Boundary values of resolvents of self-adjoint operators in Krein spaces

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BOUNDARY VALUES OF RESOLVENTS OF SELF-ADJOINT OPERATORS IN KREIN SPACES

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Abstract. We prove in this paper resolvent estimates for the boundary values of resolvents of selfadjoint operators on a Krein space: if H is a selfadjoint operator on a Krein space $\mathcal{H}$, equipped with the Krein scalar product $\langle\cdot|\cdot\rangle$, A is the generator of a C_0-group on $\mathcal{H}$ and $I \subset \mathbb{R}$ is an interval such that:

1) H admits a Borel functional calculus on I,
2) the spectral projection $\mathbb{1}_I(H)$ is positive in the Krein sense,
3) the following *positive commutator estimate* holds:

$$\mathrm{Re}\langle u|[H, \mathrm{i}A]u\rangle \geq c\langle u|u\rangle,\ u \in \mathrm{Ran}\mathbb{1}_I(H),\ c > 0.$$

then assuming some smoothness of H with respect to the group $\mathrm{e}^{\mathrm{i}tA}$, the following resolvent estimates hold:

$$\sup_{z \in I \pm \mathrm{i}]0,\nu]} \|\langle A\rangle^{-s}(H-z)^{-1}\langle A\rangle^{-s}\| < \infty,\ s > \frac{1}{2}.$$

As an application we consider abstract Klein-Gordon equations

$$\partial_t^2\phi(t) - 2\mathrm{i}k\phi(t) + h\phi(t) = 0,$$

and obtain resolvent estimates for their generators in *charge spaces* of Cauchy data.

1. Introduction

30 years ago, E. Mourre showed that a local in energy positive commutator estimate for a selfadjoint operator H entails a limiting absorption principle for this operator and thus the absence of singular continuous spectrum, see [M1]. This result had a very deep impact in scattering theory leading in particular to asymptotic completeness results for quantum $N-$ particle systems. Among many other applications we mention applications to Quantum Field Theory or sccattering problems in General Relativity. A lot of efforts had been made to weaken the original hypotheses in the work of Mourre, see e.g. [ABG]. A central requirement remained however that the hamiltonian H is a selfadjoint operator on a Hilbert space. Whereas this is a very natural requirement for the Schrödinger equation, it turns out that it is in general not fulfilled for the Klein-Gordon equation when this equation is coupled to an electric field or associated to a lorentzian metric which is not stationary. The natural setting in this situation seems to be the one of a selfadjoint operator on a so called Krein space (which is a generalization of a Hilbert space). The present paper is devoted to the proof of weighted estimates for boundary values on the real line of selfadjoint operators on Krein spaces. Our result generalizes the result of Mourre to the Krein space setting. Applications to the Klein-Gordon equation are given. Let us now briefly describe the results and methods of this work.

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1.1. **Selfadjoint operators on Krein spaces.** A *Krein space* is a hilbertizable Banach space $\mathcal{H}$ equipped with a non-degenerate hermitian form $\langle u|v\rangle$, $u, v \in \mathcal{H}$ called a *Krein scalar product*. Orthogonals to vector subspaces and adjoint of linear operators on $\mathcal{H}$ are defined with respect to $\langle\cdot|\cdot\rangle$.

In contrast to Hilbert spaces, the hermitian form is not assumed to be positive definite. Note however that the notion of positivity of a subspace $\mathcal{K} \subset \mathcal{H}$ resp. of an operator A on $\mathcal{H}$ still makes sense, by requiring that $\langle u|u\rangle \geq 0$ for all $u \in \mathcal{K}$ resp. $\langle u|Au\rangle \geq 0$ for all $u \in \mathrm{Dom}A$.

Of special interest are *selfadjoint operators* on Krein spaces. Typically a selfadjoint operator H on a Krein space arises as the generator of a C_0-group $\{\mathrm{e}^{\mathrm{i}tH}\}_{t\in\mathbb{R}}$ preserving the quadratic quantity $\langle u|u\rangle$.

In general, not much of interest can be said about the spectrum, functional calculus or the behavior of the resolvent of selfadjoint operators on a Krein space. Namely the spectrum is invariant under complex conjugation, the functional calculus is limited to the Dunford-Taylor functional calculus, and the behavior of the resolvent, both near the real axis of near infinity, can be arbitrary.

However, there is a class of selfadjoint operators, called *definitizable*, first defined and studied by Langer [La], which admit a rich (i.e. Borel outside a finite subset of $\mathbb{R}$) functional calculus. A selfadjoint operator H on $\mathcal{H}$ is definitizable if its resolvent set $\rho(H)$ is not empty and if there exists a (real) polynomial p such that $p(H) \geq 0$. Real zeroes of p in the spectrum of H are called *critical points*.

1.2. **Positive comutator method.** If H is definitizable and $I \subset \mathbb{R}$ is a bounded interval with ∂I disjoint from the critical points of H, then the spectral projection $\mathbb{1}_I(H)$ is well defined and bounded on $\mathcal{H}$. Moreover if I does not contain any critical point, then $\mathbb{1}_I(H)$ is definite in the Krein sense, i.e. $\mathbb{1}_I(H) \geq 0$ or $-\mathbb{1}_I(H) \geq 0$.

This local definiteness of the Krein scalar product opens the way for an extension to the Krein space framework of the well-known *positive commutator method*, which is a standard way to prove weighted resolvent estimates for usual selfadjoint operators on a Hilbert space. In the Hilbert space framework, the positive commutator method introduced by Mourre [M1] relies on an estimate

$$\mathbb{1}_I(H)[H, \mathrm{i}A]\mathbb{1}_I(H) \geq c\mathbb{1}_I(H),\ c > 0, \tag{1.1}$$

where H is the selfadjoint operator under study, $I \subset \mathbb{R}$ is an interval, and A is another selfadjoint operator, called a *conjugate operator*. From (1.1), assuming some regularity of H with respect to the unitary group $\mathrm{e}^{\mathrm{i}tA}$, one obtains the resolvent estimates:

$$\sup_{z\in I\pm\mathrm{i}]0,+\infty[} \|\langle A\rangle^{-s}(H-z)^{-1}\langle A\rangle^{-s}\| < \infty,\ s > \frac{1}{2}, \tag{1.2}$$

see [M1], [PSS], [ABG]. The original proofs relied on differential inequalities. Some years ago another proof, based on energy estimates was given in [Ge]. The argument in [Ge] is closer to a method of Putnam [P2], which was an ancestor of the positive commutator method. It turns out that the proof of [Ge] can be adapted to the Krein space framework.

Several difficulties must be faced before an estimate like (1.2) can be obtained for a selfadjoint operator on a Krein space. First of all H should have a Borel functional calculus in order to be able to define spectral projections. Second the conjugate operator A is in general not unitary for a compatible Hilbert space structure on $\mathcal{H}$. In particular the definition of $\langle A\rangle^{-s} = (A^2+1)^{-s/2}$ is not obvious.

However on a Krein space, an estimate like (1.1) has still a meaning, if it is understood formally as

$$\mathrm{Re}\langle u|[H,\mathrm{i}A]u\rangle \geq c\langle u|u\rangle,\ u\in \mathrm{Ran}\mathbb{1}_I(H),\ c>0. \tag{1.3}$$

The main result of this paper, Thm. 7.9, states that if H is a selfadjoint operator on a Krein space, which is of class C^α with respect to A for some $\alpha > 3/2$, and $I \subset \mathbb{R}$ is an interval such that:

1) H admits a Borel functional calculus near I, $\mathbb{1}_I(H) \geq 0$,
2) the Mourre estimate (1.1) holds,

then the resolvent estimates (1.2) hold, possibly replacing A by ϵA for $0 < \epsilon \ll 1$ and restricting z to $I \pm \mathrm{i}]0, \nu]$ for some $\nu > 0$, due to the possible presence of complex eigenvalues. We also prove a *virial theorem*, which has the same consequences as in the Hilbert space case.

1.3. **Abstract Klein-Gordon equations.** In a subsequent paper [GGH1], we apply the abstract results of this paper to the generators of abstract Klein-Gordon equations

$$\partial_t^2\phi(t) - 2\mathrm{i}k\phi(t) + h\phi(t) = 0,$$

where $\phi : \mathbb{R} \to \mathcal{H}$, $\mathcal{H}$ is a Hilbert space and h, k are self-adjoint, resp. symmetric operators on $\mathcal{H}$. The simplest example is the *Klein-Gordon equation on Minkowski space* minimally coupled with an external electric field:

$$(\partial_t - \mathrm{i}v(x))^2\phi(t,x) - \Delta_x\phi(t,x) + m^2\phi(t,x) = 0, \tag{1.4}$$

for which $\mathcal{H} = L^2(\mathbb{R}^d, dx)$, $h = -\Delta_x + m^2 - v^2(x)$, $k = v(x)$ is a (real) electric potential and $m \geq 0$ is the mass of the Klein-Gordon field.

In contrast to Schrödinger equations, there is no preferred topology on the space of Cauchy data $\begin{pmatrix} \phi(t) \\ \mathrm{i}^{-1}\partial_t\phi(t) \end{pmatrix}$. It turns out that two spaces of Cauchy data are natural, the *energy space* $\mathcal{E} = \langle h\rangle^{-\frac{1}{2}}\mathcal{H}\oplus\mathcal{H}$ and the *charge space* $\mathcal{K}_{1/4} = \langle h\rangle^{-1/4}\mathcal{H}\oplus\langle h\rangle^{1/4}\mathcal{H}$ (see Subsect. 8.1 for the notation). In [GGH1] resolvent estimates are proved on the energy space, and then extended to the charge space by duality and interpolation.

In this paper we give another application of Thm. 7.9 by directly proving resolvent estimates on the charge space. We also discuss in details various realizations of the Klein-Gordon generator starting from the dual space $\mathcal{E}^* = \mathcal{H} \oplus \langle h\rangle^{\frac{1}{2}}\mathcal{H}$, and the functional calculus of 'free' Klein-Gordon generators, corresponding to $k = 0$.

1.4. **Plan of the paper.** We now briefly describe the plan of this paper. In Sect. 2 we describe some basic results on the smooth and Borel functional calculus for linear operators on Banach spaces. The Dunford-Taylor functional calculus for a linear operator H can be extended to smooth functions on an interval $I \subset \mathbb{R}$ if the resolvent $(H - z)^{-1}$ is of polynomial growth near the real axis. If this functional calculus is continuous for the sup norm, then it uniquely extends to bounded Borel functions on I.

In Sect. 3 we recall basic results on $K-$spaces, which are natural generalizations of Krein spaces. Sect. 4 is devoted to the construction of a Borel functional calculus for definitizable selfadjoint operators on Krein spaces. Although various versions of this construction can be found in the literature (see in particular [La], [J1], or more recently [Wr]), we believe our presentation might have some interest. In particular we precise the optimal class of admissible functions, namely bounded

Borel functions on $\mathbb{R}$ having a precised asymptotic expansion at each critical point of H.

In Sect. 5 we collect some rather standard facts on the smoothness of an operator with respect to a C_0-group. In the usual Hilbert space framework, the C_0-groups of practical interest for the Mourre method are unitary, with selfadjoint generators. In this case a very comprehensive study can be found in [ABG]. In our applications to Krein spaces, no natural Hilbert space structure is present and part of the formalism has to be generalized.

These results are used in Sect. 6 to prove *commutator expansions*. Roughly speaking if H is an operator and A the generator of a C_0-group on a Banach space $\mathcal{H}$, we need to expand the commutator $[H, \mathrm{i}f(A)]$ for some class of functions f as $f'(A)[H,\ iA] + R$ with a careful estimate of the error term R. Again in the Hilbert space case, such commutator expansions are a basic tool of spectral and scattering theory, see among many other references [GoJe].

In Sect. 7 we prove the main result of this paper, Thm. 7.9, by adapting the Hilbert space proof in [Ge] to the Krein space framework. In the last section of this paper, Sect. 8, we discuss abstract Klein-Gordon operators.

2. Boundary values of resolvents and functional calculus

In this section we present some results on the smooth and Borel functional calculus for linear operators on Banach spaces, under some general assumptions on the growth of their resolvents near the real axis.

2.1. **Notations.** If $\mathcal{H}$ is a Banach space we denote $\mathcal{H}^*$ its adjoint space, i.e. the set of continuous anti-linear functionals on $\mathcal{H}$ equipped with the natural Banach space structure. The canonical anti-duality between $\mathcal{H}$ and $\mathcal{H}^*$ is denoted $\langle u, w\rangle \equiv w(u)$, where $u \in \mathcal{H}$ and $w \in \mathcal{H}^*$. So $\langle \cdot, \cdot\rangle : \mathcal{H} \times \mathcal{H}^* \to \mathbb{C}$ is anti-linear in the first argument and linear in the second one. On the other hand, we denote by $\langle \cdot | \cdot \rangle$ hermitian forms on $\mathcal{H}$, again anti-linear in the first argument and linear in the second one.

We say that $\mathcal{H}$ is *Hilbertizable* if there is a scalar product on $\mathcal{H}$ such that the norm associated to it defines the topology of $\mathcal{H}$; such a scalar product and the norm associated to it will be called *admissible*. Scalar products are denoted by $(\cdot|\cdot)$.

If $\mathcal{H}$ is a reflexive Banach space then the canonical identification $\mathcal{H}^{**} = \mathcal{H}$ is obtained by setting $u(w) = \overline{w(u)}$ for $u \in \mathcal{H}$ and $w \in \mathcal{H}^*$. In other terms, the relation $\mathcal{H}^{**} = \mathcal{H}$ is determined by the rule $\langle w, u\rangle = \overline{\langle u, w\rangle}$.

Let $\mathcal{G}, \mathcal{H}$ be reflexive Banach spaces and $\mathcal{E} = \mathcal{G} \oplus \mathcal{H}$. The usual realization $(\mathcal{G} \oplus \mathcal{H})^* = \mathcal{G}^* \oplus \mathcal{H}^*$ of the adjoint space will not be convenient later, we shall rather identify $\mathcal{E}^* = \mathcal{H}^* \oplus \mathcal{G}^*$ in the obvious way. For example, if $\mathcal{H} = \mathcal{G}^*$, so $\mathcal{H}^* = \mathcal{G}$, the adjoint space of $\mathcal{E} = \mathcal{G} \oplus \mathcal{G}^*$ is identified with itself $\mathcal{E}^* = \mathcal{E}$.

If S is a closed densely defined operator on a Banach space $\mathcal{H}$, we denote by $\rho(S)$, $\sigma(S)$ its resolvent set and spectrum.

We use the notation $\langle a\rangle = (1 + a^2)^{\frac{1}{2}}$ if a is real number or an operator for which this expression has a meaning.

