.30.

The semigroup (P_t) is called *irreducible* if for all $a \in L^1(\mathcal{M}, \tau)$ one has

$$\frac{1}{T}\int_0^T P_t a\,dt \to \tau(a)$$

in $L^1(\mathcal{M}, \tau)$ as $T \to \infty$.

The following lemma collects some well-known characterizations of irreducibility.

Lemma 7.8. The following assertions are equivalent.

(i) The semigroup (P_t) is irreducible.

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(ii) There exists a total subset D of $L^1(\mathcal{M}, \tau)$ such that for all $a \in D$ one has

$$\frac{1}{T}\int_0^T P_t a\,dt \to \tau(a)$$

weakly in $L^1(\mathcal{M}, \tau)$ as $T \to \infty$.

(iii) For all $a \in L^2(\mathcal{M}, \tau)$ one has

$$\frac{1}{T}\int_0^T P_t a\,dt \to \tau(a)$$

in $L^2(\mathcal{M}, \tau)$ as $T \to \infty$.

- (iv) The kernel of $\mathscr{L}^{(2)}$ is spanned by 1.
- (v) The kernel of $\mathscr{L}^{(\infty)}$ is spanned by 1.
- (vi) If $p \in \ker \mathscr{L}^{(\infty)}$ is a projection, then p = 0 or p = 1.

Proof. The equivalence of (i) and (ii) and of (iii) and (iv) is proven in [EN00, Theorem V.4.5]. The implication (i) \Longrightarrow (iii) follows from [EN00, Corollary V.4.6], while (iii) \Longrightarrow (ii) is obvious. Since ker $\mathscr{L}^{(\infty)} \subset \ker \mathscr{L}^{(2)}$, the implication (iv) \Longrightarrow (v) is also clear.

(v) \iff (vi): If $x \in \ker \mathscr{L}^{(\infty)}$, then

$$P_t(x^*x) \ge P_t(x)^*P_t(x) = x^*x$$

by the Kadison-Schwarz inequality (see [Tak02, Corollary IV.3.8]).

Since $\tau(P_t(x^*x)) = \tau(x^*x)$, we have $P_t(x^*x) = x^*x$. Similarly, $P_t(xx^*) = xx^*$. The equivalence of (v) and (vi) follows now from [Eva77, Theorem 3.1].

 $(v) \Longrightarrow (i)$: Since $\mathscr{L}^{(\infty)} = (\mathscr{L}^{(1)})^*$, we have $\mathbb{C} = \ker \mathscr{L}^{(\infty)} = (\operatorname{ran} \mathscr{L}^{(1)})^{\perp}$. Thus $a - \tau(a) \in \operatorname{ran} \mathscr{L}^{(1)}$. Now (i) follows from [EN00, Lemma V.4.4].

Remark 7.9. As discussed in [Yea77] (in the case of discrete time, but the arguments can easily be adopted), the semigroup (P_t) is mean ergodic on $L^p(\mathcal{M}, \tau)$ for all $p \in [1, \infty)$, that is, for all $a \in L^p(\mathcal{M}, \tau)$ the limit

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T P_t a\,dt$$

exists in L^p . In fact, this convergence even holds almost uniformly, which provides a noncommutative analog of the classical pointwise ergodic theorem. For details see [JX07, Theorem 6.8] and [CL16, Corollary 5.2]. **Proposition 7.10** (Modified log-Sobolev inequality). If (P_t) is irreducible and \mathscr{E} satisfies $\operatorname{GE}(K,\infty)$ for K > 0, then \mathscr{E} satisfies the modified logarithmic Sobolev inequality with constant K.

Proof. First assume that $\rho \in \mathcal{D}(\mathcal{M}, \tau) \cap \mathcal{M}$ is invertible. We may further assume that $\rho \in D(\mathcal{E})$ as otherwise the right-hand side is infinite.

By Propositions 4.24 and 4.25 the curve $(P_t\rho)_{t\geq 0}$ is admissible and we have $\|DP_t\rho\|_{P_t\rho}^2 \leq \mathscr{I}(P_t\rho)$ for a.e. $t\geq 0$. Hence there exists a measurable set $E \subset [0,\infty)$ such that E^c is a null set and

$$\limsup_{h \searrow 0} \frac{1}{h} \mathcal{W}(P_{t+h}\rho, P_t\rho) \leq \limsup_{h \searrow 0} \frac{1}{h} \int_t^{t+h} \|DP_r\rho\|_{P_r\rho} \, dr \leq \mathcal{I}(P_t\rho)^{1/2}$$

for $t \in E$.

Thus

$$\begin{split} -\frac{1}{2}\frac{d^{+}}{dt}\mathcal{W}(P_{t}\rho,\sigma)^{2} &= \limsup_{h \to 0} \frac{1}{2h}(\mathcal{W}(P_{t}\rho,\sigma)^{2} - \mathcal{W}(P_{t+h}\rho,\sigma)^{2}) \\ &\leq \limsup_{h \searrow 0} \frac{1}{2h}(\mathcal{W}(P_{t+h}\rho,P_{t}\rho)^{2} + 2\mathcal{W}(P_{t+h}\rho,P_{t}\rho)\mathcal{W}(P_{t+h}\rho,\sigma)) \\ &\leq \mathcal{I}(P_{t}\rho)^{1/2}\mathcal{W}(P_{t}\rho,\sigma) \end{split}$$

for all $t \in E$ and $\sigma \in \mathcal{D}(\mathcal{M}, \tau)$ with $\mathcal{W}(\rho, \sigma) < \infty$.

The evolution variational inequality from Theorem 6.15 implies

$$\begin{aligned} \operatorname{Ent}(P_t\rho) &\leq -\frac{1}{2} \frac{d^+}{dt} \mathcal{W}(P_t\rho,\sigma)^2 - \frac{K}{2} \mathcal{W}(P_t\rho,\sigma)^2 + \operatorname{Ent}(\sigma) \\ &\leq \mathcal{I}(P_t\rho)^{1/2} \mathcal{W}(P_t\rho,\sigma) - \frac{K}{2} \mathcal{W}(P_t\rho,\sigma)^2 + \operatorname{Ent}(\sigma) \\ &\leq \frac{1}{2K} \mathcal{I}(P_t\rho) + \operatorname{Ent}(\sigma) \end{aligned}$$

for all $t \in E$ and all $\sigma \in \mathcal{D}(\mathcal{M}, \tau)$ with $\mathcal{W}(\rho, \sigma) < \infty$.

In particular, if $\sigma_T = \frac{1}{T} \int_0^T P_s \rho \, ds$, then $\mathcal{W}(\sigma_T, \rho) < \infty$ and $\operatorname{Ent}(\sigma_T) \to 0$ as $T \to \infty$ by Proposition B.7 and irreducibility of (P_t) . Thus

$$\operatorname{Ent}(P_t\rho) \leq \frac{1}{2K} \mathscr{I}(P_t\rho) = \frac{1}{2K} \mathscr{E}(P_t\rho, \log P_t\rho).$$

for all $t \in E$.

Now let (t_k) be a null sequence in E. On the one hand, $\operatorname{Ent}(P_{t_k}\rho) \to \operatorname{Ent}(\rho)$ by Proposition 4.2 and Corollary 4.26. On the other hand, since $\rho \in D(\mathscr{E})$, we have $P_{t_k}\rho \to \rho$ and $\log P_{t_k}\rho \to \log \rho$ with respect to $\|\cdot\|_{\mathscr{E}}$. Hence the modified log-Sobolev inequality holds for invertible $\rho \in \mathcal{D}(\mathcal{M}, \tau) \cap \mathcal{M}$.

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If $\rho \in \mathcal{D}(\mathcal{M}, \tau) \cap \mathcal{M}$ is not necessarily invertible, let $\rho^n = (1 + 1/n)^{-1}(\rho + 1/n)$. By Propositions 4.1 and 4.2 we have $\operatorname{Ent}(\rho^n) \to \operatorname{Ent}(\rho)$. Moreover, the functions

$$C_n: [0,\infty) \to \mathbb{R}, t \mapsto \log\left(\frac{t+1/n}{1+1/n}\right)$$

satisfy the conditions from the definition of the Fisher information so that $\mathscr{I}(\rho^n)$ converges to $\mathscr{I}(\rho)$.

Finally, if $\rho \in \mathscr{D}(\mathscr{M}, \tau)$ is not necessarily bounded, let $\rho^n = (\rho \wedge n)/\tau(\rho \wedge n)$. The same continuity arguments as above show $\operatorname{Ent}(\rho^n) \to \operatorname{Ent}(\rho)$ and $\mathscr{I}(\rho^n) \to \mathscr{I}(\rho)$.

In fact, if \mathscr{E} satisfies $GE(K,\infty)$, then irreducibility is not only sufficient, but also necessary for the modified logarithmic Sobolev inequality. To see this, we need the following lemma (see [Pin64, Pages 15 and 20] for a version with a worse constant and [Kem69, Theorem 6.1] for the version with the optimal constant presented here). Since it only involves commuting density operators, the proof for the commutative case carries over to the noncommutative setting.

Lemma 7.11 (Pinsker's inequality). If $\rho \in \mathcal{D}(\mathcal{M}, \tau)$, then

$$\|\rho - 1\|_{1}^{2} \le 2\text{Ent}(\rho)$$

and the inequality is strict unless $\rho = 1$.

Proposition 7.12 (Exponential entropy decay). Let C > 0. The Dirichlet form \mathscr{E} satisfies the logarithmic Sobolev inequality with constant C if and only if

$$\operatorname{Ent}(P_t \rho) \le e^{-2Ct} \operatorname{Ent}(\rho)$$

for all $\rho \in \mathcal{D}(\mathcal{M}, \tau)$ and $t \ge 0$. In this case, $P_t \rho \to 1$ in $L^1(\mathcal{M}, \tau)$ as $t \to \infty$ for all $\rho \in \mathcal{D}(\mathcal{M}, \tau)$ and (P_t) is irreducible.

Proof. By the same approximation argument as in the proof of Proposition 7.10 we may assume that ρ is bounded and invertible. If \mathscr{E} satisfies the modified logarithmic Sobolev inequality with constant C, then the exponential entropy decay follows from Proposition 4.25 and an application of Grönwall's lemma.

Assume conversely that the exponential entropy decay inequality holds. We can additionally assume $\rho \in D(\mathscr{E})$. As seen in the proof of Proposition 7.10, we

have $\mathscr{I}(P_t\rho) \to \mathscr{I}(\rho)$ as $t \to 0$. An application of Proposition 4.25 yields

$$\begin{aligned} \mathscr{I}(\rho) &= \lim_{t \to 0} \frac{1}{t} \int_0^t \mathscr{I}(P_s \rho) ds \\ &= \lim_{t \to 0} \frac{\operatorname{Ent}(\rho) - \operatorname{Ent}(P_t \rho)}{t} \\ &\geq \lim_{t \to 0} \frac{1 - e^{-2Ct}}{t} \operatorname{Ent}(\rho) \\ &= 2C \operatorname{Ent}(\rho). \end{aligned}$$

It remains to show that $P_t \rho \to 1$ in L^1 and (P_t) is irreducible. If $\rho \in D(Ent)$, then

$$||P_t \rho - 1||_1^2 \le 2 \text{Ent}(P_t \rho) \le 2e^{-2Ct} \text{Ent}(\rho) \to 0$$

by Lemma 7.11. For arbitrary $\rho \in \mathcal{D}(\mathcal{M}, \tau)$, the convergence follows by approximation by elements of finite entropy. The irreducibility of (P_t) is clear.

Proposition 7.13 (Talagrand inequality). If \mathscr{E} satisfies the modified logarithmic Sobolev inequality with constant C, then \mathscr{E} satisfies the Talagrand inequality with constant 2/C.

Proof. We first proof the inequality for $\rho \in \mathcal{D}(\mathcal{M}, \tau) \cap \mathcal{M}$. Let $T = \sup\{t \ge 0 \mid P_t \rho \ne 1\}$ and note that $P_t \rho \ne 1$ for all $t \in [0, T)$. By Proposition 4.25 the map $t \mapsto \operatorname{Ent}(P_t \rho)^{1/2}$ is locally absolutely continuous on [0, T) and

$$-2\mathrm{Ent}(P_t\rho)^{1/2}\frac{d}{dt}\mathrm{Ent}(P_t\rho)^{1/2} = \mathscr{I}(P_t\rho)$$

for a.e. $t \in [0, T)$. The modified log-Sobolev inequality implies

$$\mathscr{I}(P_t\rho)^{1/2} \le -\left(\frac{2}{C}\right)^{1/2} \frac{d}{dt} \operatorname{Ent}(P_t\rho)^{1/2}$$
(7.2)

for a.e. $t \in [0, T)$.

Let $\vartheta: [0,1) \to [0,\infty)$ be a smooth function with $\vartheta(0) = 0$ and $\lim_{t \nearrow 1} \vartheta(t) = \infty$, and let $\rho_t = P_{\vartheta(t)}\rho$. By Proposition 7.12 we have $\rho_t \to 1$ in $L^1(\mathcal{M}, \tau)$ as $t \nearrow 1$.

Clearly $D\rho_t$ exists for a.e. $t \in [0, 1]$ and

$$\int_{0}^{1} \|D\rho_{t}\|_{\rho_{t}} dt = \int_{0}^{\infty} \|DP_{t}\rho\|_{P_{t}\rho} dt
\leq \int_{0}^{T} \mathscr{I}(P_{t}\rho)^{1/2} dt
\leq -\lim_{S \to T} \left(\frac{2}{C}\right)^{1/2} \int_{0}^{S} \frac{d}{dt} \operatorname{Ent}(P_{t}\rho)^{1/2} dt
\leq \left(\frac{2}{C}\right)^{1/2} \operatorname{Ent}(\rho)^{1/2},$$
(7.3)

where we used Proposition 4.24 for the first and (7.2) for the second inequality. In particular, ϑ can be chosen in such a way that (ρ_t) has constant speed and is therefore an admissible curve connecting ρ and 1. Then (7.3) implies

$$\mathcal{W}(\rho, 1)^2 \leq \frac{2}{C} \operatorname{Ent}(\rho).$$

In the general case $\rho \in D(\text{Ent})$ we can argue by approximation. Let $\rho^n = \frac{\rho \wedge n}{\tau(\rho \wedge n)}$. In the first part we saw that there are smooth functions $\vartheta^n : [0,1) \to [0,\infty)$ with $\vartheta^n(0) = 0$ and $\lim_{t \neq 1} \vartheta^n(t) = \infty$ such that the curve (ρ_t^n) given by $\rho_t^n = P_{\vartheta^n(t)}\rho^n$ for $t \in [0,1)$ and $\rho_t^n = 1$ for t = 1 is admissible, has constant speed and

$$\int_0^1 \|D\rho_t^n\|_{\rho_t^n}^2 dt \leq \frac{2}{C} \operatorname{Ent}(\rho^n).$$

It is easy to see that $(\text{Ent}(\rho^n))_n$ is bounded. It follows from Lemma 7.7 that there exists a strictly increasing sequence (n_k) in \mathbb{N} and an admissible curve $(\rho_t)_{t \in [0,1]}$ such that $\rho_t^{n_k} \to \rho_t$ weakly in $L^1(\mathcal{M}, \tau)$ for all $t \in [0,1]$ and

$$\begin{split} \mathcal{W}(\rho,1)^2 &\leq \int_0^1 \|D\rho_t\|_{\rho_t}^2 dt \\ &\leq \liminf_{n \to \infty} \int_0^1 \|D\rho_t^n\|_{\rho_t^n}^2 dt \\ &\leq \liminf_{n \to \infty} \mathcal{W}(\rho^n,1)^2 \\ &\leq \frac{2}{C} \lim_{n \to \infty} \operatorname{Ent}(\rho^n) \\ &= \frac{2}{C} \operatorname{Ent}(\rho). \end{split}$$

Finally, also the Poincaré inequality can be obtained as a consequence of the modified log-Sobolev inequality. Recall from Proposition 3.27 that this implies a bound for the distance \mathcal{W} .

Proposition 7.14. Let C > 0. If \mathscr{E} satisfies the modified log-Sobolev inequality with constant C, then \mathscr{E} satisfies the Poincaré inequality with constant \sqrt{C} .

Proof. By a standard approximation argument we can assume $a \in D(\mathcal{E}) \cap \mathcal{M}_h$ and furthermore $\tau(a) = 0$. Let $\rho^{\varepsilon} = 1 + \varepsilon a$. If ε is sufficiently small, then $\rho^{\varepsilon} \in \mathcal{D}(\mathcal{M}, \tau) \cap \mathcal{M}$ and ρ^{ε} is invertible. From the Taylor series for the logarithm around 1 we deduce that there exists C > 0 such that

$$\|\log(1+\varepsilon a) - (\varepsilon a - \frac{1}{2}\varepsilon^2 a^2)\|_{\mathcal{M}} \le C\varepsilon^3.$$

Thus

$$\frac{1}{\varepsilon^2} \operatorname{Ent}(\rho^{\varepsilon}) = \frac{1}{\varepsilon^2} \tau((1 + \varepsilon a)(\varepsilon a - \frac{1}{2}\varepsilon^2 a^2)) + C\varepsilon \to \frac{1}{2}\tau(a^2)$$

as $\varepsilon \to 0$.

Similarly, approximating $\log(1 + \varepsilon \cdot)$ in C^1 by polynomials we obtain

$$\lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2} \mathscr{I}(\rho^{\varepsilon}) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2} \mathscr{E}(1 + \varepsilon a, \varepsilon a) = \mathscr{E}(a).$$

Now the Poincaré inequality follows from the modified log-Sobolev inequality. \Box

7.3 Convexity of the entropy along \mathcal{W} -geodesics

In this section we establish the existence of geodesics in $(\mathcal{D}(\mathcal{M}, \tau), \mathcal{W})$ and investigate convexity properties of the entropy along geodesics.

Let (X,d) be an extended metric space. A curve $(\gamma_t)_{t\in[0,1]}$ in X is called (constant speed) *geodesic* if $d(\gamma_0,\gamma_1) < \infty$ and $d(\gamma_s,\gamma_t) = |s-t|d(\gamma_0,\gamma_1)$ for all $s,t \in [0,1]$. The extended metric space (X,d) is called *geodesic space* if any two $x, y \in X$ with $d(x,y) < \infty$ can be joined by a geodesic.

Theorem 7.15. If the entropy has regular sublevel sets and (P_t) is an EVI_K gradient flow of Ent, then for all $\rho_0, \rho_1 \in D(\text{Ent})$ with $\mathcal{W}(\rho_0, \rho_1) < \infty$ there exists a geodesic $(\rho_t)_{t \in [0,1]}$ with $\sup_{t \in [0,1]} \text{Ent}(\rho_t) < \infty$. In particular, $(D(\text{Ent}), \mathcal{W})$ is a geodesic space.

Proof. Using the contraction estimate from Lemma 6.2, one can proceed exactly as in the proof of Proposition 7.2 to see that for all $\rho_0, \rho_1 \in D(\text{Ent})$ with $\mathcal{W}(\rho_0, \rho_1) < \infty$ and all $n \in \mathbb{N}$ there exists an L_n -Lipschitz curve $(\rho_t^n)_{t \in [0,1]}$ connecting ρ_0 and ρ_1 such that $L_n^2 \leq e^{-2K/n} (\mathcal{W}(\rho_0, \rho_1)^2 + \frac{1}{n^2})$ and

$$\sup_{n\in\mathbb{N}}\sup_{t\in[0,1]}\operatorname{Ent}(\rho_t^n)<\infty.$$

Since the entropy has regular sublevel sets, the curves (ρ_t^n) are admissible and

$$\|D\rho_t^n\|_{\rho_t^n} = |\dot{\rho}_t^n|_{\mathcal{W}} \le L_n.$$

As (L_n) is bounded, we can apply Lemma 7.7 to get an admissible curve $(\rho_t)_{t \in [0,1]}$ with uniformly bounded entropy connecting ρ_0 and ρ_1 such that

$$\begin{split} \int_0^1 \|D\rho_t\|_{\rho_t}^2 dt &\leq \liminf_{n \to \infty} \int_0^1 \|D\rho_t^n\|_{\rho_t^n}^2 dt \\ &\leq \liminf_{n \to \infty} e^{-2K/n} \left(\mathcal{W}(\rho_0, \rho_1)^2 + \frac{1}{n^2} \right) \\ &= \mathcal{W}(\rho_0, \rho_1)^2. \end{split}$$

Hence (ρ_t) is a geodesic connecting ρ_0 and ρ_1 .