2.2. **Polynomial growth condition.** Let H be a closed densely defined operator on a Banach space $\mathcal{H}$. We first give a meaning to the boundary values $R(\lambda \pm \mathrm{i}0)$ of the resolvent of H as $B(\mathcal{H})$-valued distributions on a certain real open set defined by a growth condition on $\|R(\lambda \pm \mathrm{i}\mu)\|$ as $\mu \downarrow 0$. We recall that if $\mathcal{B}$ is a Banach space then a $\mathcal{B}$-valued distribution on a real open set I is a continuous linear map

$T : C_0^\infty(I) \to \mathcal{B}$. We often use the formal notation $T(\chi) = \int T(\lambda)\chi(\lambda)d\lambda$ for $\chi \in C_0^\infty(I)$. The topology on this space of distributions is defined as in the scalar case.

Lemma 2.1. *Assume that $I \subset \mathbb{R}$ is open with $I \pm \mathrm{i}]0,\nu] \subset \rho(H)$ for some $\nu > 0$ and that there exists $n \in \mathbb{N}$ and $C > 0$ such that*

$$\|R(z)\| \leq C|\mathrm{Im} z|^{1-n},\ z \in I \pm \mathrm{i}]0,\nu]. \tag{2.1}$$

Then the boundary values $R(\lambda \pm \mathrm{i}0) := \lim_{\mu\downarrow 0} R(\lambda \pm \mathrm{i}\mu)$ exist as $B(\mathcal{H})$-valued distributions of order n on I. More explicitly, if $\chi \in C_0^n(I)$ and we set

$$\chi_{(n)}(\lambda + \mathrm{i}\mu) = \sum_{k=0}^{n} \chi^{(k)}(\lambda)(\mathrm{i}\mu)^k/k!, \lambda, \mu \in \mathbb{R},$$

then

$$\begin{array}{rl} & \int_{\mathbb{R}} R(\lambda + \mathrm{i}0)\chi(\lambda)d\lambda \\ = & \int_{\mathbb{R}} \Big(R(\lambda + \mathrm{i}\nu)\chi_{(n)}(\lambda + \mathrm{i}\nu) + \int_0^\nu R(\lambda + \mathrm{i}\mu)\frac{d(\mathrm{i}\mu)^n}{n!}\chi^{(n)}(\lambda)\Big)d\lambda. \end{array} \tag{2.2}$$

Proof. We use a well-known elementary argument, valid for any holomorphic function, cf [H, Thm. 3.1.11] and the comment after its proof: make a Taylor expansion up to order n of the function $\mu \mapsto R(\lambda + \mathrm{i}\mu)$ on the interval $[\varepsilon, \nu]$ with $0 < \varepsilon < \nu$ and note that $\frac{d}{d\mu}R(\lambda + \mathrm{i}\mu) = \mathrm{i}\frac{d}{d\lambda}R(\lambda + \mathrm{i}\mu)$ by holomorphy. The remainder is the derivative of order n of a bounded function hence we may let $\varepsilon \to 0$ and get

$$R(\lambda + \mathrm{i}0) = \sum_{k=0}^{n-1} \frac{\nu^k}{k!}(-\mathrm{i}\partial_\lambda)^k R(\lambda + \mathrm{i}\nu) + (-\mathrm{i}\partial_\lambda)^n \int_0^\nu R(\lambda + \mathrm{i}\mu)\frac{d\mu^n}{n!} \tag{2.3}$$

as $B(\mathcal{H})$-valued distributions on I. This relation is equivalent to (2.2). □

In the next definition we define the maximal open real set on which the distributions $R(\cdot \pm \mathrm{i}0)$ make sense.

Definition 2.2. *Let $\beta(H)$ be the set of $\lambda \in \mathbb{R}$ such that there is a real open neighborhood I of λ and there are numbers $\nu > 0, n \in \mathbb{N}, C > 0$ such that*

$$\|R(z)\| \leq C|\mathrm{Im} z|^{1-n},\ z \in I \pm \mathrm{i}]0,\nu].$$

The boundary values $R(\lambda \pm \mathrm{i}0) = \lim_{\mu\downarrow 0} R(\lambda \pm \mathrm{i}\mu)$ of the resolvent of H are well defined $B(\mathcal{H})$-valued distributions on $\beta(H)$.

Remark 2.3. If $\mathscr{X}$ is a Banach space such that $B(\mathcal{H})$ is continuously embedded in $\mathscr{X}$ then $R(\cdot \pm \mathrm{i}0)$ may be viewed as $\mathscr{X}$-valued distributions on $\beta(H)$. It may happen that on some open set $I \subset \beta(H)$ these $\mathscr{X}$-valued distributions are defined by locally bounded $\mathscr{X}$-valued functions: this is the case if the *limiting absorption principle* holds on I relatively to $\mathscr{X}$, i.e. if $\|R(z)\|_{\mathscr{X}} \leq C$ for $z \in I \pm \mathrm{i}]0,\nu]$ for some $\nu > 0$.

The usual strategy (adopted here) is to construct Banach spaces $\mathcal{K}$ with $\mathcal{K} \subset \mathcal{H}$ continuously and densely, which allows one to take $\mathscr{X} = B(\mathcal{K}, \mathcal{K}^*)$, such that $R(\lambda \pm \mathrm{i}0)$, when viewed as a $B(\mathcal{K}, \mathcal{K}^*)$-valued distributions, is well defined and a continuous function of λ.

2.3. **Smooth functional calculus.** We now describe an elementary functional calculus which makes sense under very general conditions. In the self-adjoint case these techniques were introduced in [HeSj]. A detailed presentation may be found in [Da1] and an extension to non self-adjoint operators in [Da2].

Under the conditions of Lemma 2.1 then for any $\chi \in C_0^n(I)$ we define a bounded operator on $\mathcal{H}$ by

$$\chi(H) = \frac{1}{2\pi \mathrm{i}} \int \big(R(\lambda + \mathrm{i}0) - R(\lambda - \mathrm{i}0)\big)\chi(\lambda) d\lambda. \tag{2.4}$$

The right hand side above can be made quite explicit by using (2.3) and a similar relation for $R(\lambda - \mathrm{i}0)$.

Note that the map $\chi \mapsto \chi(H)$ is an *algebra morphism*. Indeed, linearity is obvious and in order to prove that it is multiplicative it suffices to show that $R(z)\chi(H) = (r_z\chi)(H)$ for $\mathrm{Im} z \neq 0$, where $r_z(\lambda) = (\lambda - z)^{-1}$. For this it suffices to note that $R(z)R(\lambda \pm \mathrm{i}0) = (R(z) - R(\lambda \pm \mathrm{i}0))r_z(\lambda)$.

The Helffer-Sjöstrand version of the formula for $\chi(H)$ may be obtained with the help of an almost analytic extension of χ as in [HeSj] (or see [Da1, p. 24]). For example, choose $\theta \in C_c^\infty(\mathbb{R})$ with $\theta(\lambda) = 1$ if $|\lambda| < \nu/2$ and $\theta(\lambda) = 0$ if $|\lambda| > \nu$. If for $z = \lambda + \mathrm{i}\mu$ we define $\tilde{\chi}(z) = \theta(\mu/\langle\lambda\rangle)\chi_{(n)}(z)$ and we set $\overline{\partial} = (\partial_\lambda + \mathrm{i}\partial_\mu)/2$ then $\overline{\partial}\tilde{\chi}(z) = O(|\mu|^n)$ and

$$\chi(H) = -\frac{1}{2\pi \mathrm{i}} \int_{\mathbb{C}} R(z)\overline{\partial}\tilde{\chi}(z) dz \wedge d\overline{z}. \tag{2.5}$$

2.4. **Borel functional calculus.** The functional calculus (2.4) introduced under the conditions of Lemma 2.1 is a priori well defined only for $\chi \in C_0^n(I)$ but often it extends to larger classes of functions by continuity.

We shall say that H *admits a* C^0*-functional calculus on* I if $I \subset \beta(H)$ and $\|\chi(H)\| \leq C \sup_{\lambda \in I} |\chi(\lambda)|$ for some finite number C and all $\chi \in C_0^\infty(I)$. Then clearly the smooth functional calculus has a unique continuous extension to an algebra morphism $C_0(I) \to B(\mathcal{H})$. If $\mathcal{H}$ is reflexive one can extend the functional calculus to Borel functions, as shown in Thm. 2.4 below.

Let $\mathcal{B}(I)$ be the set of bounded Borel functions on I. A sequence of functions φ_n on I is *boundedly convergent* if $\sup_{n,\lambda} |\varphi_n(\lambda)| < \infty$ and $\lim_n \varphi_n(\lambda) = \varphi(\lambda)$ exists $\forall \lambda \in I$. Note that $\varphi \in \mathcal{B}(I)$ if $\varphi_n \in \mathcal{B}(I)$ $\forall$ n. The following result is a straightforward application of the Riesz theorem, see [Wr, Cor. 9.1.10] for example.

Theorem 2.4. *Assume that* $\mathcal{H}$ *is a reflexive Banach space and let* $F_0 : C_0(I) \to B(\mathcal{H})$ *be a norm continuous algebra morphism. Then* F_0 *extends uniquely to an algebra morphism* $F : \mathcal{B}(I) \to B(\mathcal{H})$ *such that:* $\varphi_n \to \varphi$ *boundedly* $\Rightarrow F(\varphi_n) \to F(\varphi)$ *weakly.*

Remark 2.5. If H is a self-adjoint operator on a Krein space (see Def. 3.1) and if H admits a C^0-functional calculus on I then it is clear that $\chi(H)^* = \overline{\chi}(H)$ for all bounded Borel functions χ on I.

3. $K-$SPACES

In this section, we discuss $K-$*spaces*, a generalization of Krein spaces, cf. [B].

3.1. Definition of $K-$spaces.

Definition 3.1. *A* $K-$space *is a Banach space* $\mathcal{H}$ *equipped with a continuous hermitian form* $\langle\cdot|\cdot\rangle$ *such that for any continuous linear form* φ *on* $\mathcal{H}$ *there is a unique* $u \in \mathcal{H}$ *such that* $\varphi = \langle u|\cdot\rangle$. *The form* $\langle\cdot|\cdot\rangle$ *is called the* Krein structure. *If* $\mathcal{H}$ *is Hilbertizable then* $\mathcal{H}$ *is called a* Krein space.

Let $J : \mathcal{H} \to \mathcal{H}^*$ be the linear continuous map defined by $Ju = \langle\cdot|u\rangle$, so that $\langle u|v\rangle = \langle u, Jv\rangle$. Since $\langle\cdot|\cdot\rangle$ is hermitian, we have $\langle u, Jv\rangle = \overline{\langle v, Ju\rangle}$. The *topological non-degeneracy* condition imposed on $\langle\cdot|\cdot\rangle$ above means that J is bijective. Thus the Krein structure $\langle\cdot|\cdot\rangle$ allows us to identify $\mathcal{H}^*$ and $\mathcal{H}$ with the help of J.

Proposition 3.2. *A $K-$space is reflexive.*

Proof. Let $I : \mathcal{H} \to \mathcal{H}^{**}$ the canonical injection. Since $J : \mathcal{H} \to \mathcal{H}^*$ is an isomorphism, so are $J^* : \mathcal{H}^{**} \to \mathcal{H}^*$ and $(J^*)^{-1} \circ J : \mathcal{H} \to \mathcal{H}^{**}$. We note then that $(J^*)^{-1} \circ J = I$. □

Remark 3.3. One may also say that a $K-$space structure on a reflexive Banach space $\mathcal{H}$ is a hermitian isomorphism $J : \mathcal{H} \to \mathcal{H}^*$. A Hilbert structure is a positive Krein structure, i.e. a positive isomorphism $J : \mathcal{H} \to \mathcal{H}^*$.

Remark 3.4. Assume that $\langle\cdot|\cdot\rangle$ is a hermitian form on a complex vector space $\mathcal{H}$ which is algebraically non-degenerate, i.e. $u = 0$ if $\langle u|v\rangle = 0$ for all $v \in \mathcal{H}$. Then *there is at most one normed space topology on $\mathcal{H}$ such that the conditions of Definition 3.1 be satisfied*. Indeed, any such norm on $\mathcal{H}$ is complete because $\mathcal{H}^*$ is always a Banach space. And if the adjoint spaces associated to two complete norms on $\mathcal{H}$ are equal then the corresponding classes of bounded sets are identical by the uniform boundedness principle, hence the norms are equivalent. See [B, p. 60-67] for better results of this nature.

3.2. **Adjoints on K-spaces.** If $T \in B(\mathcal{H})$ then the adjoint $T^* \in B(\mathcal{H}^*)$ of T in the Banach space sense is defined on $\mathcal{H}^*$ as usual and then we may transport it on $\mathcal{H}$ with the help of J. In other terms, the Krein structure $\langle\cdot|\cdot\rangle$ allows us to define an involution $T \mapsto T^*$ on $B(\mathcal{H})$ such that $\langle T^*u|v\rangle = \langle u|Tv\rangle$. This definition extends as usual to closed densely defined operators.

Clearly $B(\mathcal{H})$ becomes a $*$-algebra with a continuous involution. The self-adjoint operators are defined as usual by the relation $S^* = S$, where S may be unbounded. We say that S is *positive* and we write $S \geq 0$ if $\langle u|Su\rangle \geq 0$ for all $u \in \mathrm{Dom}S$. If S is bounded and $S \geq 0$ then $T^*ST \geq 0$ for all $T \in B(\mathcal{H})$, but the identity operator is not positive unless $\mathcal{H}$ is a Hilbert space. So $T^*T \geq 0$ holds only in exceptional cases. To each positive bounded operator S we associate a semi-norm on $\mathcal{H}$, namely $\|u\|_S = \sqrt{\langle u|Su\rangle}$, which satisfies $|\langle u|Sv\rangle| \leq \|u\|_S\|v\|_S$.

We say that a linear subspace $\mathcal{K}$ is a *Hilbert subspace of* $\mathcal{H}$ if $\big(\mathcal{K}, \langle\cdot|\cdot\rangle|_{\mathcal{K}\times\mathcal{K}}\big)$ is a Hilbert space. Equivalently, this means that $\mathcal{K}$ is a closed subspace of $\mathcal{H}$ such that $\langle u|u\rangle \geq c\|u\|^2$ for some number $c > 0$ and all $u \in \mathcal{K}$. We equip such a subspace with the natural Hilbert norm $\|u\|_{\mathcal{K}} = \sqrt{\langle u|u\rangle}$ which is equivalent to $\|\cdot\||_{\mathcal{K}}$.

3.3. **Projections on K-spaces.** A *projection* on $\mathcal{H}$ is an element $\Pi \in B(\mathcal{H})$ such that $\Pi^2 = \Pi$. A self-adjoint projection is also called an *orthogonal projection*. A *positive projection* is a projection Π such that $\Pi \geq 0$. In particular, Π will be orthogonal. For the proof of the following fact, see [B].