Corollary 7.16. If the entropy has regular sublevel sets and (P_t) is an EVI_K gradient flow of Ent, then the metric W is lower semicontinuous with respect to weak L^1 -convergence on sublevel sets of the entropy.

Remark 7.17. Theorem 7.15 guarantees the existence of geodesics connecting density matrices with finite entropy only if their distance is finite; it does not rule out the possibility that density matrices with finite entropy have infinite distance. As we have seen in the last section, this cannot happen if \mathscr{E} satisfies $GE(K,\infty)$ for K > 0 and (P_t) is irreducible.

The last property discussed in this section is *K*-convexity of the entropy. Let (X,d) be an extended metric space. A functional $S: X \longrightarrow (-\infty,\infty]$ is called *K*-convex along the geodesic $(\gamma_t)_{t \in [0,1]}$ in (D(S),d) if

$$S(\gamma_t) \le (1-t)S(\gamma_0) + tS(\gamma_1) - \frac{K}{2}t(1-t)d(\gamma_0,\gamma_1)^2$$

for all $t \in [0, 1]$.

The functional S is called *strongly geodesically K-convex* if it is *K*-convex along every geodesic in (D(S),d). It is called *geodesically K-convex* if every pair $x_0, x_1 \in D(S)$ can be joined by a geodesic (γ_t) such that S is K-convex along (γ_t) .

Remark 7.18. If (D(S),d) is a geodesic space, then every strongly geodesically *K*-convex functional is geodesically *K*-convex. If (D(S),d) is not a geodesic space, it does not make too much sense to talk about geodesic convexity at all.

If (P_t) is an EVI_K gradient flow of the entropy and the sublevel sets of the entropy are regular, the strong *K*-convexity follows from abstract results on gradient flows in metric spaces.

Theorem 7.19. If (P_t) is an EVI_K gradient flow of Ent and Ent has regular sublevel sets, then (D(Ent), W) is a geodesic space and Ent is strongly geodesically K-convex.

Proof. This is a direct consequence of Theorem 7.15 and [AGS14b, Proposition 2.23]. \Box

Example 7.20. As discussed in Example 5.19, the noncommutative heat semigroup on the noncommutative torus satisfies $GE(0,\infty)$. Thus the von Neumann entropy is strongly geodesically convex in this case. Taking geodesic *K*-convexity as definition for a lower Ricci curvature bound *K*, this can be seen as a first step towards Ricci curvature bounds in noncommutative geometry. This aligns well with the fact that the generator of the noncommutative heat semigroup is interpreted as noncommutative analog of the Laplace–Beltrami operator for the flat metric on the torus. *Example* 7.21. Gross' fermionic Dirichlet form satisfies $GE(1,\infty)$ according to example 5.20. Hence the entropy is strongly geodesically 1-convex in this case. This complements the result by Carlen and Maas for finite-dimensional fermionic systems (see [CM17a, Theorem 8.6]).

Let us summarize the results of the last two sections.

Theorem 7.22. Assume that τ is finite, $L^1(\mathcal{M}, \tau)$ is separable and θ is the logarithmic mean, which is regular for \mathscr{E} . For $K \in \mathbb{R}$ consider the following properties.

- (i) The semigroup (P_t) satisfies the gradient estimate $GE(K,\infty)$.
- (ii) The semigroup (P_t) is an EVI_K gradient flow of Ent, the sublevel sets of Ent are regular and W is non-degenerate.
- (iii) The pseudo metric W is non-degenerate, (D(Ent), W) is geodesic and Ent is strongly geodesically K-convex.

Then $(i) \Longrightarrow (ii) \Longrightarrow (iii)$.

Remark 7.23. The properties (i), (ii) and (iii) can all be understood as lower Ricci curvature bounds for the geometry determined by \mathcal{E} . This approach has been studied intensively for metric measure spaces (see e.q. [AGS14b, LV09, Stu06a, Stu06b]) and, more recently, also for graphs (see e.g. [EM12, EHMT17]). We hope that the present framework allows to address the highly interesting question of introducing a concept of Ricci curvature (bounds) in noncommutative geometry. First steps in this direction were already taken by Hornshaw [Hor18].

CHAPTER 8

OUTLOOK AND OPEN PROBLEMS

8.1 Beyond tracial symmetry

One of the crucial assumptions on the quantum Markov semigroup throughout this thesis is that it is symmetric with respect to a trace, which in the later section is furthermore assumed to be finite. Finiteness of the trace is restrictive in that it excludes some natural examples of (noncommutative) measure spaces such as Riemannian manifolds with infinite volume and the bounded linear operators on an infinite-dimensional Hilbert space with the standard trace.

Some of the reasons to assume finiteness of the trace are merely technical. For example, this assumption allows for approximation of density operators by invertible ones and via the inclusion of L^p spaces simplifies several convergence arguments. There are, however, at least two severe challenges to overcome in the infinite case.

One is the lack of semicontinuity of the entropy in the case of an infinite reference weight. This problem occurs already in the (strongly local) commutative case and is overcome as follows. Let (X,d,m) be a metric measure space. The basic assumption that replaces finiteness of m is the existence of a Lipschitz map $V: X \longrightarrow (0,\infty)$ such that $\int e^{-V^2} dm \leq 1$. Then one restricts the attention to the set $P_V(X)$ of all Borel probability measures μ on X such that $V \in L^2(X,\mu)$.

If one endows this space with the topology of weak convergence with moments, that is, $\mu_n \to \mu$ in $P_V(X)$ if and only if $\mu_n \to \mu$ weakly and $\|V\|_{L^2(X,\mu_n)} \to \|V\|_{L^2(X,\mu)}$, the entropy becomes lower semicontinuous again. Moreover, the Lipschitz continuity of V also guarantees the lower semicontinuity of the entropy with respect to convergence in Wasserstein distance. It seems conceivable that a similar argument works in the noncommutative case if one replaces the Lipschitz continuity of *V* by a suitable weak formulation of $\Gamma(V) \in \mathcal{M}$.

Another challenge, which is especially relevant for Chapter 7, is the lack of a good compactness criterion in the case of an infinite trace. In the commutative situations treated so far, the transport distance \mathcal{W} is defined on the space of all probability measures (although possibly infinite) and Prokhorov's theorem yields a useful criterion for compactness. In contrast, in the setting of this thesis the metric \mathcal{W} is only defined on the weak^{*} dense subset of probability densities. In Chapter 7 we could rectify the lack of compactness in the space of density operators by considering sublevel sets of the entropy, which are compact by the noncommutative version of Vallée-Poussin's criterion. It is not clear how to modify this argument to work in the infinite case as well.

Besides finiteness, another assumption one might want to weaken is the trace property of the invariant weight. This does not make a difference in the commutative case, as every weight is automatically tracial, but is very relevant for applications to mathematical physics and noncommutative geometry. In particular, not every von Neumann algebra admits an n.s.f. trace.

There are three closely related relaxations of tracial symmetry, called GNS, KMS and BKM symmetry (named after Gelfand–Naimark–Segal, Kubo–Martin– Schwinger and Bogoliubov–Kubo–Mori respectively). Let us describe these conditions in the case when (\mathcal{M}, τ) is a tracial von Neumann algebra. Let $\sigma \in \mathcal{D}(\mathcal{M}, \tau)$ and define

$$\langle \cdot, \cdot \rangle_s : \mathcal{M} \times \mathcal{M} \longrightarrow \mathbb{C}, \langle x, y \rangle_s = \tau(x\sigma^s y^* \sigma^{1-s})$$

for $s \in [0, 1]$.

A quantum Markov semigroup (P_t) on \mathcal{M} is called *GNS symmetric* (or said to satisfy the *detailed balance condition*) if it is symmetric with respect to $\langle \cdot, \cdot \rangle_s$ for some $s \neq 1/2$. In this case, (P_t) is symmetric with respect to $\langle \cdot, \cdot \rangle_s$ for all $s \in [0, 1]$. The semigroup is called *KMS symmetric* if it is symmetric with respect to $\langle \cdot, \cdot \rangle_{1/2}$. It is called *BKM symmetric* if it is symmetric with respect to $\int_0^1 \langle \cdot, \cdot \rangle_s ds$. Note that the BKM inner product occurring in the last condition is nothing but $\langle \cdot, \cdot \rangle_\sigma$ for $\theta = \text{LM}$ and left and right action on $L^2(\mathcal{M}, \tau)$ given by left and right multiplication.

In each of these cases, σ is invariant under the predual semigroup of (P_t) . Of course, if $\sigma = 1$, then all of these three notions coincide with tracial symmetry.

In the finite-dimensional case, Carlen and Maas [CM17a] gave a construction of a Riemannian metric on the space of invertible density matrices for GNSsymmetric quantum Markov semigroups such that the semigroup is the gradient flow of the relative entropy

$$\operatorname{Ent}(\rho \| \sigma) = \tau(\rho(\log \rho - \log \sigma)).$$

Moreover, in [CM18, Theorem 2.9] they showed that for the existence of such a metric it is necessary that the semigroup (P_t) is BKM symmetric.

If \mathcal{M} does not admit an n.s.f. trace, GNS symmetry with respect to an invariant state ω can be expressed as symmetry with respect to the embedding $\mathcal{M} \hookrightarrow H_{\omega}$ into the GNS Hilbert space. KMS symmetry can be rephrased in terms of the modular automorphism group as

$$\omega\left(P_t(x)\sigma_{-\frac{i}{2}}(y)\right) = \omega\left(\sigma_{\frac{i}{2}}(x)P_t(y)\right)$$

for all $t \ge 0$ and $x, y \in \mathcal{M}_{\sigma}$. Here (σ_t) is the modular automorphism group associated with ω and \mathcal{M}_{σ} the algebra of analytic elements for (σ_t) .

More generally, if one replaces the parameter i/2 of the modular automorphism group by $i\beta/2$, one obtains the notion of β -KMS symmetry. In physics, the parameter β plays the role of the inverse temperature. Clearly, tracially symmetric semigroups correspond to the case $\beta = 0$, which can be understood as an infinite temperature limit. In noncommutative geometry, β -KMS-symmetric quantum Markov semigroups appear for example as conformal defomration of the noncommutative heat semigroup on the noncommutative torus (see [CC92, CT11]). As such they are crucial for the understanding of non-flat noncommutative geometries. Both these possible applications give a strong motivation to study possible extensions of the theory developed in this thesis beyond the tracially symmetric case.