Proposition 3.5. *The range of a positive projection is a Hilbert subspace of $\mathcal{H}$. Reciprocally, if $\mathcal{K}$ is a Hilbert subspace of $\mathcal{H}$ then there is a unique self-adjoint projection Π such that $\Pi\mathcal{H} = \mathcal{K}$ and this projection is positive.*

If Π is a positive projection then $\|u\|_\Pi = \|u\|_{\Pi\mathcal{H}}$ for all $u \in \Pi\mathcal{H}$. If $S \in B(\mathcal{H})$ we denote $\|S\|_\Pi$ the norm of the operator $\Pi S\Pi$ on the Hilbert space $\Pi\mathcal{H}$. If $S = S^*$ then $\|S\|_\Pi = \sup\{|\langle u|Su\rangle| \mid u \in \Pi\mathcal{H}, \langle u|u\rangle = 1\}$. It follows that if $S \in B(\mathcal{H})$ and $S = S^*$ then

$$\pm\langle\Pi u|S\Pi u\rangle \leq \|S\|_\Pi\langle\Pi u|\Pi u\rangle,\ u \in \mathcal{H}. \tag{3.1}$$

3.4. **Phase spaces.** A typical construction of $K-$spaces starts with a reflexive Banach space $\mathcal{G}$ thought as configuration space of a system. Then the *phase space of* $\mathcal{G}$ is $\mathcal{H} = \mathcal{G} \oplus \mathcal{G}^*$ and its $K-$space structure is

$$\langle u|v\rangle = v_1(u_0) + \overline{u_1(v_0)} = \langle u_0, v_1\rangle + \langle u_1, v_0\rangle,\ u = \left(\begin{smallmatrix} u_0 \\ u_1 \end{smallmatrix}\right),\ v = \left(\begin{smallmatrix} v_0 \\ v_1 \end{smallmatrix}\right) \in \mathcal{H}. \tag{3.2}$$

Recall that according to the convention adopted in Subsect. 2.1 we identify $\mathcal{H}^* = \mathcal{G} \oplus \mathcal{G}^* = \mathcal{H}$. Thus J is the identity operator and (3.2) satisfies the required topological non-degeneracy condition.

Note that we think of elements of $\mathcal{H}$ as column matrices hence we may represent operators on $\mathcal{H}$ as matrices

$$S = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

where $a : \mathcal{G} \to \mathcal{G}$, $b : \mathcal{G}^* \to \mathcal{G}$, $c : \mathcal{G} \to \mathcal{G}^*$, $d : \mathcal{G}^* \to \mathcal{G}^*$. A computation gives

$$S^* = \begin{pmatrix} d^* & b^* \\ c^* & a^* \end{pmatrix} \tag{3.3}$$

hence

(3.4)

$$S = S^* \Longleftrightarrow S = \begin{pmatrix} a & b \\ c & a^* \end{pmatrix} \quad \text{with} \quad a \in B(\mathcal{G}),\ b = b^* : \mathcal{G}^* \to \mathcal{G},\ c = c^* : \mathcal{G} \to \mathcal{G}^*.$$

Lemma 3.6. *An operator $S : \mathcal{H} \to \mathcal{H}$ is positive if and only if it is as in* (3.4) *with $b \geq 0$, $c \geq 0$, and*

$$|\langle au_0|u_1\rangle|^2 \leq \langle u_1|bu_1\rangle\langle u_0|cu_0\rangle \quad \textit{for all } u_0 \in \mathcal{G}, u_1 \in \mathcal{G}^*. \tag{3.5}$$

If $\mathcal{G}$ is a Hilbert space and $\mathcal{G}^* = \mathcal{G}$ then this means $a, b, c \in B(\mathcal{G})$ with $b, c \geq 0$ and $\|c^{-1/2}ab^{-1/2}\| \leq 1$.

Proof. The symmetric operator S as given in (3.4) is positive if and only $\langle u|Su\rangle \geq 0$ for all $u \in \mathcal{H}$ with

$$\langle u|Su\rangle = 2\mathrm{Re}\langle au_0|u_1\rangle + \langle u_1|bu_1\rangle + \langle u_0|cu_0\rangle.$$

Taking successively $u_0 = 0$ and $u_1 = 0$ we see that $b \geq 0$ and $c \geq 0$ are necessary conditions. Then by changing u_1 in $-\omega u_1$ with $\omega = \overline{\langle au_0|u_1\rangle}|\langle au_0|u_1\rangle|^{-1}$ if the denominator is not zero and $\omega = 1$ otherwise, we see that positivity of S is equivalent to $2|\langle au_0|u_1\rangle| \leq \langle u_1|bu_1\rangle + \langle u_0|cu_0\rangle$ for all $u_0 \in \mathcal{G}$ and $u_1 \in \mathcal{G}^*$. Replace u_0, u_1 by $\varepsilon^{1/2}u_0$ and $\varepsilon^{-1/2}u_1$ with $\varepsilon > 0$. If one of the terms in the right hand side is zero then we get $\langle au_0|u_1\rangle = 0$ by making $\varepsilon \to 0$ or $\varepsilon \to \infty$. If not then $\varepsilon = \langle u_0|cu_0\rangle^{1/2}\langle u_1|bu_1\rangle^{-1/2}$ gives (3.5). □

Remark 3.7. If $\mathcal{G}$ is a Hilbert space identified with its adjoint space $\mathcal{G}^*$ with the help of the Riesz isomorphism then on the phase space $\mathcal{H} = \mathcal{G} \oplus \mathcal{G}$ we have the direct sum Hilbert structure $(u|v)_H = (u_0|v_0) + (u_1|v_1)$ and the Krein structure $\langle u|v\rangle_K$ defined by (3.2). Clearly $\langle u|v\rangle_K = \langle u|Jv\rangle_H$ with $J = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$. Observe that now we have two natural ways of identifying $\mathcal{H}$ with its adjoint space, namely by using $(\cdot|\cdot)_H$ (i.e. the Riesz isomorphism) or $\langle\cdot|\cdot\rangle_K$. In our framework it is more convenient to use the second one which could be called *Krein isomorphism*. This is coherent with the convention $(X \oplus Y)^* = Y^* \oplus X^*$ adopted in Subsect. 2.1.

4. Definitizable operators on Krein spaces

The definitizable operators on a Krein space are remarkable because they admit a functional calculus almost as rich as that of self-adjoint operators on a Hilbert space. In fact the functions φ for which $\varphi(H)$ may be given a natural meaning can be arbitrary bounded Borel functions outside a finite set of "critical points". In this section we shall consider only continuous functions because, thanks to Thm. 2.4, this is sufficient to our needs. The main point in the approach we present below is the estimate in Prop. 4.10 due to P. Jonas [J1, Thm. 1]. Another presentation of the Langer-Jonas functional calculus may be found in [Wr, Ch. 9].

4.1. **Definitizable operators.** In this section we fix a Krein space $\mathcal{H} \equiv (\mathcal{H}, \langle\cdot|\cdot\rangle)$.

Definition 4.1. *A self-adjoint operator H on $\mathcal{H}$ is* definitizable *if $\rho(H) \neq \emptyset$ and there is a real polynomial $p \neq 0$ such that $p(H) \geq 0$, i.e. $\langle u|p(H)u\rangle \geq 0$ for all $u \in \mathrm{Dom}H^n$ where n is the degree of p. Such a p is called a* definitizing polynomial *for H.*

Remark 4.2. The assumption $\rho(H) \neq \emptyset$ is important, natural self-adjoint operators on a Krein space have empty resolvent set, see [B, p. 148]. For example, let $\mathcal{H}$ be the phase space of a Hilbert space $\mathcal{G}$ (cf. Remark 3.7) and let b be a positive injective operator on $\mathcal{G}$. If b or $c := b^{-1}$ is unbounded, then $\left(\begin{smallmatrix} 0 & b \\ c & 0 \end{smallmatrix}\right)$ is strictly positive, i.e. $\langle u|Hu\rangle > 0$ for all $u \neq 0$ in the domain of H, and $\rho(H) = \emptyset$.

The next result gives informations on the non-real spectrum of a definitizable operator. The proof is easy, see [J1, Lemma 1].

Proposition 4.3. *Let H be definitizable. Then:*

1. *If $z \in \sigma(H)\backslash\mathbb{R}$ then $p(z) = 0$ for each definitizing polynomial p.*
2. *There is a definitizing polynomial p such that $\sigma(H) \setminus \mathbb{R}$ is exactly the set of non-real zeroes of p.*
3. *Moreover, this p may be chosen such that if $\lambda \notin \mathbb{R}$ is a zero of multiplicity k of p then λ is an eigenvalue of H of Riesz index k.*
4. *The non-real spectrum of H consists of a finite number of eigenvalues of finite Riesz index distributed symmetrically with respect to the real axis.*

The following consequence is easily proved with the help of the Riesz projection associated to the finite set $\sigma(H) \setminus \mathbb{R}$. A *Krein subspace of $\mathcal{H}$* is a closed subspace which is a Krein space when equipped with the hermitian form induced by $\langle\cdot|\cdot\rangle$.

Corollary 4.4. *There are Krein subspaces $\mathcal{H}_1, \mathcal{H}_2$ of $\mathcal{H}$ such that $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$, where the sum is direct and orthogonal with respect to the Krein structure of $\mathcal{H}$, such that $H = H_1 \oplus H_2$ with H_1 a bounded self-adjoint operator in $\mathcal{H}_1$ with finite spectrum and H_2 a definitizable operator in $\mathcal{H}_2$ with $\sigma(H_2) \subset \mathbb{R}$.*

The above decomposition is canonical in a sense easy to make precise. Thus for any "reasonable" function φ we should have $\varphi(H) = \varphi(H_1) \oplus \varphi(H_2)$. Since the definition of $\varphi(H_2)$ is rather obvious, when we discuss the functional calculus of a definitizable operator it suffices to consider the case when it has only real spectrum.

4.2. **Rational functional calculus.** Before going on we make a general remark concerning the rational functional calculus associated to an arbitrary closed operator H with non-empty resolvent set on a Banach space $\mathcal{H}$. This makes things completely elementary and avoids the use of the (analytic) Dunford calculus. In the sequel we denote by $\hat{\mathbb{C}}$, $\hat{\mathbb{R}}$ the one-point compactifications of $\mathbb{C}$, $\mathbb{R}$.

Denote $\mathcal{R}_H$ the set of rational functions whose poles belong to $\rho(H)$ and which are bounded near infinity. This space is an unital algebra. If $\rho(H) = \overline{\rho(H)}$, as in the case of a self-adjoint operator on a Krein space, then $\mathcal{R}_H$ becomes a $*$-algebra if we define the adjoint $\overline{\varphi}$ of φ by $\overline{\varphi}(\lambda) = \overline{\varphi(\overline{\lambda})}$.

Lemma 4.5. *There is a unique unital algebra morphism $\mathcal{R}_H \ni \varphi \mapsto \varphi(H) \in B(\mathcal{H})$ with $\varphi(H) = (H-z)^{-1}$ if $\varphi(\lambda) = (\lambda - z)^{-1}$ for some $z \in \rho(H)$. If $\mathcal{H}$ is a Krein space and H is self-adjoint then $\varphi \mapsto \varphi(H)$ is a $*$-morphism.*

Proof. Let $\Omega \subset \hat{\mathbb{C}} \times \mathbb{N}$ be the set of couples $\omega = (z, s)$ with $z \in \rho(H)$ and $s \in \mathbb{N}^*$ or $\omega = (\infty, 0) \equiv \infty$. For $\omega \in \Omega$ we set:

$$\rho_\omega(\lambda) := (\lambda - z)^{-s} \text{ if } \omega \in \rho(H) \times \mathbb{N}^*,\ \rho_\omega(\lambda) := 1 \text{ if } \omega = (\infty, 0).$$

Then $\{\rho_\omega\}_{\omega\in\Omega}$ is a vector space basis in $\mathcal{R}_H$. Hence there is a unique linear map $\varphi \mapsto \varphi(H)$ from $\mathcal{R}_H$ into $B(\mathcal{H})$ which sends ρ_ω into $\varphi(H) = (H-z)^{-s}$ if $\omega \neq \infty$ and 1 into the identity operator. From the first resolvent identity it follows that this map is an algebra morphism. In the Krein space case note that $\varphi(H)^* = \overline{\varphi}(H)$ for any φ follows from the fact that the adjoint of $(H-z)^{-1}$ is $(H - \overline{z})^{-1}$. □

4.3. C^α **functional calculus.** The set $\mathcal{R}$ of *bounded rational functions* $\varphi : \mathbb{R} \to \mathbb{C}$ is a unital $*$-algebra for the usual algebraic operations. By Lemma 4.5 if H is a definitizable operator with only real spectrum then there is a unique unital $*$-morphism $\varphi \mapsto \varphi(H)$ of $\mathcal{R}$ into $\in B(\mathcal{H})$ such that $\varphi(H) = (H-z)^{-1}$ if $\varphi(\lambda) = (\lambda - z)^{-1}$ with $z \in \mathbb{C} \setminus \mathbb{R}$. We now extend this calculus to a class of continuous functions $\varphi : \mathbb{R} \to \mathbb{C}$ which have a certain degree of regularity at a finite set of real points and/or at infinity.

Definition 4.6. *Let $\omega = (\xi, s) \in \hat{\mathbb{R}} \times \mathbb{N}$ and $\varphi : \mathbb{R} \to \mathbb{C}$.*

1. *If $\xi \in \mathbb{R}$, then φ* is of class C^s at ξ *if there is a polynomial P such that $\varphi(x) = P(x-\xi) + o(|x-\xi|^s)$.*
2. *φ* is of class C^s at infinity *if there is a polynomial P such that $\varphi(x) = P(1/x) + o(|x|^{-s})$.*

Denote $C^\omega(\mathbb{R}) = \{\varphi \in C(\hat{\mathbb{R}}) \mid \varphi \text{ is of class } C^s \text{ at } \xi\}$, for $\omega = (\xi, s)$

Under the conditions of the definition, the terms of degree $\leq s$ of P are uniquely determined hence if $\xi \in \mathbb{R}$ there is a unique polynomial $T^+_\omega\varphi$ of degree $\leq s$ such that $\varphi(x) = T^+_\omega\varphi(x) + o(|x-\xi|^s)$ and if $\xi = \infty$ there is a unique rational function of the form $T^+_\omega\varphi(x) = \sum_{k\leq s} a_k x^{-k}$ such that $\varphi(x) = T^+_\omega\varphi(x) + o(|x|^{-s})$. Some new notations will allow us to write this in a more convenient form.

Equip $\hat{\mathbb{R}} \times \mathbb{N}$ with the following order relation: $\mu \leq \nu$ means $\mu = (\xi, s)$ and $\nu = (\eta, t)$ with $\xi = \eta$ and $s \leq t$. If $\omega = (\xi, s) \in \hat{\mathbb{R}} \times \mathbb{N}$ let χ_ω be the rational function defined by $\chi_\omega(x) = (x-\xi)^s$ if $\xi \in \mathbb{R}$ and $\chi_\omega(x) = x^{-s}$ if $\xi = \infty$. Set $\rho_\omega = \chi_\omega^{-1}$

Now it is clear that there is a unique sequence of complex numbers $\{\delta_\mu(\varphi)\}_{\mu\leq\omega}$ such that $T^+_\omega\varphi = \sum_{\mu\leq\omega} \delta_\mu(\varphi)\chi_\mu$. Set $T_\omega\varphi = \sum_{\mu<\omega} \delta_\mu(\varphi)\chi_\mu$ and

$$R_\omega\varphi = \rho_\omega(\varphi - T_\omega\varphi) \quad \text{hence} \quad \varphi = T_\omega\varphi + \chi_\omega R_\omega\varphi. \tag{4.1}$$

Since $C^\omega \subset C^\mu$ if $\mu \leq \omega$ the quantity $\|\varphi\|_\omega = \sum_{\mu\leq\omega} \sup |R_\mu\varphi|$ is a well defined real number if $\varphi \in C^\omega$.