8.2 Possible equivalence of $GE(K,\infty)$, EVI_K and *K*-convexity of the entropy

Let us recall Theorem 7.22.

Theorem. Assume that τ is finite, $L^1(\mathcal{M}, \tau)$ is separable and θ is the logarithmic mean, which is regular for \mathscr{E} . For $K \in \mathbb{R}$ consider the following properties.

- (i) The semigroup (P_t) satisfies the gradient estimate $GE(K,\infty)$.
- (ii) The semigroup (P_t) is an EVI_K gradient flow of Ent, the sublevel sets of Ent are regular and W is non-degenerate.
- (iii) The pseudo metric W is non-degenerate, (D(Ent), W) is geodesic and Ent is strongly geodesically K-convex.

Then $(i) \Longrightarrow (ii) \Longrightarrow (iii)$.

The properties (i), (ii) and (iii) are equivalent for the Dirichlet energy on complete Riemannian manifolds [vRS05, Theorems 1.1, 1.3] (and more generally for the Cheeger energy on infinitesimally Hilbertian length metric measure spaces [AGS15, Theorem 1.1]) as well as the Dirichlet forms associated with finite graphs ([EM12, Theorem 4.5] and [EF18, Theorem 3.1]). It seems therefore natural to conjecture that the same is true, at least under suitable technical conditions, in the framework of this thesis. Let us elaborate on the possible implication (iii) \implies (i). The following discussion is informal, but it can be made rigorous at least in the finite-dimensional case.

Via a Ledoux ansatz, the gradient estimate

$$\|\partial P_t a\|_{\rho}^2 \le e^{-2Kt} \|\partial a\|_{P_t \rho}^2$$

is equivalent to

$$\operatorname{Hess}_{\rho}(\operatorname{Ent})[\partial a, \partial a] \geq K \|\partial a\|_{\rho}^{2},$$

where the Hessian is understood with respect to the (formal) Riemannian structure on $\mathcal{D}(\mathcal{M},\tau)$ induced by \mathcal{W} (see Section 8.5). This inequality in turn follows from the *K*-convexity of the entropy along the geodesic starting at ρ with initial velocity ∂a (even for finite graphs one has to take additional care since the simplex of probability densities is a manifold with boundary and the Riemannian metric induced by \mathcal{W} degenerates at the boundary).

In this argument it is crucial that there exists a geodesic starting in ρ with initial velocity ∂a for sufficiently many $\rho \in \mathscr{D}(\mathcal{M}, \tau)$ and $a \in \mathscr{A}_{AM}$. In the finite-dimensional case (away from the boundary of the simplex of probability densities), this follows from classical existence theory of ODE, but it is not at all clear in the infinite-dimensional case.

For strongly local Dirichlet forms it was proven by Ambrosio, Erbar and Savaré [AES16] that the contraction estimate $\mathcal{W}(P_t\rho,P_t\sigma) \leq e^{-Kt}\mathcal{W}(\rho,\sigma)$, which follows from (ii), implies the gradient estimate $GE(K,\infty)$. Their argument relies on the recent extension of the DiPerna–Lions theory to abstract metric measure spaces (see [AT14]). In [OW05, Section 3] one can find a heuristic discussion how to deduce the contraction estimate for the gradient flow from geodesic *K*-convexity of the functional.

So it seems like one needs a better existence theory for solutions of the abstract continuity equation or even W-geodesics to get any sufficient conditions for (i) and, in particular, to prove the equivalence of (i), (ii) and (iii).

The analysis of the noncommutative continuity equation in this thesis relies on some simple estimates under quite restrictive assumptions as in Proposition 3.27, the stability result from Theorem 3.30 and the (up to technicalities) explicit solution in the case when ρ is a heat flow trajectory. A key difficulty compared to the local case lies of course in the non-linearity of the equation in ρ . Moreover, the analysis of the classical continuity equation typically relies strongly on the underlying spatial structure. However, there is simply no spatial structure in the noncommutative framework.

8.3 Dual formulation

Both for the Dirichlet energy on Euclidean space (see e.g. [Vil03, Proof of Theorem 8.1]) and for Dirichlet forms associated with graphs (see [GLM17, Theorem 5.10],[EMW19, Theorem 3.4]), the optimization problem in the definition of \mathcal{W} admits a dual formulation in terms of subsolutions of a Hamilton–Jacobi equation. This dual formulation has, among other things, been used in the description of the geometry of \mathcal{W} -geodesics discussed below and features in most proofs of the gradient flow characterization.

More precisely, define a metric \mathcal{W}_* by

$$\frac{1}{2}\mathcal{W}_{*}(\rho_{0},\rho_{1})^{2} = \sup \int_{X} (u_{1}\rho_{1} - u_{0}\rho_{0}) dm,$$
(DP)

where the supremum is taken over all curves (u_t) in \mathcal{A}_{AM} that satisfy

$$\frac{d}{dt} \int_{X} u_t \sigma \, dm + \frac{1}{2} \|\partial u_t\|_{\sigma}^2 \le 0 \tag{HJE}$$

for all probability densities σ in a suitable weak sense. The duality result asserts $W_* = W$.

In the strongly local case (or when θ is the arithmetic mean), the inequality (HJE) is linear in σ and is simply a weak formulation of the differential inequality

$$\dot{u}_t + \frac{1}{2}\Gamma(u_t) \le 0.$$

In other words, the admissible curves in the optimization problem for \mathcal{W}_* are subsolutions of a Hamilton–Jacobi equation.

In the noncommutative framework of this thesis, the inequality $\mathcal{W} \geq \mathcal{W}_*$ is still true, at least if (u_t) is sufficiently regular in t. Indeed, let (ρ_t) be a smooth admissible curve connecting ρ_0 and ρ_1 . Then

$$\begin{aligned} \tau(u_1\rho_1 - u_0\rho_0) &= \int_0^1 \frac{d}{dt} \tau(u_t\rho_t) dt \\ &\leq \int_0^1 \left(-\frac{1}{2} \|\partial u_t\|_{\rho_t}^2 + \langle \partial u_t, D\rho_t \rangle_{\rho_t} \right) dt \\ &\leq \frac{1}{2} \int_0^1 \|D\rho_t\|_{\rho_t}^2 dt. \end{aligned}$$

The converse inequality is considerably harder and it is not clear under which conditions it holds for noncommutative or just non-local commutative Dirichlet forms.

8.4 Hopf-Lax formula

One way to prove the equivalence of the Benamou–Brenier formulation and the Monge–Kantorovich formulation of the Wasserstein metric (on Euclidean space for the sake of simplicity) is to pass through the dual formulation from the last section and use the Hopf-Lax formula, which asserts that the (viscosity) solution of the initial-value problem

$$\dot{u}_t + \frac{1}{2} |\nabla u_t|^2 = 0$$
$$u_0 = g$$

is given by

$$u_t(x) = \inf_{y} \left(g(y) + \frac{|x-y|^2}{2t} \right).$$

This way, the Hopf-Cole formula links the dynamical and static optimization problems for the Wasserstein distance. One could therefore hope that an explicit formula for the solutions of the Hamilton–Jacobi equation (HJE) similarly leads to a static formulation of the transport metric \mathcal{W} on graphs, which might bear a more direct connection to the geometry of the underlying graph than the dynamical formulation does.

8.5 Otto calculus

The Benamou-Brenier formula of the Wasserstein metric has the form of the distance function induced by a Riemannian metric, except for the fact that the Borel probability measures on Euclidean space do not form a (finite-dimensional) differential manifold. On this basis, Otto ([Ott01], see also [Lot08, OV00] for further extensions) developed what is now known as *Otto calculus*, a set of calculations on this formal Riemannian manifold. Despite their formal nature, these have proven useful in obtaining rigorous estimates for diffusion equations.

If one does not restrict to local Dirichlet forms, the situation improves as it makes sense to consider the finite-dimensional case. In this case, the transport metric \mathcal{W} is induced by a Riemannian metric on the invertible density matrices and one can perform calculations from Otto calculus rigorously. For example, the geodesic equations on this manifold are

$$\dot{\rho}_{t} = \partial^{*}(\theta(L(\rho_{t}), R(\rho_{t}))\partial a_{t}) \dot{a}_{t} = \langle \theta_{1}(L(\rho_{t}), R(\rho_{t}))\partial a_{t}, \partial a_{t} \rangle_{\mathcal{H}},$$
 (Geo)

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where $\theta_1(s,t) = \frac{\partial}{\partial s} \theta(s,t)$.

Carlen and Maas [CM17a, CM18] performed some of these calculations and showed that they can also serve as a formal calculus for the infinite-dimensional case very much like the original Otto calculus. Nevertheless it would be interesting to see if one can make some of the calculations such as the geodesics equations (Geo) rigorous in the infinite-dimensional setting.

8.6 The geometry of \mathcal{W}

The geometry of the L^2 -Wasserstein space over length or geodesic metric spaces has been understood quite well by now (see e.g. [Lis07, Vil09]). As the underlying metric space embeds isometrically into the Wasserstein space, the link between geometric properties of the underlying space and the space of probability measures is often quite direct. This connection has played a pivotal role in the study of the geometry of metric spaces with lower bounded Ricci curvature (see e.g. [LV09, Stu06a, Stu06b, CM17b]). For example, the Wasserstein space is geodesic if and only if the underlying space is geodesic, and in this case, the midpoint of a geodesic between two probability measures is supported on the midpoints of geodesics between the points in their supports. This fact implies almost immediately the Brunn–Minkowski inequality for CD(K,N) spaces.

The situation is less clear and much less is known about the transport metric \mathcal{W} if the Dirichlet form is non-local. Already the simplest case of Dirichlet forms associated with finite graphs exhibits some interesting and unexpected features. For example, if one considers the complete graph on three vertices, any geodesic connecting two distinct Dirac measures is supported on all vertices at intermediate times. In other words, the optimal way to transport mass from one vertex to a neighbor is not only along the connecting edge, but along all edges.

In a joint article with Jan Maas and Matthias Erbar [EMW19] we examined under which conditions \mathcal{W} -geodesics can be localized, that is, if the start and endpoint are supported on a certain subgraph, so is some/any geodesic between them at intermediate times. One sufficient condition is that the subgraph is connected to the rest of the graph through a "bottleneck", that is, a single vertex. Another sufficient condition covers so-called *retracts* and includes the cases of hypercubes in finite subgraphs of \mathbb{Z}^d as well as edges in complete graphs on four and more vertices.