An element $\omega \in \hat{\mathbb{R}} \times \mathbb{N}$ may be thought as a function $\hat{\mathbb{R}} \to \mathbb{N}$ with support containing at most one point. More generally, consider functions with finite support $\alpha : \hat{\mathbb{R}} \to \mathbb{N}$, which we also call *order functions*. We write $\omega \preceq \alpha$ if $\omega = (\xi, s) \in \hat{\mathbb{R}} \times \mathbb{N}$ and $s \leq \alpha(\xi)$. Then $\omega \prec \alpha$ means $\omega \preceq \alpha$ and $s < \sum_\eta \alpha(\eta)$.

Lemma 4.7. *If α is an order function then $C^\alpha(\mathbb{R}) = \cap_{\omega\preceq\alpha} C^\omega(\mathbb{R})$ is an involutive Banach algebra with unit for the usual algebraic operations and the norm $\|\varphi\|_\alpha = \sup_{\omega\preceq\alpha}\|\varphi\|_\omega$. The space $\mathcal{R}$ is a dense $*-$sub-algebra of C^ω.*

The proof is elementary and will not be given. Next we show that the functional calculus for definitizable operators extends to an algebra of the form $C^\alpha(\mathbb{R})$. We start by associating an order function α to each definitizable operator.

Definition 4.8. *Let H be a definitizable operator on $\mathcal{H}$ with $\sigma(H)\subset\mathbb{R}$.*

1. *To each definitizing polynomial p for H we associate an order function β as follows: if $\xi\in\mathbb{R}$ then $\beta(\xi)$ is the multiplicity of ξ as zero of p and $\beta(\infty)=0$ if p is of even degree and $\beta(\infty)=1$ if p is of odd degree.*
2. *The order function α_H of H is the infimum over all definitizing polynomials for H of the above functions β.*

Theorem 4.9. *Let H be a self-adjoint definitizable operator on the Krein space $\mathcal{H}$ with $\sigma(H)\subset\mathbb{R}$.Then there is a unique linear continuous map $\varphi\mapsto\varphi(H)$ from $C^{\alpha_H}(\mathbb{R})$ into $B(\mathcal{H})$ such that if $\varphi(\lambda)=(\lambda-z)^{-1}$ for $z\in\mathbb{C}\backslash\mathbb{R}$ then $\varphi(H)=(H-z)^{-1}$. This map is a morphism of unital $*$-algebras.*

The theorem follows from the next proposition and Lemma 4.7.

Proposition 4.10. *There is a constant C such that $\|\varphi(H)\|\le C\|\varphi\|_\alpha\ \forall\ \varphi\in\mathcal{R}$.*

The rest of this section is devoted to the proof of this proposition. We begin with three simple observations concerning the $*$-algebra $\mathcal{R}$.

Lemma 4.11. *If $\varphi\in\mathcal{R}$ then $\varphi\ge 0$ as function on $\mathbb{R}$ if and only if there is $\psi\in\mathcal{R}$ such that $\varphi=\overline{\psi}\psi$.*

Proof. We have $\varphi=P/Q$ where P,Q are polynomials, Q has no real zeroes, and the degree of P is less or equal to that of Q. Since $\varphi=P\overline{Q}/Q\overline{Q}$, we may assume $Q\ge 0$. Then the degree of Q is $2n$ and one may write $Q=\overline{Q}_0Q_0$ where Q_0 is a polynomial of degree n whose zeroes are exactly the zeroes of Q in the upper half-plane. If $\varphi\ge 0$ then P is a positive polynomial hence its degree is $2m$ with $m\le n$ and one may similarly factorize $P=\overline{P}_0P_0$ (the real zeroes of P being of even multiplicity). Then we take $\psi=P_0/Q_0$. □

As a consequence, if θ is a positive linear form on $\mathcal{R}$ then $|\theta(\varphi)|\le\theta(1)\sup|\varphi|$. The following version of this assertion is more convenient for our purposes.

Lemma 4.12. *Let $\mathcal{H}$ be a complex vector space equipped with a positive sesquilinear form $(\cdot,\cdot)$ and the associated semi-norm $|u|=(u,u)^{1/2}$. Let $M:\mathcal{R}\to L(\mathcal{H})$ be a unital algebra morphism such that $(u,M(\varphi)v)=(M(\overline{\varphi})u,v)$. Then $|M(\varphi)u|\le\sup|\varphi||u|$ for all $\varphi\in\mathcal{R}$ and $u\in\mathcal{H}$.*

Proof. It suffices to show that $|M(\varphi)u|^2=(u,M(|\varphi|^2)u)\le(u,u)$ if $\sup|\varphi|=1$. We have $1-|\varphi|^2\ge 0$ as function on $\mathbb{R}$ and $1-|\varphi|^2\in\mathcal{R}$ hence by Lemma 4.11 there is $\psi\in\mathcal{R}$ such that $1-|\varphi|^2=\overline{\psi}\psi$. Since $M(1)=1$ we obtain $(u,(1-M(|\varphi|^2)u)=(u,M(\overline{\psi}\psi)u)=|M(\psi)u|^2\ge 0$ which proves the assertion. □

The third observation is an analogue of the division algorithm in the algebra $\mathcal{R}$. To each $\psi\in\mathcal{R}$ we associate an order function α_ψ by defining $\alpha_\psi(\xi)$ as the multiplicity of ξ as zero of ψ. In other terms, $\alpha_\psi(\xi)=k$ means that the limit $\lim_{\lambda\to\xi}\psi(\lambda)\rho_\omega(\lambda)$ exists in $\mathbb{C}$ and is not zero for $\omega=(\xi,k)$. The proof of the next lemma is quite elementary and we skip the details.

Lemma 4.13. *Let $\psi \in \mathcal{R}$ with only real zeros and set $\alpha = \alpha_\psi$. Then there are numbers $a_\omega \in \mathbb{C}$ and functions $b_\omega \in \mathcal{R}$ such that for each $\varphi \in \mathcal{R}$ we have:*

$$\varphi = \psi \sum_{\omega \preceq \alpha} a_\omega R_\omega \varphi + \sum_{\omega \prec \alpha} \delta_\omega(\varphi) b_\omega. \tag{4.2}$$

Proof of Prop. 4.10. By a simple argument its suffices to show that $\|\varphi(H)\| \leq C\|\varphi\|_\alpha$ where α is the order function of a definitizing polynomial p with only real zeros. Let n be the degree of p, define $m = \left[\frac{n+1}{2}\right]$, let $\lambda \in \mathbb{C} \setminus \mathbb{R}$, and let $\psi(x) = p(x)(x-\lambda)^{-m}(x-\overline{\lambda})^{-m}$. Then $\psi \in \mathcal{R}$ and $(u|u) := \langle u|\psi(H)u\rangle \geq 0$ for all $u \in \mathcal{H}$. Set $|u| = (u|u)^{1/2}$. Since the rational functional calculus is an algebra morphism we get from (4.2):

$$\varphi(H) = \psi(H) \sum_{\omega \preceq \alpha} a_\omega (R_\omega \varphi)(H) + \sum_{\omega \prec \alpha} \delta_\omega(\varphi) b_\omega(H),\ \varphi \in \mathcal{R}. \tag{4.3}$$

Since the $b_\omega(H)$ are bounded operators, there is a constant C such that for any $u, v \in \mathcal{H}$:

$$|\langle u|\varphi(H)v\rangle| \leq \Big|\Big(u\Big|\sum_{\omega \preceq \alpha} a_\omega (R_\omega\varphi)(H)v\Big)\Big| + C\sum_{\omega\prec\alpha} |\delta_\omega(\varphi)|\,\|u\|\|v\|,\ \varphi \in \mathcal{R}, \tag{4.4}$$

where we used the positive scalar product $(f|g) := \langle f|\psi(H)g\rangle$ introduced above. It is easy to prove that $\sum_{\omega\prec\alpha} |\delta_\omega(\varphi)| \leq \|\varphi\|_\alpha$. On the other hand, by Cauchy-Schwarz inequality and Lemma 4.12 we get:

$$\Big|\Big(u\Big|\sum_{\omega\preceq\alpha} a_\omega(R_\omega\varphi)(H)v\Big)\Big| \leq \sup\Big|\sum_{\omega\preceq\alpha} a_\omega R_\omega\varphi\Big| |u||v| \leq C\|\varphi\|_\alpha \|u\|\|v\|.$$

Thus $|\langle u|\varphi(H)v\rangle| \leq C\|\varphi\|_\alpha\|u\|\|v\|$, which finishes the proof of Prop. 4.10. □

From Thm. 4.9 we can deduce an optimal estimate of the resolvent of a definitizable operator. We first introduce some terminology.

Definition 4.14. *We set $\sigma_{\mathbb{C}}(H) := \sigma(H)\backslash\mathbb{R}$. We set $c(H) := \{\omega \in \hat{\mathbb{R}} \ :\ \alpha_H(\xi) \neq 0\}$. The set $c(H)$ is called the set of* critical points *of H.*

Let H be a definitizable operator. Recall that α_H is defined in Def. 4.8.

Proposition 4.15. *With the preceding notations, there exists $c > 0$ such that*

$$c\|(H-z)^{-1}\| \leq \sum_{\xi\in\sigma_{\mathbb{C}}(H)} |z-\xi|^{-\alpha_H(\xi)} + |\mathrm{Im}z|^{-1}\Big(1 + \sum_{\xi\in c(H)} |z-\xi|^{-\alpha_H(\xi)} + |z|^{\alpha_H(\infty)}\Big) \tag{4.5}$$

for all $z \notin \sigma_c \cup \mathbb{R}$. Note that $\alpha_H(\infty)$ is either 0 or 1.

Proof. It is clearly sufficient to assume that the spectrum of H is real. If $z \notin \mathbb{R}$ and $\varphi(x) = (z-x)^{-1}$ then $\varphi \in \mathcal{R}$ and thus $\|(z-H)^{-1}\| \leq C\|\varphi\|_{\alpha_H}$ by Thm. 4.9. To simplify notations we set $\alpha_H(\xi) = k_\xi$ and $T_{(\xi,k)} = T_\xi^k$. Since $\varphi(\infty) = 0$ we have

$$\|\varphi\|_{\alpha_H} \leq \sup|\varphi| + \sup_{\xi\in\sigma_r}\sum_{k\leq k_\xi} \sup_{x\in\mathbb{R}} \big|\varphi(x) - T_\xi^k\varphi(x)\big|\,|x-\xi|^{-k} + \alpha_H(\infty)\sup_{x\in\mathbb{R}}|x\varphi(x)|.$$

We have $\sup|\varphi| = |\mathrm{Im}z|^{-1}$ and $\sup|x\varphi(x)| = |z||\mathrm{Im}z|^{-1}$ hence it remains to estimate $(\varphi(x) - T_\xi^k\varphi(x))(x-\xi)^{-k}$. We shall prove the following extension of the first order resolvent identity:

$$\varphi(x) - T_\xi^k\varphi(x) = (x-\xi)^k\varphi^k(\xi)\varphi(x) \quad \text{if } x, \xi \neq z. \tag{4.6}$$

This implies the next estimate, which proves the proposition:

$$\sup_x \big|\varphi(x) - T_\xi^k\varphi(x)\big||x-\xi|^{-k} = \sup_x |z-\xi|^{-k}|z-x|^{-1} = |z-\xi|^{-k}|\mathrm{Im}z|^{-1}.$$

Observe that (4.6) is trivial if $k = 0$ because $T^0_\xi\varphi = 0$ and is just the first order resolvent identity if $k = 1$. Now assume (4.6) holds for k. Since $\varphi^{(k)} = k!\varphi^{k+1}$ we have

$$T^{k+1}_\xi\varphi(x) = T^k_\xi\varphi(x) + \frac{1}{k!}\varphi^{(k)}(\xi)(x-\xi)^k = T^k_\xi\varphi(x) + \varphi^{k+1}(\xi)(x-\xi)^k,$$

which when used in (4.6) gives the same identity with k replaced by $k+1$. □

Remark 4.16. The interpretation of the points $\xi \in \mathbb{R}$ with $\alpha_H(\xi) > 0$ as "critical points" of H is misleading from the point of view of the functional calculus. For example, the operator of q of multiplication by x in the Krein space $L^2(\mathbb{R},\ \mathrm{sign}\, x\, dx)$ is positive and α_q has value 1 at 0 and ∞ but the functional calculus extends continuously from the algebra C^{α_q} to $C(\hat{\mathbb{R}})$ defined by the order function $\alpha = 0$.

5. C_0-groups and regular operators

In this section we collect some standard facts on smoothness of operators with respect to C_0-groups.

5.1. $C^\alpha(A)$ **classes of bounded operators.** Let $W = \{W_t\}$ be a C_0-group on a Banach space $\mathcal{H}$ with generator A defined such that $W_t = \mathrm{e}^{\mathrm{i}tA}$. Then there are numbers $M \geq 1$ and $\gamma \geq 0$ such that

$$\|W_t\| \leq M\mathrm{e}^{\gamma|t|} \quad \text{for all} \ \ t \in \mathbb{R}. \tag{5.1}$$

The spectrum of the operator A is included in the strip $\{z \in \mathbb{C} \mid \ |\mathrm{Im}z| \leq \gamma\}$ and it could be equal to this strip.

One may naturally associate to A three operators acting on the Banach space $B(\mathcal{H})$, namely *left multiplication* by A, denoted $\mathcal{A}_\ell$, *right multiplication* by A, denoted $\mathcal{A}_r$, and *commutation* by A, denoted $\mathcal{A}$ and defined by $\mathcal{A}(T) = [T, A]$, so that $\mathcal{A} = \mathcal{A}_r - \mathcal{A}_\ell$. Since A is unbounded, it is convenient to define these operators as generators of one parameter groups of bounded operators on $B(\mathcal{H})$. More precisely, if $t \in \mathbb{R}$ and $T \in B(\mathcal{H})$ we have:

$$\mathrm{e}^{\mathrm{i}t\mathcal{A}_\ell}(T) = \mathrm{e}^{\mathrm{i}tA}T, \quad \mathrm{e}^{\mathrm{i}t\mathcal{A}_r}(T) = T\mathrm{e}^{\mathrm{i}tA}, \quad \mathrm{e}^{\mathrm{i}t\mathcal{A}}(T) = \mathrm{e}^{-\mathrm{i}tA}T\mathrm{e}^{\mathrm{i}tA} \equiv T(t). \tag{5.2}$$

These operators commute in the sense that the elements of the groups they generate are pairwise commuting, and $\mathcal{A} = \mathcal{A}_r - \mathcal{A}_\ell$ i.e. $\mathrm{e}^{\mathrm{i}t\mathcal{A}} = \mathrm{e}^{-\mathrm{i}t\mathcal{A}_\ell}\mathrm{e}^{\mathrm{i}t\mathcal{A}_r}$.