A natural follow-up problem is of course to consider the case of infinite graphs. This is also interesting for computational purposes, as it would allow to compute distances between finitely supported probability measures on finite graphs without any error. It seems that the methods from [EMW19] are sufficiently robust to carry over at least to the case of graphs with bounded Laplacian. Another question about \mathcal{W} -geodesics concerns their uniqueness. For the Wasserstein metric, geodesics with a given starting and endpoint are not unique if they are not unique in the underlying space. Whether \mathcal{W} -geodesics on probability densities on graphs are always unique or uniqueness depends on the graph structure is subject of current investigation.

Even less is known about the geometry of \mathcal{W} in the noncommutative case, apart from the existence of geodesics proven in this thesis (Theorem 7.19) and a decomposition result of geodesics for the case when the underlying algebra is a C(X)-algebra obtained in [Hor18]. In this context it would be particularly interesting to find connections to other fields of noncommutative geometry.

8.7 Approximation

One motivation for a unified treatment of the transport distance \mathcal{W} in the local and non-local setting was to have a convenient framework for approximation, for example of unbounded Dirichlet forms by bounded ones, or of Dirichlet forms on infinite spaces by ones on finite spaces. In each of these instances, the approximating forms are necessarily non-local.

Approximation has turned out to be a delicate matter with only a few results available so far. In [GM13] it was shown that if one equips the discrete torus $(\mathbb{Z}/n\mathbb{Z})^d$ with suitable weights, the space of probability measures with the corresponding transport metric converges in the Gromov-Hausdorff sense to the Wasserstein space on the continuous torus as $n \to \infty$. In [GKM18], Gromov-Hausdorff convergence was shown for the transport distance on certain isotropic meshes approximating bounded convex domains in Euclidean space. As demonstrated in [GKM18] and [Gar17], the convergence/non-convergence of the space of probability measures depends quite subtly on the structure of the underlying graphs.

All the cited sources have in common that they infer Gromov-Hausdorff convergence of the space of probability measures directly from geometric properties of the underlying spaces. While this approach comes in handy to construct approximating graphs or check Gromov-Hausdorff convergence for a given approximation, it somehow obscures the analytic aspect and is hard to generalize to other forms of approximations.

It would therefore be interesting to break up the approximation results into two parts: one part to deduce Gromov-Hausdorff convergence of the space of density operators from a suitable convergence of the underlying Dirichlet forms, and a second part (in the commutative case) to deduce the convergence of Dirichlet forms from some form of convergence of the underlying spaces. Depending on the mode of convergence needed for the Dirichlet forms, the second step might in many situations even follow from known convergence results for Laplace operators. Moreover, the first step is also applicable to the noncommutative case without any underlying space.

One difficulty with this approach lies in the rather indirect dependence of the transport metric on the Dirichlet form through the first-order differential calculus and curves of density operators. As a good toy example one could test the bounded approximating forms $\mathscr{E}_{\varepsilon}$ generated by $\frac{1}{\varepsilon}(1-P_{\varepsilon})$.

APPENDIX A

NONCOMMUTATIVE L^p SPACES

In this section we give a short overview over the theory of noncommutative integration and noncommutative L^p spaces. The material in this appendix is wellknown. Standard references for the basic theory of operator algebras are [Bla06, Sak98, Tak02]. The approach to noncommutative L^p spaces presented here was developed by Segal [Seg53a, Seg53b], Nelson [Nel74] and Yeadon [Yea75]; a good overview is given in [Ter81, PX03].

Let *H* be a Hilbert space and let $\mathscr{L}(H)$ denote the space of all bounded linear operators on *H*. The *commutant* of a subset \mathscr{M} of $\mathscr{L}(H)$ is

$$\mathcal{M}' = \{ y \in \mathcal{L}(H) \mid yx = xy \text{ for all } x \in \mathcal{M} \}.$$

A von Neumann algebra is a C^* -subalgebra \mathcal{M} of $\mathcal{L}(H)$ such that $\mathcal{M}'' = \mathcal{M}$. We denote the cone of positive elements of \mathcal{M} by \mathcal{M}_+ .

A *weight* on a von Neumann algebra \mathcal{M} is a map $\omega \colon \mathcal{M}_+ \longrightarrow [0,\infty]$ such that

- $\omega(x+y) = \omega(x) + \omega(y)$ for all $x, y \in \mathcal{M}_+$,
- $\omega(\lambda x) = \lambda \omega(x)$ for all $\lambda \ge 0$, $x \in \mathcal{M}_+$ (with the convention $0 \cdot \infty = 0$).

The weight ω is called

- *normal* if $\omega(\sup_i x_i) = \sup_i \omega(x_i)$ for every increasing net (x_i) in \mathcal{M}_+ ,
- *semi-finite* if $\omega(x) = \sup\{\omega(y) \mid 0 \le y \le x, \tau(y) < \infty\}$ for all $x \in \mathcal{M}_+$,
- *faithful* if $\omega(x^*x) = 0$ implies x = 0,
- *tracial* or a *trace* if $\omega(x^*x) = \omega(xx^*)$ for all $x \in \mathcal{M}$.

We say that τ is an *n.s.f. trace* if it is an normal, semi-finite, faithful, tracial weight and call the pair (\mathcal{M}, τ) a *tracial von Neumann algebra*.

If the weight ω is finite, then it extends linearly to \mathcal{M} and is in fact continuous. Conversely, every positive linear functional on \mathcal{M} restricts to a finite weight on \mathcal{M}_+ . We will usually identify finite weights and positive linear functionals. A finite weight ω is called a *state* if $\omega(1) = 1$.

Example A.1 (Standard trace). The functional

tr:
$$\mathscr{L}(H)_+ \longrightarrow [0,\infty], tr(x) = \begin{cases} \sum_{\lambda} \lambda \dim \ker(x-\lambda) & \text{if } x \text{ is compact}, \\ \infty & \text{otherwise} \end{cases}$$

is an n.s.f. trace on the von Neumann algebra $\mathcal{L}(H)$.

Example A.2 (Commutative von Neumann algebras). Let (X, \mathcal{B}, m) be a measure space. The measure *m* is called semi-finite if

$$m(A) = \sup\{m(B) \mid B \in \mathcal{B}, B \subset A, m(B) < \infty\}$$

for all $A \in \mathcal{B}$. The measure space (X, \mathcal{B}, m) is called localizable if m is semi-finite and $L^{\infty}(X, m)$ is Dedekind complete. For example, σ -finite measure spaces are localizable.

If (X, \mathcal{B}, m) is localizable, then the space $\mathcal{M}(X, m)$ formed by the operators

$$M_f: L^2(X,m) \longrightarrow L^2(X,m), M_f \varphi = f \varphi$$

for $f \in L^{\infty}(X,m)$ is a von Neumann algebra and the functional

$$\tau_m \colon \mathscr{M}_+ \longrightarrow [0,\infty], \, \tau_m(M_f) = \int_X f \, dm$$

is an n.s.f. trace. The weight τ_m is a state if and only if *m* is a probability measure.

Conversely, if \mathcal{M} is a commutative von Neumann algebra and τ an n.s.f. trace on \mathcal{M} , then there exist a localizable measure space (X, \mathcal{B}, m) and a *-isomorphism $\Phi: \mathcal{M} \longrightarrow \mathcal{M}(X, m)$ such that $\tau_m \circ \Phi|_{\mathcal{M}_+} = \tau$ (see [Seg51] or [Sak98, Section1.18] for details). In this sense the theory of n.s.f. traces on commutative von Neumann algebras is equivalent to measure theory on localizable measure spaces.

Every n.s.f. trace τ on \mathcal{M} induces a faithful normal representation π_{τ} of M on a Hilbert space H_{τ} , the GNS representation, as follows:

The set

$$\mathcal{N}_{\tau} = \{ x \in \mathcal{M} \mid \tau(x^* x) < \infty \}$$

is a σ -weakly closed left ideal of \mathcal{M} and the map

$$\langle \cdot, \cdot \rangle_{\tau} : \mathcal{N}_{\tau} \times \mathcal{N}_{\tau} \longrightarrow \mathbb{C}, \langle x, y \rangle_{\tau} = \tau(y^* x)$$

is an inner product on \mathcal{N}_{τ} . Moreover, \mathcal{M} acts by bounded operators on \mathcal{N}_{τ} by left multiplication. This action extends to a faithful normal representation π_{τ} on the completion H_{τ} of \mathcal{N}_{τ} . We will routinely identify \mathcal{M} with $\pi_{\tau}(\mathcal{M})$. The same construction works if τ is merely an n.s.f. weight (not a trace), but we concentrate on the tracial case in this thesis.

Sometimes it is more convenient to start with a C^* -algebra A instead of a von Neumann algebra. If one assumes τ to be lower semicontinuous instead of normal, then the same construction as above yields a faithful non-degenerate representation π_{τ} of A and τ extends to an n.s.f. trace on the von Neumann algebra $\pi_{\tau}(A)''$.

Example A.3 (Noncommutative Torus). Let $\vartheta \in (0,1)$ be irrational and let $U, V \in \mathscr{L}(H)$ be unitaries with $VU = e^{2\pi i \vartheta}UV$. The unital C^* -algebra A_ϑ generated by U, V is called *noncommutative torus* (and, up to *-isomorphism, it is indeed independent of the choice of U, V). Alternatively, A_ϑ can be obtained as the crossed product $C(S^1) \rtimes \mathbb{Z}$ induced by the rotation with angle ϑ on S^1 .

Let \mathscr{A}_{ϑ} be the linear hull of $\{U^m V^n \mid m, n \in \mathbb{Z}\}$, which is clearly a dense *subalgebra of A_{ϑ} . The map

$$\mathscr{A}_{\vartheta} \longrightarrow \mathbb{C}, \sum_{m,n} \alpha_{mn} U^m V^n \mapsto \sum_{m,n} \delta_{m,0} \delta_{n,0} \alpha_{mn}$$

extends to a faithful tracial state τ on A_{ϑ} , and this tracial state is unique. For more details see for example [Rie81].