These are C_0-groups if we equip $B(\mathcal{H})$ with the strong operator topology. If we assume (5.1) then

$$\|\mathrm{e}^{\mathrm{i}t\mathcal{A}_\ell}\| \leq M\mathrm{e}^{\gamma|t|},\ \|\mathrm{e}^{\mathrm{i}t\mathcal{A}_r}\| \leq M\mathrm{e}^{\gamma|t|},\ \|\mathrm{e}^{\mathrm{i}t\mathcal{A}}\| \leq M^2\mathrm{e}^{2\gamma|t|} \quad \text{for all} \ \ t \in \mathbb{R}. \tag{5.3}$$

Let $0 < \alpha < 1$. We say that $S \in B(\mathcal{H})$ is of class $C^\alpha(A)$, and we write $S \in C^\alpha(A)$, if the map $\mathbb{R} \ni t \mapsto S(t) = \mathrm{e}^{\mathrm{i}t\mathcal{A}}S \in B(\mathcal{H})$ is of class C^α (i.e. is Hölder continuous of order α) for the strong operator topology of $B(\mathcal{H})$. By the uniform boundedness principle, this is equivalent to $\|S(t) - S\| \leq C|t|^\alpha$ for $|t| \leq 1$ and from this estimate we easily get that

$$\|S(t) - S(s)\| \leq C\mathrm{e}^{2\gamma|t|}|t-s|^\alpha, \ \text{for}\ |t-s| \leq 1. \tag{5.4}$$

We say that $S \in B(\mathcal{H})$ is of class $C^1(A)$ if $t \mapsto S(t)$ is of class C^1 for the strong operator topology. If $\mathcal{H}$ is reflexive then $S \in C^1(A)$ if and only if $t \mapsto S(t)$ is locally Lipschitz (this property holds in the strong topology if and only if it holds in the norm topology). Then we may define

$$S' := \frac{d}{dt}S(t)_{|t=0} \tag{5.5}$$

so that $S(b)-S(a)=\int_a^b S'(t)dt$ in the strong sense. Note that $S\in C^1(A)$ if and only if $S\mathrm{Dom}A\subset\mathrm{Dom}A$ and the operator $[S,\mathrm{i}A]$ with domain $\mathrm{Dom}A$ extends to a bounded operator on $\mathcal{H}$ which is exactly S'. For this reason we often abuse notation and denote $S'=\mathrm{i}\mathcal{A}S=[S,\mathrm{i}A]$.

If $1<\alpha\leq 2$, we say that S is of class $C^\alpha(A)$ if $S\in C^1(A)$ and $S'\in C^{\alpha-1}(A)$. The class $C^\alpha(A)$ is similarly defined for $\alpha>2$. Note however that for integer α it would be more natural to define this class in terms of Zygmund type conditions. The next lemma follows easily from the fact that $\mathrm{e}^{\mathrm{i}t\mathcal{A}}$ are automorphisms of $B(\mathcal{H})$.

Lemma 5.1. *The following properties hold for any number $\alpha>0$:*

(1) *the classes $C^\alpha(A)$ are sub-algebras of $B(\mathcal{H})$,*
(2) *$\mathcal{A}$ is a derivation of $B(\mathcal{H})$, i.e. $(S_1S_2)'=S_1'S_2+S_1S_2'$ if $S_1,S_2\in C^1(A)$,*
(3) *if $S\in B(\mathcal{H})$ is boundedly invertible and $S\in C^\alpha(A)$ then $S^{-1}\in C^\alpha(A)$. Moreover if $S\in C^1(A)$ then $(S^{-1})'=-S^{-1}S'S^{-1}$.*

5.2. $C^\alpha(A)$ **classes of unbounded operators.** In this subsection we fix $0<\alpha\leq 2$ and S a closed, densely defined operator on $\mathcal{H}$ with $\rho(S)\neq\emptyset$. We set $R(z)=(S-z)^{-1}$ for $z\in\rho(S)$.

We say that S is *regular* if there is a sequence $(z_n)\in\rho(S)$ with $\lim|z_n|=+\infty$ and

$$\|(S-z_n)^{-1}\|\leq C|z_n|^{-1}\quad\text{for some constant}\quad C\geq 0.$$

Note that this is not an innocent condition, some natural realizations of the free Klein-Gordon operator considered later do not have this property: if $S=H_0$ as in Remark 8.10 we may have $\sigma(S)=\mathbb{R}$ and $\|(S-z)^{-1}\|\geq 1$ for all $z\notin\mathbb{R}$.

Definition 5.2. *We say that $S\in C^\alpha(A)$ for $0<\alpha\leq 2$ if $R(z_0)\in C^\alpha(A)$ for some $z_0\in\rho(S)$.*

Lemma 5.3. (1) *if $R(z_0)\in C^\alpha(A)$ for some $z_0\in\rho(S)$ then $R(z)\in C^\alpha(A)$ for all $z\in\rho(S)$,*
(2) *If $S\in C^1(A)$ then*

$$[A,R(z)]=(S-z_0)R(z)[A,R(z_0)]R(z)(S-z_0),\ \ z_0,z\in\rho(S).$$

(3) *If $S\in C^1(A)$ then the space $D:=R(z)\mathrm{Dom}A$ is independent on $z\in\rho(S)$, included in $\mathrm{Dom}A\cap\mathrm{Dom}S$ and is a core for S.*
(4) *If moreover S is regular, then D is dense in $\mathrm{Dom}A\cap\mathrm{Dom}S$.*

Proof. (1) follows from (3) of Lemma 5.1 and the first resolvent formula. Then (2) follows from (2) of Lemma 5.1 and again the first resolvent formula. Let us prove (3). Since $\mathrm{Dom}A$ is dense in $\mathcal{H}$, the set $D_z:=R(z)\mathrm{Dom}A$ is a core for S. By Subsect. 5.1 we know that $D_z\subset\mathrm{Dom}A$. Using the first resolvent formula, we see that $D_{z_1}\subset D_{z_2}$ for all $z_1,z_2\in\rho(S)$, hence D_z is independent on z.

If S is regular, then $J_n:=-z_nR(z_n)$ tends strongly to the identity in $\mathcal{H}$ and in $\mathrm{Dom}S$. Let $u\in\mathrm{Dom}A\cap\mathrm{Dom}S$. Then $u_n:=J_nu\in D$ and $u_n\to u$ in $\mathrm{Dom}S$. From (2) we obtain that:

$$[A,J_n]=(S-z_0)R(z_n)[A,R(z_0)]J_n(S-z_0).$$

Since S is regular, we see that $(S-z_0)R(z_n)\to 0$ strongly on $\mathcal{H}$. So $[A,J_n]\to 0$ strongly on $\mathcal{H}$ hence $u_n\to u$ in $\mathrm{Dom}A$ and D is dense in $\mathrm{Dom}A\cap\mathrm{Dom}S$. □

We now assume that the Banach space $\mathcal{H}$ is reflexive. Then

$$\begin{aligned}\|u\|&=\sup_{w\in\mathcal{H}^*,\|w\|=1}|\langle w,u\rangle|\quad\text{if } u\in\mathcal{H},\\ \|S\|&=\sup_{u\in\mathcal{H},w\in\mathcal{H}^*,\|u\|=\|w\|=1}|\langle w,Su\rangle|\quad\text{if } S\in B(\mathcal{H}).\end{aligned}\tag{5.6}$$

From (5.6) we obtain that for $S \in B(\mathcal{H})$ we have $S \in C^\alpha(A) \Leftrightarrow S^* \in C^\alpha(A^*)$. This extends to S closed and densely defined. Moreover, if S is closed densely defined and regular, then so is S^*.

We consider the sesquilinear form:

$$[A,S](w,u) := \langle A^*w, Su\rangle - \langle S^*w, Au\rangle,\ u \in \mathrm{Dom}S \cap \mathrm{Dom}A,\ w \in \mathrm{Dom}S^* \cap \mathrm{Dom}A^*.$$

We equip $\mathrm{Dom}S$ and $\mathrm{Dom}S^*$ with their graph norms.

Proposition 5.4. *Let S be regular. Then the following are equivalent:*

(1) *S is of class $C^1(A)$,*
(2) *the following three conditions are satisfied:*
   (i) $|[A,S](w,u)| \leq C\|w\|_{\mathrm{Dom}S^*}\|u\|_{\mathrm{Dom}S}$, $u \in \mathrm{Dom}S \cap \mathrm{Dom}A$, $w \in \mathrm{Dom}S^* \cap \mathrm{Dom}A^*$,
   (ii) $\{u \in \mathrm{Dom}A\ :\ R(z)u \in \mathrm{Dom}A\}$ *is a core for A for some $z \in \rho(S)$,*
   (iii) $\{w \in \mathrm{Dom}A^*\ :\ R(z)^*w \in \mathrm{Dom}A^*\}$ *is a core for A^* for some $z \in \rho(S)$.*

For the proof, see [GGM, Props. 2.19, 2.21].

Assume that $S \in C^1(A)$ is regular. Then by Lemma 5.3 $\mathrm{Dom}A \cap \mathrm{Dom}S$ is dense in $\mathrm{Dom}S$ and $\mathrm{Dom}A^* \cap \mathrm{Dom}S^*$ in $\mathrm{Dom}S^*$. As in the proof of [GGM, Prop. 2.19] we see that $[A,S]$ uniquely extends to a bounded sesquilinear form $[A,S]^\circ$ on $\mathrm{Dom}S^* \times \mathrm{Dom}S$ and $[A,R(z)] = -R(z)[A,S]^\circ R(z)$. Here, the left $R(z)$ acts on $\mathcal{H}^*$ as $R(z)^*$.

Remark 5.5. On a Krein space (see Sect. 3.1), if $S = S^*$ and if the Krein structure is of class $C^1(A)$, (see Subsect. 5.5), then (iii) follows from (ii), because we can consider S^*, A^* as operators on $\mathcal{H}$ and $A - A^*$ is bounded.

We now give some regularity properties with respect to A of a function of S.

Lemma 5.6. *If $S \in C^\alpha(A)$ then $\chi(S) \in C^\alpha(A)$ for any $\chi \in C_0^\infty(\beta(S))$.*

Proof. We prove more, namely that $\int R(\lambda \pm \mathrm{i}0)\chi(\lambda)d\lambda$ are of class C^α. From the definition of $\beta(S)$ (see Def. 2.2) and using a partition of unity, we may assume that the assumptions of Lemma 2.1 are fulfilled. We begin with the case $0 < \alpha \leq 1$. We claim first that

$$\|\mathrm{e}^{\mathrm{i}t\mathcal{A}}R(z) - R(z)\| \leq C|\mathrm{Im}z|^{-2n}|t|^\alpha,\ 0 \leq |t| \leq 1,\ z \in I \pm \mathrm{i}]0,\nu]. \tag{5.7}$$

This implies the lemma if $0 < \alpha \leq 1$ using (2.2) with n replaced by $2n$.

We now prove (5.7). If $T \in B(\mathcal{H})$ with $T^{-1} \in B(\mathcal{H})$ then from $\mathrm{e}^{\ it\mathcal{A}}T^{-1} = (\mathrm{e}^{\mathrm{i}t\mathcal{A}}T)^{-1}$ we get

$$\|\mathrm{e}^{\mathrm{i}t\mathcal{A}}T^{-1} - T^{-1}\| \leq C\|T^{-1}\|^2\|\mathrm{e}^{\mathrm{i}t\mathcal{A}}T - T\|,\ |t| \leq 1. \tag{5.8}$$

The same argument gives for $T_1, T_2 \in B(\mathcal{H})$:

$$\|\mathrm{e}^{\mathrm{i}t\mathcal{A}}(T_1T_2) - T_1T_2\| \leq C\|T_1\|\|\mathrm{e}^{\mathrm{i}t\mathcal{A}}T_2 - T_2\| + C\|T_2\|\|\mathrm{e}^{\mathrm{i}t\mathcal{A}}T_1 - T_1\|,\ |t| \leq 1. \tag{5.9}$$

For $z_0 \in \rho(S)$ and $z \in I \pm \mathrm{i}]0,\nu]$ we have:

$$R(z) = R(z_0)(1 + (z - z_0)R(z_0))^{-1}.$$

Applying (5.8), (5.9) and the hypothesis that $R(z_0) \in C^\alpha(A)$, we obtain

$$\|\mathrm{e}^{\mathrm{i}t\mathcal{A}}R(z) - R(z)\| \leq C\|R(z)\|^2|t|^\alpha,\ 0 \leq |t| \leq 1,$$

which proves (5.7). Note that in the case $\alpha = 1$ the formula (2.2) gives an explicit expression for the commutator $[\int R(\lambda + \mathrm{i}0)\chi(\lambda)d\lambda, A]$ involving expressions of the form $R(z)[S,A]^0R(z)$. In the case $1 < \alpha \leq 2$ we repeat the same arguments applied to the first derivative, using again (2.2). □

5.3. **Some Fourier transforms.** For simplicity of future notation, we normalize the Fourier transform of tempered distributions in such a way that $f(\tau) = \int \mathrm{e}^{\mathrm{i}\tau t}\widehat{f}(t)dt$. We set

$$f_s(\tau) := f(s\tau),\ f \in \mathcal{S}'(\mathbb{R}),\ s \in \mathbb{R}. \tag{5.10}$$

Then $\widehat{f_s}(t) = s^{-1}\widehat{f}(s^{-1}t)$. If $\delta := \tau\frac{d}{d\tau}$, then $f_s = \mathrm{e}^{-t\delta}f$ for $s = \mathrm{e}^{-t}$. We will set

$$\tilde{f}(\tau) := \delta f(\tau) = \tau f'(\tau),\ f \in \mathcal{S}'(\mathbb{R}). \tag{5.11}$$

We denote by $S^\sigma(\mathbb{R})$ for $\sigma \in \mathbb{R}$ the space of functions $f \in C^\infty(\mathbb{R})$ such that $|f^{(n)}(\tau)| \leq C_n\langle\tau\rangle^{\sigma-n},\ n \in \mathbb{N}$.

Lemma 5.7. *The classes S^σ have the following properties:*

(1) *If $f \in S^\sigma(\mathbb{R})$ then $\widehat{f} \in C^\infty(\mathbb{R}\backslash\{0\})$ and*

$$|\widehat{f}(t)| \leq C_n\langle t\rangle^{-n} \text{ in } |t| \geq 1,\ \forall\ n \in \mathbb{N}.$$

(2) *If $f \in S^\sigma(\mathbb{R})$ for $\sigma < 0$ then $\widehat{f} \in L^1(\mathbb{R})$,*
(3) *If $f \in S^\sigma(\mathbb{R})$ for $-1 < \sigma < 0$ then*

$$|t^k\widehat{f}^{(k)}(t)| \leq C_k|t|^{-\sigma-1},\ \forall\ k \in \mathbb{N}.$$

These facts are well known. The typical example of a symbol in $S^{-\sigma}(\mathbb{R})$ is the function $\langle\cdot\rangle^{-\sigma}$ whose Fourier transform is the *Bessel potential* G_σ. For all $t \neq 0$, $G_\sigma(t)$ is given by the following absolutely convergent integral (see e.g. [S, Sect. V.3]):

$$G_\sigma(t) = \frac{1}{2^\sigma\sqrt{\pi}\Gamma(\sigma/2)}\int_0^{+\infty}\mathrm{e}^{-t^2/r-r/4}r^{(\sigma-1)/2}\frac{dr}{r}. \tag{5.12}$$

The following lemma is easy.

Lemma 5.8. *The distributions G_σ have the following properties:*

(1) $G'_\sigma(t) = C_\sigma tG_{\sigma-2}(t),\ t \neq 0,\ \sigma \in \mathbb{R}$,
(2) $|t^kG_\sigma^{(k)}(t)| \leq C_{k,\sigma}|t|^{\sigma-1},\ t \neq 0,\ \sigma \in \mathbb{R},\ k \in \mathbb{N}$,
(3) $|G_\sigma^{(k)}(t)| \leq C_{k,\sigma}|t|^k\mathrm{e}^{-|t|/2},\ |t| \geq 1, \sigma \in \mathbb{R},\ k \in \mathbb{N}$,
(4) $\mathrm{e}^{c|t|}\delta^kG_\sigma \in L^1(\mathbb{R}),\ \sigma > 0,\ c < \frac{1}{2},\ k \in \mathbb{N}$,
(5) $\mathrm{e}^{c|t|}G'_\sigma \in L^1(\mathbb{R}),\ \sigma > 1,\ c < \frac{1}{2}$.

Proof. We get (1) by differentiating (5.12) under the integral sign. Relation (2) for $k = 0$ follows from

$$\mathrm{e}^{-t^2/r-r/4} \leq \mathrm{e}^{-t^2/r}.$$

Using (1) we obtain (2) for arbitrary k. Similarly using the inequality

$$t^2/r + r/4 \geq |t|/2 + 1/2r + r/8,\ |t| \geq 1,$$

and the fact that the integral $\int_0^{+\infty}\mathrm{e}^{-1/2r-r/8}r^{(\sigma-1)/2}\frac{dr}{r}$ is finite for all $\sigma \in \mathbb{R}$ we obtain (3) for $k = 0$, and then for arbitrary k using (1). Finally, (4) and (5) follow from (2) and (3). □

5.4. **Functional calculus associated to A.** Let us fix a C_0-group W on the Banach space $\mathcal{H}$ with generator A.

Let $\mathcal{M}_\gamma$ be the set of functions $f : \mathbb{R} \to \mathbb{C}$ whose Fourier transforms are complex measures such that:

$$\|f\|_{\mathcal{M}} := \int \mathrm{e}^{\gamma|t|}|\widehat{f}(t)|dt < \infty. \tag{5.13}$$

$\mathcal{M}$ is a unital Banach $*$-algebra for the usual operations of addition and multiplication and the involution $f^*(\tau) = \overline{f}(-\tau)$. Such functions f admit a holomorphic extension in the strip $\{\tau \ : \ |\mathrm{Im}\tau| < \gamma\}$, in particular do not have compact support. We define

$$f(A) := \int \mathrm{e}^{\mathrm{i}tA}\widehat{f}(t)dt$$

and note that $\mathcal{M} \ni f \mapsto f(A) \in B(\mathcal{H})$ is a linear multiplicative map. Clearly $f \in \mathcal{M}_\gamma \Rightarrow f_s \in \mathcal{M}_\gamma$ if $0 \leq s \leq 1$ and

$$\|f(sA)\| \leq M\|f\|_{\mathcal{M}_\gamma} \quad \text{where } f(sA) = f_s(A). \tag{5.14}$$

By Lemma 5.8 we see that if $\sigma > 0$ then $\langle\cdot\rangle^{-\sigma} \in \mathcal{M}_\gamma$ if $\gamma < 1/2$ hence $\langle sA\rangle^{-\sigma}$ is a well defined bounded operator on $\mathcal{H}$ if $0 \leq 2s\gamma < 1$.

A similar assertion holds for a large class of analytic symbols of strictly negative order but the problem of the boundedness of the operator $f(A)$ for symbols of class S^0 which are not Fourier transforms of measures is much more delicate.

We will be interested in the apparently trivial case when the derivative of f satisfies $f'(\tau) = \langle\tau\rangle^{-\sigma}$ with $\sigma > 1$. To understand the nature of the problem note that for such an f the operator $f(P)$ with $P = -\mathrm{i}\frac{d}{dx}$ is bounded in $L^p(\mathbb{R})$ if $1 < p < \infty$ but not in $L^1(\mathbb{R}), L^\infty(\mathbb{R})$, or $C_0(\mathbb{R})$.

If W is a bounded C_0-group and $\mathcal{H}$ is Hilbertizable then $\|f(A)\| \leq C \sup|f|$ because such a group is unitary for an admissible Hilbert norm. In our applications this is not sufficient because W is of exponential growth. But we have:

Proposition 5.9. *If $\mathcal{H}$ is Hilbertizable and f is holomorphic on the strip $\{z \ : \ |\mathrm{Im}z| < \gamma'\}$ for some $\gamma' > \gamma$ then*

$$\|f(A)\| \leq C \sup_{\mathbb{R}+\mathrm{i}]-\gamma',\gamma'[} |f(z)| \tag{5.15}$$

For the proof, see [ABG, Prop. 3.7.1]. The hilbertizability assumption is rather annoying but we expect that the result remains true in UMD spaces.

One may define $f(A)$ for unbounded functions f by allowing $\widehat{f}$ to be a distribution of exponential decay instead of a measure. In other terms, $\widehat{f}$ may be a sum of derivatives of exponentially decaying measures, or f a sum of functions in $\mathcal{M}_\gamma$ multiplied by polynomials. We assume $\gamma < 1/2$ and explain this in detail only for the functions $f(\tau) = \langle\tau\rangle^s$ with $0 < s < 1$ which are important here. Let us set $\sigma = 2 - s$, so that $1 < \sigma < 2$. Note that from

$$\langle\tau\rangle^{-s}\langle\tau\rangle^{-\sigma} = \langle\tau\rangle^{-2} = (1 - \mathrm{i}\tau)^{-1}(1 + \mathrm{i}\tau)^{-1},$$

identity valid in the algebra $\mathcal{M}_\gamma$, we get by the already defined functional calculus

$$\langle A\rangle^{-s}\langle A\rangle^{-\sigma} = (1 + A^2)^{-1} = (1 - \mathrm{i}A)^{-1}(1 + \mathrm{i}A)^{-1}.$$

Thus $B = \langle A\rangle^{-\sigma}(1 + A^2)$ is a well defined operator on $\mathrm{Dom}A^2$ and there we have $\langle A\rangle^{-s}B = B\langle A\rangle^{-s} = 1$. Hence we must define $\langle A\rangle^s$ as the closure of B. Then we have on $\mathrm{Dom}A^2$:

$$\langle A\rangle^s = \int (1 + A^2)\mathrm{e}^{\mathrm{i}tA}G_\sigma(t)dt = \int \Big((1 - \partial_t^2)\mathrm{e}^{\mathrm{i}tA}\Big)G_\sigma(t)dt = \int \mathrm{e}^{\mathrm{i}tA}\big(G_\sigma(t) - G''_\sigma(t)\big)dt \tag{5.16}$$

where we interpret the derivatives in the sense of distributions. If we set $P = -\mathrm{i}\frac{d}{dt}$ as operator acting on $\mathcal{H}$-valued distributions then we may write

$$\langle A\rangle^s u = \langle A\rangle^{-\sigma} u - \int \mathrm{e}^{\mathrm{i}tA} u G''_\sigma(t)dt = \int W_t u \cdot (1+P^2)G_\sigma(t)dt, \ , \ u \in \mathrm{Dom}A^2.$$

This representation gives the following useful estimate:

Proposition 5.10. *If $\gamma < 1/2$ and $0 < s < m < 1$ then there exists $C \geq 0$ such that*

$$\|\langle A\rangle^s u\| \leq C\|u\| + C\mathrm{sup}_{|x|<1}|x|^{-m}\|(W(x)-1)u\|. \tag{5.17}$$

Proof. Let θ be a C^∞ function such that $\theta(t) = 1$ for $|t| < 1$ and $\theta(t) = 0$ if $|t| > 2$. Set $V(t) = \theta(t)W_t u$. Then

$$\langle A\rangle^s u = \int V(t)\cdot(1+P^2)G_\sigma(t)dt + \int (1-\theta)W_t u(1+P^2)G_\sigma(t)dt.$$

By Lemma 5.8 (3) the second term is bounded by $C\|u\|$. Since V is a continuous function with compact support, for any $s < \mu < m$ we have:

$$\int V(t)\cdot(1+P^2)G_\sigma(t)dt = \int \langle P\rangle^\mu V(t)\cdot\langle P\rangle^{2-\mu}G_\sigma(t)dt.$$

Since $\widehat{Pf}(t) = t\widehat{f}(t)$ and $\sigma = 2-s$ we have $\langle P\rangle^{2-\mu}G_\sigma = G_{\mu-s}$, hence

$$\left\|\int V(t)\cdot(1+P^2)G_\sigma(t)dt\right\| = \left\|\int \langle P\rangle^\mu V(t)\cdot G_{\mu-s}(t)dt\right\| \leq \|\langle P\rangle^\mu V\|_{L^\infty}\|G_{\mu-s}\|_{L^1},$$

where we used that $\mu - s > 0$ and Lemma 5.8 (4). Then it remains to note that $\|\langle P\rangle^\mu V\|_{L^\infty} \leq C\|V\|_{C^m}$ if $0 < \mu < m < 1$, V has compact support, and

$$\|V\|_{C^m} = \sup_t \|V(t)\| + \sup_{t\neq s}|t-s|^{-m}\|V(t)-V(s)\|.$$

This is easy to prove by a standard Littlewood-Paley type argument. □

5.5. **C_0-groups on $K-$spaces.** In this subsection $\mathcal{H}$ is a $K-$space equipped with the hermitian form $\langle\cdot|\cdot\rangle$. Since $\mathcal{H}$ is reflexive $W^* = \{W_t^*\}$ is also a C_0-group of operators on $\mathcal{H}$ whose generator is $-A^*$. In other terms, $W_t^* = \mathrm{e}^{-\mathrm{i}tA^*}$. Clearly $\|W_t^*\| \leq M'\mathrm{e}^{\gamma|t|}$ with the same γ hence the operators A, A^* admit an $\mathcal{M}_\gamma$ functional calculus and we have $f(A)^* = \overline{f}(A^*)$ for all $f \in \mathcal{M}_\gamma$. For example, $(\langle\varepsilon A\rangle^{-\sigma})^* = \langle\varepsilon A^*\rangle^{-\sigma}$ for $\varepsilon > 0$ small enough.

We shall say that *the Krein structure is of class $C^1(A)$* if the conditions of the next proposition are verified.

Proposition 5.11. *The following assertions are equivalent:*

1. *the function $t \mapsto \langle W_t u|W_t u\rangle$ is derivable at zero for each $u \in \mathcal{H}$,*
2. *the function $t \mapsto \langle W_t u|W_t u\rangle$ is of class C^1 for each $u \in \mathcal{H}$,*
3. *the map $t \mapsto W_t^* W_t$ is locally Lipschitz,*
4. *$A^* = A + B$ where B is a bounded operator.*

Proof. For $u, v \in \mathrm{Dom}A$ we have

$$-\mathrm{i}\frac{d}{dt}\langle W_t u|W_t u\rangle = \langle W_t u|AW_t u\rangle - \langle AW_t u|W_t u\rangle. \tag{5.18}$$

If the derivative in the left hand side exists at zero for each $u, v \in \mathcal{H}$ then the map $t \mapsto W_t^* W_t$ is weakly differentiable at $t = 0$, hence by the uniform boundedness principle the derivative is a bounded operator and so there is a number C such that $|\langle u|Av\rangle - \langle Au|v\rangle| \leq C\|u\|\|v\|$ for all $u, v \in \mathrm{Dom}A$. Thus if we fix $v \in \mathrm{Dom}A$ then $|\langle Au|v\rangle| \leq C'\|u\|$ for all $u \in \mathrm{Dom}A$ hence $v \in \mathrm{Dom}A^*$ and $|\langle u|(A-A^*)v\rangle| \leq$

$C\|u\|\|v\|$ for $u, v \in \mathrm{Dom}A$. Thus $\mathrm{Dom}A \subset \mathrm{Dom}A^*$ and $\|(A - A^*)v\| \leq C''\|v\|$ for $v \in \mathrm{Dom}A$. If we denote A_0^* the restriction of A^* to $\mathrm{Dom}A$ then we get $A_0^* = A + B$ for a bounded operator B. If $a > 0$ is large enough then

$$A_0^* + \mathrm{i}a = (A + \mathrm{i}a) + B = [1 + B(A + \mathrm{i}a)^{-1}](A + \mathrm{i}a)$$

and $\|B(A + \mathrm{i}a)^{-1}\| < 1$ hence $A_0^* + \mathrm{i}a : \mathrm{Dom}A \to \mathcal{H}$ is bijective. But $A^* + \mathrm{i}a : \mathrm{Dom}A^* \to \mathcal{H}$ is also bijective for large a, so $\mathrm{Dom}A = \mathrm{Dom}A^*$ and $A^* = A + B$. This proves (1) $\Rightarrow$ (4). Then (4) $\Rightarrow$ (2) $\Rightarrow$ (1) follows from

$$\langle W_{t_2}u|W_{t_2}v\rangle - \langle W_{t_1}u|W_{t_1}v\rangle = \mathrm{i}\int_{t_1}^{t_2} \big(\langle W_t u|AW_t v\rangle - \langle AW_t u|W_t v\rangle\big)dt \tag{5.19}$$

which holds for $u, v \in \mathrm{Dom}A$ and extends to all $u, v \in \mathcal{H}$ under the assumption (4). Finally, (2) $\Rightarrow$ (3) follows from uniform boundedness principle and (3) $\Rightarrow$ (2) follows from (5.19) and a density argument. □

Remark 5.12. Note that $B = \mathrm{i}\frac{d}{dt}W_t^* W_t|_{t=0}$.

Remark 5.13. If A is self-adjoint for a Hilbert norm $(\cdot|\cdot)^{1/2}$ and $\langle u|v\rangle = (u|Jv)$ then (4) means $J \in C^1(A)$.