Example A.4 (Fermionic Clifford algebra). Let H be a separable infinite-dimensional *real* Hilbert space. The Clifford C^* -algebra $\mathbb{C}\ell(H)$ is the universal unital C^* -algebra generated by self-adjoint elements $x_{\xi}, \xi \in H$, subject to the conditions

- (C1) $x_{\alpha\xi+\beta\eta} = \alpha x_{\xi} + \beta x_{\eta}$ for $\alpha, \beta \in \mathbb{R}, \xi, \eta \in H$,
- (C2) $x_{\xi}x_{\eta} + x_{\eta}x_{\xi} = 2\langle \xi, \eta \rangle_H$ for $\xi, \eta \in H$.

This means that $\mathbb{C}\ell(H)$ contains self-adjoint elements x_{ξ} , $\xi \in H$, that satisfy (C1) and (C2), and whenever A is a C^* -algebra with elements y_{ξ} , $\xi \in H$, that also satisfy (C1) and (C2), then there exists a unique unital *-homomorphism $\varphi : \mathbb{C}\ell(H) \longrightarrow A$ such that $\varphi(x_{\xi}) = y_{\xi}$ for all $\xi \in H$.

In fact, the Clifford C^* -algebra is simple and hence every unital C^* -algebra generated by elements $y_{\xi}, \xi \in H$, that satisfy (C1) and (C2) is *-isomorphic to $\mathbb{C}\ell(H)$.

Let (e_j) be an orthonormal basis of H. The unital algebra $\mathbb{C}\ell_0(H)$ generated by (e_j) is a dense *-subalgebra of $\mathbb{C}\ell(H)$ and

$$\tau \colon \mathbb{C}\ell_0(H) \longrightarrow \mathbb{C}, \sum_{j_1 < \cdots < j_k} \alpha_{j_1, \dots, j_k} e_{j_1} \dots e_{j_k} \mapsto \alpha_{\emptyset}$$

extends to a faithful tracial state on $\mathbb{C}\ell(H)$. The von Neumann algebra $\pi_{\tau}(\mathbb{C}\ell(H))''$ is the (up to *-isomorphism unique) hyperfinite type II₁ factor.

Let $\mathscr{F}_{-}(H)$ be the fermionic Fock space over H, that is, $\mathscr{F}_{-}(H) = \bigoplus_{k \ge 0} \bigwedge^{k} H$. The map

$$\mathbb{C}\ell_0(H) \longrightarrow \mathscr{F}_{-}(H), \sum_{j_1 < \cdots < j_k} \alpha_{j_1 \dots j_k} e_{j_1} \dots e_{j_k} \mapsto \sum_{j_1 < \cdots < j_k} \alpha_{j_1 \dots j_k} e_{j_1} \wedge \cdots \wedge e_{j_k}$$

extends to an isometric isomorphism $\Phi: H_{\tau} \longrightarrow \mathscr{F}_{-}(H)$, the Chevalley–Segal isomorphism. For more details see for example [SS64].

Let us now turn to noncommutative Lebesgue spaces. There are several equivalent definitions. Here we present an approach pioneered by Segal and Nelson.

Let \mathcal{M} be a von Neumann algebra on H. A closed, densely defined operator x on H is called *affiliated with* \mathcal{M} if ux = xu for every unitary $u \in \mathcal{M}'$. In particular, the set of bounded operators affiliated with \mathcal{M} is just \mathcal{M} .

An operator with polar decomposition x = v|x| is affiliated with \mathcal{M} if and only if $v \in \mathcal{M}$ and |x| is affiliated with \mathcal{M} . For a self-adjoint operator x on H, the following properties are equivalent:

- (i) x is affiliated with \mathcal{M} .
- (ii) $\mathbb{1}_E(x) \in \mathcal{M}$ for every Borel set $E \subset \mathbb{R}$.
- (iii) $\varphi(x) \in \mathcal{M}$ for every bounded Borel function $\varphi \colon \mathbb{R} \longrightarrow \mathbb{R}$.

In general, the set of affiliated operators does not have any nice algebraic properties. However, in the presence of an n.s.f. trace this can be rectified by considering the smaller space of measurable affiliated operators.

An operator *x* affiliated with the tracial von Neumann algebra (\mathcal{M}, τ) is called τ -*measurable* if $\tau(\mathbb{1}_{(\lambda,\infty)}(|x|)) < \infty$ for some $\lambda \ge 0$. The space of all τ -measurable operators is denoted by $L^0(\mathcal{M}, \tau)$. For an operator *x* affiliated with \mathcal{M} , the following properties are equivalent:

- (i) x is τ -measurable.
- (ii) |x| is τ -measurable.
- (iii) For all $\delta > 0$ there exists $\varepsilon > 0$ and a projection $e \in \mathcal{M}$ such that $||xe||_{\mathcal{M}} < \varepsilon$ and $\tau(1-e) < \delta$.
- (iv) For all $\delta > 0$ there exists $\varepsilon > 0$ such that $\tau(\mathbb{1}_{(\varepsilon,\infty)}(|x|)) < \delta$.

The sum and product of two τ -measurable operators is closable, and the closure is again a τ -measurable operator. These closures are called the strong sum and strong product of two measurable operators. Moreover, also the adjoint of a τ measurable operator is τ -measurable. In other words, $L^0(\mathcal{M}, \tau)$ is a *-algebra when endowed with these operations. Products and sums in $L^0(\mathcal{M}, \tau)$ are always to be understood in the strong sense.

The noncommutative L^p spaces can now be defined as

$$L^{p}(\mathcal{M},\tau) = \{x \in L^{0}(\mathcal{M},\tau) \mid \tau(|x|^{p}) < \infty\}$$

for $p \in [1,\infty)$. Endowed with the norm $\|\cdot\|_p = \tau(|\cdot|^p)^{1/p}$ these spaces are Banach spaces. For $p = \infty$ one sets $L^{\infty}(\mathcal{M}, \tau) = \mathcal{M}$.

Example A.5. Since $\mathscr{L}(H)' = \mathbb{C}1$, every closed densely defined operator on H is affiliated with $\mathscr{L}(H)$. In contrast, since a projection has only finite trace if it is finite-dimensional, the algebra of trace measurable operators coincides with $\mathscr{L}(H)$. Consequently, the spaces $L^p(\mathscr{L}(H), \mathrm{tr})$ coincide with the usual Schatten classes.

Example A.6. The von Neumann algebra \mathcal{M} from Example A.2 is maximally abelian, that is, $\mathcal{M}' = \mathcal{M}$. Therefore a closed densely defined operator on $L^2(X,m)$ is affiliated with \mathcal{M} if and only if it is of the form

$$D(M_f) = \{\varphi \in L^2(X,m) \mid f\varphi \in L^2(X,m)\}, M_f\varphi = f\varphi$$

for some measurable $f: X \longrightarrow \mathbb{C}$.

The operator M_f is τ_m -measurable if and only if f is bounded on the complement of a set of finite measure. Thus $L^0(\mathcal{M}, \tau_m)$ is in general a proper subset of the set of all measurable functions on \mathbb{C} . However, if m is finite, then the set of all τ_m -measurable operators and the set of all measurable functions on \mathbb{C} coincide. In any case,

$$L^p(X,m) \longrightarrow L^p(\mathcal{M},\tau_m), f \mapsto M_f$$

is an isometric isomorphism.

Proposition A.7 ([Yea75, Theorem 3.7]). Let (\mathcal{M}, τ) be a tracial von Neumann algebra. For all $p \in [1,\infty]$ the set $L^p(\mathcal{M}, \tau) \cap \mathcal{M}$ is dense in $L^p(\mathcal{M}, \tau)$.

As a consequence one can equivalently define $L^p(\mathcal{M}, \tau)$ as the completion of

$$\{x \in \mathcal{M} \mid \tau(|x|^p) < \infty\}$$

with respect to the norm $\tau(|\cdot|^p)^{1/p}$ without having to go through the framework of measurable operators. However, it often comes in handy to work with (possibly unbounded) operators instead of abstract elements of the completion.

One advantage of the representation of the L^p spaces by measurable operators is that they inherit some multiplicative structure. Of course the product of two elements of L^p is in general not in L^p , but it always makes sense as measurable operator. This allows to extend the following classical result to the noncommutative setting.

Theorem A.8 (Hölder's inequality and duality, [Yea75, Theorems 3.4, 4.4]). Let (\mathcal{M}, τ) be a tracial von Neumann algebra and $p, q \in [1, \infty]$ with 1/p + 1/q = 1.

(a) If $x \in L^p(\mathcal{M}, \tau)$ and $y \in L^q(\mathcal{M}, \tau)$, then $xy \in L^1(\mathcal{M}, \tau)$ and

$$||xy||_1 \le ||x||_p ||y||_q.$$

(b) If p > 1, then

$$L^p(\mathcal{M},\tau) \longrightarrow (L^q(\mathcal{M},\tau))^*, x \mapsto \tau(x \cdot)$$

is an isometric isomorphism.

Theorem A.9 (Interpolation scale [PX03, Theorem 2.1]). Let (\mathcal{M}, τ) be a tracial von Neumann algebra and $p, q, r \in [1, \infty]$. If $\vartheta \in [0, 1]$ such that

$$\frac{1}{r} = \frac{1-\vartheta}{q} + \frac{\vartheta}{q},$$

then the complex interpolation space $(L^p(\mathcal{M},\tau), L^q(\mathcal{M},\tau))_{\vartheta}$ is isometrically isomorphic to $L^r(\mathcal{M},\tau)$.

This theorem yields yet another possibility to define the noncommutative Lebesgue spaces:

$$L^p(\mathcal{M},\tau) \cong (\mathcal{M},\mathcal{M}_*)_{1/p}.$$

APPENDIX B

OPERATOR TOPOLOGIES

Let H be a Hilbert space. If H is finite-dimensional, then so is $\mathcal{L}(H)$ and it therefore carries a unique Hausdorff topological vector space topology. In contrast, in the infinite-dimensional case there is a plethora of different operator topologies. In this section we recall the definitions and review some properties of the topologies we use in this thesis. With the possible exception of Proposition B.3 and Lemma B.9, the results in this appendix are well-known and can be found in standard texts like [Bla06, Sak98, Tak02]

Definition B.1 (Operator topologies). The *norm topology* on $\mathcal{L}(H)$ is the topology generated by the operator norm

$$\|\cdot\|_{\mathscr{L}(H)}\colon \mathscr{L}(H) \longrightarrow [0,\infty), \|x\|_{\mathscr{L}(H)} = \sup_{\xi \in H} \frac{\|x\xi\|_{H}}{\|\xi\|_{H}}.$$

The strong (operator) topology on $\mathcal{L}(H)$ is the topology generated by the seminorms

$$p_{\xi} \colon \mathscr{L}(H) \longrightarrow [0,\infty), p_{\xi}(x) = \|x\xi\|_{H}$$

for $\xi \in H$. In other words, the strong topology is the topology of pointwise strong convergence in *H*.