Corollary 5.14. *If the Krein structure is of class $C^1(A)$ then the Besov scales $\mathcal{H}_{s,p}$ associated to the groups W and W^* coincide for $-1 < s < 1$.*

Proof. We have $\mathrm{Dom}A = \mathrm{Dom}A^*$ by (4) of Prop. 5.11. The spaces $\mathcal{H}^A_{s,p}$ with $0 < s < 1$ associated to W are obtained by interpolation between $\mathrm{Dom}A$ and $\mathcal{H}$ and similarly for W^*, hence $\mathcal{H}^A_{s,p} = \mathcal{H}^{A^*}_{s,p}$ if $0 < s < 1$. Then $\mathcal{H}^A_{s,p} = \mathcal{H}^{A^*}_{s,p}$ follows by duality if $-1 < s < 0$ (supplemented by an obvious density argument if $p = \infty$). The case $s = 0$ is covered by interpolating between $\mathcal{H}^A_{1/2,p}$ and $\mathcal{H}^A_{-1/2,p}$. □

Proposition 5.15. *If the Krein structure is of class $C^1(A)$ then for $0 < \sigma < 1$ and $\varepsilon > 0$ small we have:*

$$\|\langle \varepsilon A\rangle^\sigma - \langle \varepsilon A^*\rangle^\sigma\| \leq C\varepsilon, \tag{5.20}$$

$$\langle \varepsilon A\rangle^{-\sigma} - \langle \varepsilon A^*\rangle^{-\sigma} = \langle \varepsilon A\rangle^{-\sigma} - \big(\langle \varepsilon A\rangle^{-\sigma}\big)^* = \langle \varepsilon A\rangle^{-\sigma} O(\varepsilon)\langle \varepsilon A\rangle^{-\sigma}. \tag{5.21}$$

Proof. Set for simplicity of notation $\mathcal{H}_s = \mathcal{H}^A_{s,2}$. From (5.16) we get

$$\langle \varepsilon A\rangle^\sigma - \langle \varepsilon A^*\rangle^\sigma = \varepsilon \int \frac{\mathrm{e}^{\mathrm{i}t\varepsilon A} - \mathrm{e}^{\mathrm{i}t\varepsilon A^*}}{\varepsilon t} t\big(G_{2-\sigma}(t) - G''_{2-\sigma}(t)\big)dt.$$

This holds in $B(\mathcal{H}_1, \mathcal{H}_{-1})$ by Corollary 5.14. Using that $\|\mathrm{e}^{\mathrm{i}\varepsilon tA} - \mathrm{e}^{\mathrm{i}\varepsilon tA^*}\| \leq C|\varepsilon t|\mathrm{e}^{a\varepsilon|t|}$ since $A - A^*$ is bounded, and the estimates for $G_{2-\sigma}$ in Lemma 5.8, we obtain (5.20). This implies $\|\langle \varepsilon A\rangle^\sigma u\| \leq c\|\langle \varepsilon A^*\rangle^\sigma u\|$ hence by using a similar estimate with A and A^* interchanged and then taking adjoints we obtain:

$$\begin{aligned} &\|\langle \varepsilon A\rangle^\sigma \langle \varepsilon A^*\rangle^{-\sigma}\| \leq C,\ \|\langle \varepsilon A^*\rangle^\sigma \langle \varepsilon A\rangle^{-\sigma}\| \leq C, \\ &\|\langle \varepsilon A\rangle^{-\sigma} \langle \varepsilon A^*\rangle^\sigma\| \leq C,\ \|\langle \varepsilon A^*\rangle^{-\sigma} \langle \varepsilon A\rangle^\sigma\| \leq C, \end{aligned} \tag{5.22}$$

where the number C is independent of ε. The left hand side of (5.21) is

$$\langle \varepsilon A\rangle^{-\sigma}\big(\langle \varepsilon A^*\rangle^\sigma - \langle \varepsilon A\rangle^\sigma\big)\langle \varepsilon A^*\rangle^{-\sigma},$$

and so if we use (5.20) and (5.22) we get (5.21). □

6. Commutator expansions

In this section we prove some results on commutator expansions. These results are well-known in the Hilbert space setting. In the Banach space setting considered here they seem to be new.

6.1. **Functional calculus associated to $\mathcal{A}$.** We now discuss the functional calculus associated to the operator $\mathcal{A}$ acting on $B(\mathcal{H})$ introduced in (5.2). By (5.3) the operator $f(\mathcal{A}) = \int \mathrm{e}^{\mathrm{i}t\mathcal{A}}\widehat{f}(t)dt$ is well defined if $f \in \mathcal{M}_{2\gamma}$ and $f \mapsto f(\mathcal{A})$ is a linear multiplicative map with values in the Banach algebra of bounded operators on $B(\mathcal{H})$ such that

$$\|f(\mathcal{A})\| \leq M^2\|f\|_{\mathcal{M}_{2\gamma}}. \tag{6.1}$$

Let $\mathcal{N}$ be the set of functions whose Fourier transforms are measures supported in $|t| \leq 1$. Then $\mathcal{N}$ is a linear subspace of $\mathcal{M}_{2\gamma}$ which contains the constants, is stable under derivations, and:

$$\|f_s\|_{\mathcal{M}_{2\gamma}} \leq \mathrm{e}^{2\gamma|s|}\|\widehat{f}\|_{L^1(\mathbb{R})},\ s \in \mathbb{R},\ f \in \mathcal{N}. \tag{6.2}$$

Below we use the notation $\widetilde{f}$ introduced in (5.11).

Lemma 6.1. (1) *If $f \in \mathcal{N}$ then*

$$\|f(s\mathcal{A})\| \leq C\mathrm{e}^{2\gamma|s|},\ s \in \mathbb{R}.$$

(2) *If $f, \widetilde{f} \in \mathcal{N}$ and $T \in C^\alpha(A)$ for some $0 < \alpha < 1$ then*

$$\|f(s_2\mathcal{A})T - f(s_1\mathcal{A})T\| \leq C|s_2 - s_1|^\alpha \mathrm{e}^{2\gamma|s_1|} \text{ for } |s_2 - s_1| \leq 1.$$

Proof. (1) follows from (6.1), (6.2). Let us now prove (2). We first claim that if $T \in C^\alpha(A)$ and $g \in \mathcal{N}$ with $g(0) = 0$ then:

$$\|g(s\mathcal{A})T\| \leq C|t|^\alpha \mathrm{e}^{2\gamma|t|},\ t \in \mathbb{R}. \tag{6.3}$$

In fact since $\|\big(\mathrm{e}^{\mathrm{i}t\mathcal{A}} - 1\big)T\| \leq C|t|^\alpha\mathrm{e}^{2\gamma|t|}$ if $T \in C^\alpha$, we have:

$$\|g(s\mathcal{A})T\| = \|g(s\mathcal{A})T - g(0\mathcal{A})T\| = \|\int \big(\mathrm{e}^{\mathrm{i}st\mathcal{A}} - 1\big)T\widehat{g}(t)dt\|$$
$$\leq \int \|\big(\mathrm{e}^{\mathrm{i}st\mathcal{A}} - 1\big)T\||\widehat{g}(t)|dt \leq C\int |st|^\alpha \mathrm{e}^{2\gamma|st|}|\widehat{g}(t)|dt \leq C'|s|^\alpha\mathrm{e}^{2\gamma|s|}.$$

We write now

$$f(s_2\mathcal{A}) - f(s_1\mathcal{A}) = \int_{s_1}^{s_2} \frac{d}{ds}f(s\mathcal{A})ds = \int_{s_1}^{s_2} \mathcal{A}f'(s\mathcal{A})ds = \int_{s_1}^{s_2} \widetilde{f}(s\mathcal{A})\frac{ds}{s}.$$

Since $\widetilde{f} \in \mathcal{N}$ and $\widetilde{f}(0) = 0$ we get $\|\widetilde{f}(s\mathcal{A})T\| \leq C|s|^\alpha\mathrm{e}^{2\gamma|s|}$ by (6.3). So if $0 \leq s_1 < s_2 < s_1 + 1$:

$$\|f(s_2\mathcal{A})T - f(s_1\mathcal{A})T\| \leq \int_{s_1}^{s_2} \|\widetilde{f}(s\mathcal{A})T\|\frac{ds}{s} \leq \int_{s_1}^{s_2} C|s|^\alpha\mathrm{e}^{2\gamma s}\frac{ds}{s}$$
$$\leq \frac{C}{\alpha}\big(s_2^\alpha - s_1^\alpha\big)\mathrm{e}^{2\gamma(s_1+1)} \leq \frac{C}{\alpha}(s_2 - s_1)^\alpha\mathrm{e}^{2\gamma(s_1+1)}.$$

If $s_1 < s_2 \leq 0$ the argument is similar. The case $s_1 < 0 < s_2$ follows from the preceding ones. □

The next lemma will be needed later on.

Lemma 6.2. *Let $\mathcal{B}$ a normed vector space. Let $\xi = \theta\eta$ where $\theta : \mathbb{R} \to \mathcal{B}$ with $\theta(0) = 0$ and $\eta : \mathbb{R} \setminus \{0\} \to \mathbb{C}$ is a function of class C^1. Assume that for some real numbers a, b, β, m, μ satisfying $0 < m < \beta < 1$ and $\mu \geq 3\gamma$ we have:*

$$\|\theta(s_1) - \theta(s_2)\| \leq a|s_1 - s_2|^\beta\mathrm{e}^{2\gamma|s_1|} \quad \text{if } |s_1 - s_2| \leq 1, \tag{6.4}$$

$$|\eta(s)| + |\widetilde{\eta}(s)| \leq b|s|^{-m-1}\mathrm{e}^{-\mu|s|}. \tag{6.5}$$

Then:

$$\int \mathrm{e}^{\gamma|s|}\|\xi(s+t) - \xi(s)\|ds \leq C_{\beta,m}ab|t|^{\beta-m},\ |t| < 1.$$

Proof. It suffices to consider the case $0 < t < 1$. From $\|\xi(s)\| \leq ab|s|^{\beta-m-1}$ and since $\beta - m > 0$ we get:

$$\int_{|s|\leq 2t} \|\xi(s+t) - \xi(s)\| ds \leq 2 \int_{|s|\leq 3t} \|\xi(s)\| ds \leq 2ab(\beta - m)^{-1}(3t)^{\beta-m}.$$

We estimate next $\int_{2t}^{+\infty}$, the integral $\int_{-\infty}^{-2t}$ is treated similarly. Clearly

$$\begin{aligned}
&\int_{2t}^{\infty} \mathrm{e}^{\gamma s} \|\xi(s+t) - \xi(s)\| ds \\
\leq &\int_{2t}^{\infty} \mathrm{e}^{\gamma s} \|\theta(s+t) - \theta(s)\| |\eta(s+t)| ds + \int_{2t}^{\infty} \mathrm{e}^{\gamma s} \|\theta(s)\| |\eta(s+t) - \eta(s)| ds \\
\leq &ab \int_{t}^{\infty} \mathrm{e}^{\gamma s} t^{\beta} \mathrm{e}^{2\gamma s} (s+t)^{-m-1} \mathrm{e}^{-\mu(s+t)} ds + a \int_{2t}^{\infty} \mathrm{e}^{\gamma s} s^{\beta} \mathrm{e}^{2\gamma s} \left| \int_{s}^{s+t} \eta'(y) dy \right| ds.
\end{aligned}$$

The first integral is less than $abm^{-1}t^{\beta-m}$ and the last integral is less than

$$\begin{aligned}
& ab \int_{2t}^{\infty} \int_{s}^{s+t} s^{\beta} \mathrm{e}^{3\gamma s} y^{-m-2} \mathrm{e}^{-\mu y} dy ds \\
\leq \; & ab \int_{2t}^{\infty} s^{\beta-m-2} t ds \leq \tfrac{ab}{1-\beta+m} (2t)^{\beta-m-1} t \\
= \; & C_{\beta,m} abt^{\beta-m}.
\end{aligned}$$

This completes the proof of the lemma. □

In the next lemma we will use Lemma 6.2 for $\mathcal{B} = B(\mathcal{H})$.

Lemma 6.3. *Assume that either $K \in \mathcal{N}$ with $K(0) = 0$ and $\widetilde{K} \in \mathcal{N}$ or that $K(\tau) = 1 - \mathrm{e}^{-\mathrm{i}\tau}$. Let ζ be a complex function in $C^1(\mathbb{R}\backslash\{0\})$ such that $|\zeta(s)| + |\widetilde{\zeta}(s)| \leq C|s|^{-m}\mathrm{e}^{-\mu|x|}$ with $0 < m < 1$ and $\mu > 3\gamma$. Set*

$$\mathcal{J}_{\varepsilon} = \int \mathrm{e}^{\mathrm{i}\varepsilon s \mathcal{A}_r} K(\varepsilon s \mathcal{A}) \zeta(s) \frac{ds}{s} \quad \text{for} \;\; 0 < \varepsilon < 1.$$

Then for $T \in C^{\beta}(A)$ with $m < \beta < 1$ we have $\mathcal{J}_{\varepsilon}(T) \in B(\mathcal{H})$ and

$$\|\mathcal{J}_{\varepsilon}(T)(W(\varepsilon t) - 1)\| \leq C\varepsilon^{\beta}|t|^{\beta-m}, \;\; |t| < 1.$$

In particular $\|\mathcal{J}_{\varepsilon}(T)\langle \varepsilon A \rangle^{s}\| \leq C\varepsilon^{\beta}$ if $s < \beta - m$ and $2\varepsilon\gamma < 1$.

Proof. The function K is such that $K(0) = 0$ and

$$\|K(s_1\mathcal{A})T - K(s_2\mathcal{A})T\| \leq C|s_1 - s_1|^{\beta} \mathrm{e}^{2\gamma|s_1|}$$

if $|s_1 - s_1| < 1$. Indeed, this follows from Lemma 6.1 for the first choice of K and is obvious in the second case. Since $K(0) = 0$ we obviously get $\|K(s\mathcal{A})T\| \leq C|s|^{\beta}\mathrm{e}^{2\gamma|s|}$ for any s. Then

$$\|\mathrm{e}^{\mathrm{i}\varepsilon s A} K(\varepsilon s \mathcal{A})(T) \zeta(s)\| \leq C\varepsilon^{\beta}|s|^{\beta-m} \mathrm{e}^{-|s|(\mu - 3\varepsilon\gamma)},$$

hence the integral defining $\mathcal{J}_{\varepsilon}(T)$ is absolutely convergent in norm and $\|\mathcal{J}_{\varepsilon}(T)\| \leq C\varepsilon^{\beta}$. Then we put $\xi(s) = K(\varepsilon s\mathcal{A})(T)\zeta(s)/s$ and we write

$$\|\mathcal{J}_{\varepsilon}(T)(\mathrm{e}^{-\mathrm{i}\varepsilon t A} - 1)\| = \left\| \int \xi(s) \mathrm{e}^{\mathrm{i}\varepsilon s A} ds (\mathrm{e}^{-\mathrm{i}\varepsilon t A} - 1) \right\| = \left\| \int \big(\xi(s+t) - \xi(s)\big) \mathrm{e}^{\mathrm{i}\varepsilon s A} ds \right\|$$

which is less than $\int \mathrm{e}^{\varepsilon\gamma|s|} \|\xi(s+t) - \xi(s)\| ds$. Now we apply Lemma 6.2 with $\theta(s) = K(\varepsilon s\mathcal{A})(T)$ and $\eta(s) = \zeta(s)/s$. The last assertion follows from Prop. 5.10 by using the estimates $\|\mathcal{J}_{\varepsilon}(T)\| \leq C\varepsilon^{\beta}$ and $\|\mathcal{J}_{\varepsilon}(T)(W(\varepsilon t) - 1)\| \leq C\varepsilon^{\beta}|t|^{\beta-m}$ for $|t| < 1$. □

6.2. **Commutator expansions.** Our proof of Thm. 7.9 is based on the strategy introduced in [Ge] and involves two ingredients: a version of the Putnam argument, cf. Props. 7.3 and 7.6 below, and a commutator expansion estimate, cf. [Ge, Sec. 2], which we discuss in this and next subsections.