The weak (operator) topology on $\mathcal{L}(H)$ is the topology generated by the seminorms

$$p_{\xi,\eta} \colon \mathscr{L}(H) \longrightarrow [0,\infty), \, p_{\xi,\eta}(x) = |\langle x\xi,\eta\rangle_H|$$

for $\xi, \eta \in H$. In other words, the weak topology is the topology of pointwise weak convergence in H. This topology should not be confused with the weak topology

in the sense of Banach spaces (we do not use the weak topology in the sense of Banach spaces on $\mathcal{L}(H)$ in this thesis).

The σ -weak or ultraweak (operator) topology on $\mathcal{L}(H)$ is the topology generated by the seminorms

$$p_{(\xi_n),(\eta_n)} \colon \mathscr{L}(H) \longrightarrow [0,\infty), \, p_{(\xi_n),(\eta_n)}(x) = \left| \sum_{n=1}^{\infty} \langle x\xi_n, \eta_n \rangle_H \right|$$

for sequences (ξ_n) , (η_n) in *H* with

$$\sum_{n=1}^{\infty} (\|\xi_n\|_H^2 + \|\eta_n\|_H^2) < \infty.$$

Let tr denote the standard trace and $\mathcal{L}_1(H)$ the space of trace-class operators on H. The map

$$\mathscr{L}(H) \longrightarrow \mathscr{L}_1(H)^*, x \mapsto \operatorname{tr}(x \cdot)$$

is an isometric isomorphism. Under this isomorphism, the σ -weak topology on $\mathscr{L}(H)$ coincides with the weak^{*} topology. Conversely, the space $\mathscr{L}(H)_*$ of all σ -weakly continuous linear functionals on $\mathscr{L}(H)$ is isomorphic to $\mathscr{L}_1(H)$ via the isomorphism

$$\mathscr{L}_1(H) \longrightarrow \mathscr{L}(H)_*, x \mapsto \operatorname{tr}(x \cdot).$$

Let $\mathscr{C}_h(H)$ be the set of all (possibly unbounded) self-adjoint operators on H. The *norm resolvent topology* on $\mathscr{C}_h(H)$ is the topology induced by the metric

$$d: \mathscr{C}_h(H) \times \mathscr{C}_h(H) \longrightarrow [0,\infty), d(x,y) = \|(x+i)^{-1} - (y+i)^{-1}\|_{\mathscr{M}}$$

The strong resolvent topology on $\mathcal{C}_h(H)$ is the topology generated by the pseudo metrics

$$d_{\xi} \colon \mathscr{C}_h(H) \times \mathscr{C}_h(H) \longrightarrow [0,\infty), d_{\xi}(x,y) = \|(x+i)^{-1}\xi - (y+i)^{-1}\xi\|_H$$

for $\xi \in H$.

Let (\mathcal{M}, τ) be a tracial von Neumann algebra. The *measure topology* on the space $L^0(\mathcal{M}, \tau)$ is the topological vector space topology generated by the neighborhood basis of zero given by

$$U(\varepsilon,\delta) = \{x \in L^0(\mathcal{M},\tau) \mid \exists \text{ projection } p \in \mathcal{M} : \|xp\|_{\mathcal{M}} < \varepsilon, \tau(1-p) < \delta\}$$

for $\varepsilon, \delta > 0$.

Let $p,q \in [1,\infty)$ with 1/p + 1/q = 1. The strong L^p topology on $L^p(\mathcal{M},\tau)$ is the topology generated by the norm

$$\|\cdot\|_p: L^p(\mathcal{M}, \tau) \longrightarrow [0, \infty), \|x\|_p = \tau(|x|^p)^{1/p}.$$

The weak L^p topology on $L^p(\mathcal{M},\tau)$ is the topology generated by the seminorms

$$p_{\gamma}: L^p(\mathcal{M}, \tau) \longrightarrow [0, \infty), x \mapsto |\tau(xy)|$$

for $y \in L^q(\mathcal{M}, \tau)$.

Continuity of multiplication and taking adjoints

Multiplication is jointly continuous in the norm topology and in the measure topology. It is also jointly continuous in the strong L^p topology when viewed as a map

$$L^p(\mathcal{M},\tau) \times L^q(\mathcal{M},\tau) \longrightarrow L^1(\mathcal{M},\tau)$$

with 1/p + 1/q = 1. Multiplication is in general not jointly continuous in the strong, weak and σ -weak topology.

Multiplication is jointly continuous on norm bounded sets and jointly sequentially continuous in the strong topology, but neither of these holds for the weak or σ -weak topology in general.

Multiplication is separately continuous in the strong, weak and σ -weak topology.

Taking adjoints is continuous in the norm topology, the weak topology, the σ -weak topology, the measure topology and the strong and weak L^p topology, but in general not continuous in the strong topology.

Taking adjoints is continuous on the set of normal operators in the strong topology.

Metrizability

The norm topology, the norm resolvent topology, the measure topology and the strong L^p topology are metrizable. If H is separable, then the strong resolvent topology is metrizable. If \mathcal{M} is separable, then the strong topology, the weak topology, the σ -weak topology and the weak L^p topology for $p \in (1,\infty)$ are all metrizable on norm bounded subsets (with respect to $\|\cdot\|_p$ in the latter case).

Local convexity

Except for the norm resolvent and strong resolvent topology, all of the mentioned topologies are Hausdorff topological vector space topologies. Except for the measure topology, all of them are locally convex. Depending on the trace, the measure topology may or may not be locally convex.

Compactness criteria

Norm bounded subsets are precompact in the weak, σ -weak and weak L^p topology for $p \in (1,\infty)$. For compactness in the weak L^1 topology, the Dunford–Pettis and the Vallée Poussin theorem extend to the noncommutative setting.

Theorem B.2 (Noncommutative Dunford–Pettis theorem, see [Tak02, Theorem III.5.4]). Let (\mathcal{M}, τ) be a tracial von Neumann algebra. For a subset \mathscr{F} of $L^1(\mathcal{M}, \tau)$, the following properties are equivalent:

- (i) The set \mathscr{F} is precompact in the weak L^1 topology.
- (ii) The set \mathcal{F} is norm bounded and

$$\sup_{x\in\mathcal{F}}|\tau(p_nx)|\to 0$$

for every decreasing sequence (p_n) of projections such that $p_n \rightarrow 0$ weakly.

Proposition B.3 (Noncommutative Vallée Poussin theorem). Let (\mathcal{M}, τ) be a tracial von Neumann algebra and assume that τ is finite. A subset \mathscr{F} of $L^1(\mathcal{M}, \tau)$ is precompact in the weak L^1 topology if there exists a nonnegative measurable function f on $[0,\infty)$ such that $f(t)/t \to \infty$ as $t \to \infty$ and

$$\sup_{x\in\mathscr{F}}\tau(f(|x|))<\infty.$$

Proof. First note that \mathscr{F} is norm bounded. By the noncommutative Dunford–Pettis theorem it suffices to show

$$\sup_{x\in\mathscr{F}}|\tau(p_nx)|\to 0$$

whenever (p_n) is a decreasing sequence of projections such that $p_n \rightarrow 0$ weakly.

Let $C = \sup_{x \in \mathscr{F}} \tau(f(|x|))$. For $\varepsilon > 0$ let $M = \frac{2C}{\varepsilon}$. By assumption there exists T > 0 such that $f(t) \ge Mt$ for $t \ge T$. Moreover, since τ is normal, we can choose $N \in \mathbb{N}$ such that $\tau(p_n) < \frac{\varepsilon}{2T}$ for $n \ge N$.

Let $x \in \mathcal{F}$ with polar decomposition x = u|x|. It follows that

$$\begin{aligned} |\tau(p_n x)| &= |\tau(p_n u | x | (\mathbb{1}_{[0,T)}(|x|) + \mathbb{1}_{[T,\infty)}(|x|)))| \\ &\leq T \tau(p_n) + \tau(|x| \mathbb{1}_{[T,\infty)}(|x|)) \\ &< \frac{\varepsilon}{2} + \frac{1}{M} \tau(f(|x|)) \\ &\leq \varepsilon \end{aligned}$$

for all $n \ge N$.

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Continuity of functional calculus

Let \mathscr{M} be a von Neumann algebra. For $F \subset \mathbb{C}^n$ closed let \mathscr{M}_F^n denote the set of all commuting *n*-tuples of normal elements of \mathscr{M} with joint spectrum in F. Analog notation will be used for \mathscr{M} replaced by $L^p(\mathscr{M}, \tau)$ or $L^0(\mathscr{M}, \tau)$.

Proposition B.4 (Strong continuity of functional calculus, see [Tak02, Theorem II.4.7]). Let \mathcal{M} be a von Neumann algebra and $F \subset \mathbb{C}^n$ be closed. If $f: F \longrightarrow \mathbb{C}$ is continuous and there exists C > 0 such that $|f(z)| \leq C(1+|z|)$ for $z \in F$, then the map

$$\mathcal{M}_F^n \longrightarrow \mathcal{M}, (a_1, \dots, a_n) \mapsto f(a_1, \dots, a_n)$$

is strongly continuous.

Proposition B.5 (Strong resolvent continuity of functional calculus [RS78, Theorem VIII.20]). Let $F \subset \mathbb{R}^n$ be a closed set and $\mathscr{C}(H)_F^n$ the set of all strongly commuting n-tuples of self-adjoint operators with joint spectrum in F. If $f: F \longrightarrow \mathbb{R}$ is continuous, then the map

$$\mathscr{C}(H)_F^n \longrightarrow \mathscr{C}_h(H), (a_1, \dots, a_n) \mapsto f(a_1, \dots, a_n)$$

is strongly resolvent continuous.

Proposition B.6 (Continuity of functional calculus in the measure topology, see [Tik87, Theorem 2.6]). Let (\mathcal{M}, τ) be a tracial von Neumann algebra and $F \subset \mathbb{R}$ be closed. If $f: F \longrightarrow \mathbb{R}$ is continuous, then the map

$$L^{0}(\mathcal{M},\tau)_{F} \longrightarrow L^{0}(\mathcal{M},\tau), a \mapsto f(a)$$

is continuous in the measure topology.

Proposition B.7 (Continuity of functional calculus in L^p [Tik87, Theorem 3.3]). Let (\mathcal{M}, τ) be a tracial von Neumann algebra, $1 \le p, q < \infty$ and $F \subset \mathbb{R}$ be closed.

(a) If $f: F \longrightarrow \mathbb{R}$ is continuous and there exists C > 0 such that $|f(\lambda)| \le C|\lambda|^{p/q}$ for all $\lambda \in F$, then the map

$$L^p(\mathcal{M},\tau)_F \longrightarrow L^q(\mathcal{M},\tau), a \mapsto f(a)$$

is continuous in the norm topology on L^p .

(b) If τ is finite, then it suffices to assume that there exist $C_1, C_2 > 0$ such that $|f(\lambda)| \le C_1 + C_2 |\lambda|^{p/q}$ for all $\lambda \in F$ to obtain the same conclusion as in (a).

Relations between the operator topologies

The norm topology on $\mathscr{L}(H)$ is stronger than the strong topology, the σ -weak topology and the measure topology. The norm topology is stronger than the norm resolvent topology on $\mathscr{L}_h(H)$. They coincide on norm bounded subsets of $\mathscr{L}_h(H)$. The norm topology is stronger than the strong L^p topology if and only if τ is finite.

The strong topology is stronger than the weak topology. A net (x_i) in $\mathcal{L}(H)$ converges to 0 strongly if and only if $(x_i^*x_i)$ converges to 0 weakly. A linear functional is strongly continuous if and only if it is weakly continuous and the strong and weak closure of convex subsets coincide. The strong topology is stronger than the strong resolvent topology on $\mathcal{L}_h(H)$. They coincide on norm bounded subsets of $\mathcal{L}_h(H)$.

The σ -weak topology is stronger than the weak topology. They coincide on norm bounded subsets. If τ is finite, then the σ -weak topology is stronger than the weak L^p topology for $p \in [1,\infty)$. The set \mathcal{M}_* of σ -weakly continuous linear functionals on \mathcal{M} is a norm closed subset of \mathcal{M}^* , the set of all norm continuous linear functionals on \mathcal{M} .

The strong L^p topology is stronger than the weak L^p topology and the measure topology. The following result gives a partial converse for the measure topology.

Proposition B.8 ([Tik87, Proposition 3.1]). Let (\mathcal{M}, τ) be a tracial von Neumann algebra and $p \in [1, \infty)$. A sequence (a_n) in $L^p(\mathcal{M}, \tau)$ that converges to $a \in L^p(\mathcal{M}, \tau)$ in measure is convergent in $L^p(\mathcal{M}, \tau)$ if and only if the following two conditions are satisfied:

- (a) For all $\varepsilon > 0$ there exists $\delta > 0$ such that $||a_n e||_p < \varepsilon$ for all $n \in \mathbb{N}$ and all projections $e \in \mathcal{M}$ with $\tau(e) < \delta$.
- (b) For all $\varepsilon > 0$ there exists a projection $e \in \mathcal{M}$ such that $||a_n e||_p < \varepsilon$ for all $n \in \mathbb{N}$ and $\tau(1-e) < \infty$.

The relation between the strong L^p topology and the strong resolvent topology is clarified by the following result.

Lemma B.9. Let (\mathcal{M}, τ) be a tracial von Neumann algebra. The strong L^p topology on $L^p_h(\mathcal{M}, \tau)$ is stronger than the strong resolvent topology.

Proof. Let (x_n) be a sequence in $L_h^p(\mathcal{M}, \tau)$ converging to x in $L^p(\mathcal{M}, \tau)$. By [Wei00, Satz 9.22] it suffices to show that $(x_n + i)^{-1}$ converges weakly to $(x + i)^{-1}$. Since $((x_n + i)^{-1})_n$ is bounded in $\mathcal{L}(H)$, it is therefore enough to prove that

$$\tau(a((x_n+i)^{-1}-(x+i)^{-1})b) \to 0$$

for $a, b \in L^2(\mathcal{M}, \tau) \cap L^{2q}(\mathcal{M}, \tau)$, where *q* is the dual exponent of *p*.

Using the resolvent formula, we see

$$\begin{aligned} |\tau(a((x_n+i)^{-1}-(x+i)^{-1})b)| &= |\tau(a(x+i)^{-1}(x-x_n)(x_n+i)^{-1}b)| \\ &\leq \|x_n-x\|_p \|a(x+i)^{-1}\|_{2q} \|(x_n+i)^{-1}b\|_{2q} \\ &\leq \|x-x_n\|_p \|a\|_{2q} \|b\|_{2q} \\ &\to 0. \end{aligned}$$

Two more classical results concerning the relations between operator topologies are the von Neumann bicommutant theorem and the Kaplansky density theorem. For the first recall that a subset *E* of $\mathscr{L}(H)$ is called *non-degenerate* if $x\xi = 0$ for all $x \in E$ implies $\xi = 0$.

Theorem B.10 (Von Neumann bicommutant theorem [Bla06, Theorem I.9.1.2]). For a non-degenerate *-subalgebra \mathcal{M} of $\mathcal{L}(H)$, the following statements are equivalent:

- (i) \mathcal{M} is a von Neumann algebra.
- (ii) \mathcal{M} is strongly closed.
- (iii) *M* is weakly closed.
- (iv) \mathcal{M} is σ -weakly closed.

In the following theorem we denote by \mathcal{M}_1 the closed unit ball in \mathcal{M} .

Theorem B.11 (Kaplansky density theorem [Bla06, Theorem I.9.1.3]). If \mathcal{M} is a von Neumann algebra and A a weakly dense *-subalgebra, then $A \cap \mathcal{M}_1$ is strongly dense in \mathcal{M}_1 and $A_h \cap \mathcal{M}_1$ is strongly dense in $\mathcal{M}_h \cap \mathcal{M}_1$

SYMBOLS

\mathcal{M}_h	set of all self-adjoint elements of \mathcal{M} .
\mathcal{M}_+	set of all positive elements of \mathcal{M} .
\mathcal{M}_1	closed unit ball of \mathcal{M} .
\mathcal{M}_{*}	predual of ${\mathscr M}$ (set of all σ -weakly continuous linear function-
	als on \mathcal{M}).
E^*	dual of E (set of all norm continuous linear functionals on E).
$M_n(\mathbb{C})$	set of complex $n \times n$ matrices.
$\mathscr{L}(H)$	set of bounded linear operators on H .
$\alpha \wedge \beta, \alpha \vee \beta$	minimum, maximum of α and β .
A°	opposite algebra of A (see Definition 1.15).
$ ilde{f}$	quantum derivative of f (see Def. 1.18).
Γ, Γ	carré du champ operators (see Section 1.3).
AM	arithmetic mean, $AM(s,t) = (s+t)/2$.
$\mathbf{L}\mathbf{M}$	logarithmic mean, $LM(s, t) = (s - t)/(\log s - \log t)$.
$\hat{ ho}$	twisted multiplication by ρ , $\hat{\rho} = \theta(L(\rho), R(\rho))$ (see Def. 2.1).
$\ \cdot\ _{ ho}^2$	quadratic form associated with ρ , $\ \xi\ _{\rho}^2 = \ \hat{\rho}^{1/2}\xi\ _{\mathcal{H}}^2$ (see Def.
	2.4).
$\ \cdot\ _{ heta}$	norm on the space $\mathscr{A}_{ heta}$ (see Def. 2.6).
$\mathscr{A}_{ heta}$	algebra of test elements (see Def. 2.6).
$\mathscr{D}(\mathscr{M}, \tau)$	set of density matrices (elements of $L^1_+(\mathcal{M}, au)$ with trace 1, see
	Def. 3.1).
$ ilde{\mathcal{H}}_{ ho}$	Hilbert space obtained from $D(\hat{ ho}^{1/2})$ after separation and com-
	pletion w.r.t. $\ \cdot\ _{\rho}$ (see Section 3.1).
$\mathscr{H}_{ ho}$	closure of $\partial \mathscr{A}_{\mathrm{AM}}$ in $ ilde{\mathscr{H}}_{ ho}$ (see Section 3.1).
$D ho_t$	velocity vector field of the curve (ρ_t) (see Def. 3.4).

W	transport metric on $\mathscr{D}(\mathscr{M}, \tau)$ (see Def. 3.12).
$\mathrm{AC}^p(I;(X,d))$	space of <i>p</i> -absolutely continuous curves (see Def. 3.25).
$ \dot{\gamma}_t _d$	metric derivative of the curve γ (see Def. 3.25).
Ent	von Neumann entropy (see Def. 4.7).
I	Fisher information (see Def. 4.19).
$\mathbb{C}\ell(H)$	fermionic Clifford algebra (see Example A.4).
$\mathscr{F}_{-}(H)$	fermionic Fock space (see Exampe A.4).
$L^0(\mathcal{M}, \tau)$	space of all τ -measurable operators (see Appendix A).
$L^p(\mathcal{M},\tau)$	noncommutative L^p space (see Appendix A).
$L^p_h(\mathcal{M}, \tau)$	set of all self-adoint elements of $L^p(\mathcal{M}, \tau)$.
$L^{p}_{+}(\mathcal{M}, au)$	set of all positive elements of $L^p(\mathcal{M}, \tau)$.
\mathcal{M}_{F}^{n}	set of all commuting <i>n</i> -tuples of normal elements of \mathcal{M} with
*	joint spectrum in F (see Appendix B).

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- [3] Bobo Hua, Matthias Keller, Michael Schwarz, and Melchior Wirth. Sobolev-Type Inequalities and Eigenvalue Growth on Graphs with Finite Measure, accepted by *Proceedings of the American Mathematical Society*
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EHRENWÖRTLICHE ERKLÄRUNG

Hiermit erkläre ich,

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Bei der Auswahl und Auswertung des Materials sowie bei der Herstellung des Manuskripts haben mich Oleksiy Sukaylo durch die Übersetzung der Referenz [Tik87] und Simon Puchert durch den vereinfachten Beweis des Lemmas 4.13 unterstützt. Die Beiträge sind im Text gekennzeichnet.

Ich habe weder die gleiche noch eine in wesentlichen Teilen ähnliche Abhandlung an einer anderen Hochschule als Dissertation eingereicht.

Jena, 15. Oktober 2019