More precisely, we are interested in developing the commutator $[S, f(A)]$ in terms of iterated commutators $\mathcal{A}^j(S)$ with estimates on the remainder for "nice" functions $f : \mathbb{R} \to \mathbb{C}$. If A is self-adjoint such results were obtained in [GoJe] using the Helffer-Sjöstrand formula (2.5) (with H replaced by A). If A is the generator of a C_0-group then $f(A)$ cannot be expressed by a relation of the type (2.5) (the imaginary part of the spectrum of A may be too large) but a version of the Dunford functional calculus could certainly be used. On the other hand, the method we use below is quite classical and elementary (a detailed presentation in the case of groups of polynomial growth may be found in [ABG, Sect. 5.5]).

In this section we make some general remarks on commutator expansions. We first discuss the "truncated exponentials" E_k defined for any $k \in \mathbb{N}$ as follows:

$$E_k(\tau) = \frac{1}{(\mathrm{i}\tau)^k}\left(\mathrm{e}^{\mathrm{i}\tau} - \textstyle\sum_{0\leq j<k}(\mathrm{i}\tau)^j/j!\right). \tag{6.6}$$

The following properties are easy to check.

Lemma 6.4.

(1) $E_k(0) = \frac{1}{k!}$,

(2) $E_k(\tau) = \frac{1}{k!} + \mathrm{i}\tau E_{k+1}(\tau)$,

(3) $E_k(\tau) = \int_0^1 \mathrm{e}^{\mathrm{i}\tau\theta}\frac{(1-\theta)^{k-1}}{(k-1)!}d\theta = -\int_0^1 \mathrm{e}^{\mathrm{i}\tau\theta}d\frac{(1-\theta)^k}{k!}$,

(4) $\mathrm{i}E_k' = kE_{k+1} - E_k$,

(5) $\delta E_k = E_{k-1} - kE_k$, *for* $1 \leq k$, *where* $\delta = \tau\partial_\tau$,

(6) $\tau^m\partial_\tau^m E_k = \sum_{n=0}^m C_k^m(n)E_{k-j}$, *for each* $0 \leq m \leq k$, *and* $C_k^m(n) \in \mathbb{N}$,

(7) $\tau^m\partial_\tau^m E_k \in \mathcal{N}$, *for* $m \in \mathbb{N}$..

Proof. For example, (3) is clearly true if $k = 0, 1$ and the function defined by the right hand side of (3) satisfies the induction relation (2), hence (3) holds for any k. To prove (6) observe first that $\tau^m\partial_\tau^m = \sum_{l=1}^m b_\ell^m\delta^\ell$ for some integers b_ℓ^m and then use (5). Since $E_k \in \mathcal{N}$ because of (3), we get (7). □

We write $[S, f(A)] = \big(f(\mathcal{A}_r) - f(\mathcal{A}_\ell)\big)(S)$ and develop the operator $f(\mathcal{A}_r) - f(\mathcal{A}_\ell)$ acting on $B(\mathcal{H})$ in terms of powers of $\mathcal{A} = \mathcal{A}_r - \mathcal{A}_\ell$ by using a Taylor expansion. The class of functions $f : \mathbb{R} \to \mathbb{C}$ for which this makes sense is easy to specify and depends only on the behavior for large t of the group $\mathrm{e}^{\mathrm{i}tA}$, for example f could be the Fourier transform of an exponentially decaying distribution.

Lemma 6.5. *For any integer* $k \geq 1$ *we have*

$$f(\mathcal{A}_r) = \sum_{0\leq j<k} \mathcal{A}^j f^{(j)}(\mathcal{A}_\ell)/j! + \mathcal{A}^k\mathcal{R}_k(f^{(k)}), \tag{6.7}$$

where

$$\mathcal{R}_k(g) = \int \mathrm{e}^{\mathrm{i}t\mathcal{A}_\ell}E_k(t\mathcal{A})\widehat{g}(t)\,dt. \tag{6.8}$$

Proof. We use the notation:

$$\mathcal{A}_0 := \mathcal{A}_\ell, \quad \mathcal{A}_1 := \mathcal{A}_r, \quad \mathcal{A}_\theta := \mathcal{A}_0 + \theta\mathcal{A} = (1-\theta)\mathcal{A}_0 + \theta\mathcal{A}_1.$$

We have the following Taylor formula for $f(\mathcal{A}_1) = f(\mathcal{A}_0 + \mathcal{A})$:

$$f(\mathcal{A}_1) = \sum_{0\le j<k} \frac{\mathcal{A}^j}{j!} f^{(j)}(\mathcal{A}_0) - \frac{\mathcal{A}^k}{k!}\int_0^1 f^{(k)}(\mathcal{A}_\theta)\, d(1-\theta)^k. \tag{6.9}$$

This is easy to prove by induction: if $k = 1$ then

$$f(\mathcal{A}_1) = f(\mathcal{A}_0) + \int_0^1 \frac{d}{d\theta} f(\mathcal{A}_0 + \theta\mathcal{A})d\theta = f(\mathcal{A}_0) + \int_0^1 f'(\mathcal{A}_\theta)\mathcal{A}\, d\theta \tag{6.10}$$

and to pass from the k to the $k+1$ step of the induction process it suffices to integrate by parts the last term in (6.9). If we set $g = f^{(k)}$ we get (6.7) with

$$\mathcal{R}_k(g) = \int_0^1 g(\mathcal{A}_\theta)\frac{(1-\theta)^{k-1}}{(k-1)!}\, d\theta \tag{6.11}$$

From $\mathcal{A}_\theta = \mathcal{A}_0 + \theta\mathcal{A}$ we get

$$g(\mathcal{A}_\theta) = \int \mathrm{e}^{\mathrm{i}t\mathcal{A}_\theta}\widehat{g}(t)\, dt = \int \mathrm{e}^{\mathrm{i}t\mathcal{A}_0}\mathrm{e}^{\mathrm{i}\theta t\mathcal{A}}\widehat{g}(t)\, dt$$

which inserted in (6.11) gives (6.8). This proves the lemma. Another easy proof by induction follows from $\mathcal{R}_k(g) = \frac{1}{k!}g(\mathcal{A}_0) + \mathcal{A}\mathcal{R}_{k+1}(g')$ which is an immediate consequence of the definition (6.8) and of the relation (2) in Lemma 6.4. □

We now explain how to estimate an operator like $\mathcal{R}_k(g)T$ when $T \in B(\mathcal{H})$; in our case $T = \mathcal{A}^k S$ for some bounded operator S of class $C^k(A)$. Observe that $\mathcal{R}_k(g)$ looks like the Fourier transform of the function $t \mapsto E_k(t\mathcal{A})\widehat{g}(t)$ evaluated at the point $\mathcal{A}_\ell$. Hence we expect that decay of $\mathcal{R}_k(g)$ with respect to $\mathcal{A}_\ell$ follows from regularity of the function $t \mapsto E_k(t\mathcal{A})\widehat{g}(t)$. In fact, an integration by parts argument which can easily be justified under convenient conditions on g gives:

$$\begin{aligned}(-\mathrm{i}\mathcal{A}_\ell)^j\mathcal{R}_k(g) &= \int \Big((-\partial_t)^j\mathrm{e}^{\mathrm{i}t\mathcal{A}_\ell}\Big)E_k(t\mathcal{A})\widehat{g}(t)\, dt = \int \mathrm{e}^{\mathrm{i}t\mathcal{A}_\ell}\partial_t^j\Big(E_k(t\mathcal{A})\widehat{g}(t)\Big)\, dt \\ &= \sum_{m=0}^{j} C_m^j \int \mathrm{e}^{\mathrm{i}t\mathcal{A}_\ell}E_k^m(t\mathcal{A})\frac{\widehat{g}^{(j-m)}(t)}{t^m}\, dt\end{aligned}$$

with $E_k^m(\tau) = \tau^m\partial_\tau^m E_k$. We saw before that $E_k^m \in \mathcal{N}$ if $m \le k$ and then $\|E_k^m(t\mathcal{A})\| \le C\mathrm{e}^{2\gamma|t|}$ by Lemma 6.1. The exponential decay of $\widehat{g}^{(j-m)}(t)$ will compensate the divergence of this factor hence there are no problems at infinity if $j \le m$. Only the singularity at 0 of $\widehat{g}^{(j-m)}(t)t^{-m}$ could make the integral divergent.

Our main purpose in the next subsection is to show that $\|\langle A\rangle^s X\langle A\rangle^s\|$ is finite for some $X = \mathcal{R}_k(g)T \in B(\mathcal{H})$ and $0 < s < 1$. For this it suffices to prove that X sends $\mathcal{H}_{-\mu,1}$ into $\mathcal{H}_{\mu,\infty}$ for a number μ with $s < \mu < 1$. If $\mathcal{H}$ is reflexive then this is a consequence of an estimate of the form $\|(\mathrm{e}^{\mathrm{i}xA} - 1)T(\mathrm{e}^{\mathrm{i}yA} - 1)\| \le C|x|^\mu|y|^\mu$ for small x, y. Hence $(\mathrm{e}^{\mathrm{i}x\mathcal{A}_\ell} - 1)(\mathrm{e}^{\mathrm{i}y\mathcal{A}_r} - 1)\mathcal{R}_k(g)$ is the object one has to estimate.

6.3. **First order estimates.** The main results of this subsection concern estimates of the remainders in some commutator expansions of interest later on. We will denote $O(\varepsilon)$ any bounded operator on $\mathcal{H}$ depending on the parameter $\varepsilon > 0$, defined at least for small ε, and such that $\|O(\varepsilon)\| \le C\varepsilon$.

Proposition 6.6. *If $0 < s < \beta < 1$ and $S \in B(\mathcal{H})$ is of class $C^\beta(A)$ then $[\langle\varepsilon A\rangle^{-s}, S] = \langle\varepsilon A\rangle^{-s}O(\varepsilon^\beta)\langle\varepsilon A\rangle^{-s}$.*

Proof. The idea of the proof is very simple at a formal level: we write

$$[\langle\varepsilon A\rangle^{-s}, S] = \langle\varepsilon A\rangle^{-s}[S, \langle\varepsilon A\rangle^s]\langle\varepsilon A\rangle^{-s}$$

and show that $[S, f(\varepsilon A)] = O(\varepsilon^\beta)$ for $f(\tau) = \langle\tau\rangle^s$. In order to justify this formal computation we first take $\varepsilon = 1$ (we assume, without loss of generality, $\gamma < 1/2$) and assume $S \in C^2(A)$, so that S leaves invariant $\mathrm{Dom}A^2$. If $B = \langle A\rangle^{-\sigma}(1 + A^2)$ with $\sigma = 2 - s$ (see Subsect. 5.4) then on $\mathrm{Dom}A^2$ we have:

$$[\langle A\rangle^{-s}, S] = \langle A\rangle^{-s} SB\langle A\rangle^{-s} - \langle A\rangle^{-s} BS\langle A\rangle^{-s} = \langle A\rangle^{-s}[S, B]\langle A\rangle^{-s}.$$

Then by (5.16) we have $[S, B] = \int [S, \mathrm{e}^{\mathrm{i}tA}]\big(G_\sigma(t) - G''_\sigma(t)\big)dt$ on $\mathrm{Dom}A^2$ hence

$$[\langle A\rangle^{-s}, S] = \langle A\rangle^{-s}\left(\int [S, \mathrm{e}^{\mathrm{i}tA}]G_\sigma(t)dt - \int [S, t^{-1}\mathrm{e}^{\mathrm{i}tA}]tG''_\sigma(t)dt\right)\langle A\rangle^{-s}, \tag{6.12}$$

where $G_\sigma(t)$ is the Bessel potential considered in Subsect. 5.3. By Lemma 5.8, $|tG''_\sigma(t)| \leq C|t|^{-s}$ for $t \neq 0$ and $|tG''_\sigma(t)| \leq C|t|^3\mathrm{e}^{-|t|/2}$ for $|t| > 1$.

We observe next that the relation (6.12) remains valid for any bounded operator S of class $C^\beta(A)$. Indeed using

$$[S, \mathrm{e}^{\mathrm{i}tA}] = \mathrm{e}^{\mathrm{i}t\mathcal{A}_\ell}(\mathrm{e}^{\mathrm{i}t\mathcal{A}} - 1)S,$$

and (5.3), we have $\|[S, \mathrm{e}^{\mathrm{i}tA}]\| \leq C\mathrm{e}^{|t|/8}|t|^\beta$ and it is easy to construct a sequence of operators $S_n \in C^2(A)$ satisfying a similar estimate uniformly in n and $\|S_n - S\| \to 0$ as $n \to \infty$. We apply (6.12) to each S_n and then pass to the limit.

Replacing A by εA in (6.12) and using

$$\|[S, t^{-1}\mathrm{e}^{\mathrm{i}t\varepsilon A}]\| \leq C\mathrm{e}^{\varepsilon\gamma|t|}\varepsilon^\beta|t|^{\beta-1},$$

we complete the proof of the proposition. □

We set now

$$\begin{aligned} E(\tau) :=&\quad E_1(\tau) = \tfrac{\mathrm{e}^{\mathrm{i}\tau} - 1}{\mathrm{i}\tau} = \textstyle\int_0^1 \mathrm{e}^{\mathrm{i}\tau t}dt, \\ F(\tau) :=&\quad E(\tau) - 1 = \tfrac{\mathrm{e}^{\mathrm{i}\tau} - 1 - i\tau}{\mathrm{i}\tau}. \end{aligned} \tag{6.13}$$

From Lemma 6.4 we know that $E, F \in \mathcal{N}$. Moreover $\widetilde{F}(\tau) = \tau F'(\tau) = \mathrm{e}^{\mathrm{i}\tau} - E(\tau)$ so $\widetilde{F} \in \mathcal{N}$.

Proposition 6.7. *Let $S \in C^\alpha(A)$ for $\frac{3}{2} < \alpha < 2$ and set $S' = [S, iA]$. Then for any number s such that $1/2 < s < \alpha - 1$ and any function f such that $f'(\tau) = \langle\tau\rangle^{-2s}$ we have*

$$[S, \mathrm{i}f(\varepsilon A)] = \langle\varepsilon A\rangle^{-s}\left(\varepsilon S' + O(\varepsilon^\alpha)\right)\langle\varepsilon A\rangle^{-s}. \tag{6.14}$$

In the usual Hilbert space setup when A is a self-adjoint operator and S is of class $C^2(A)$, this proposition was proved in [Ge, Prop. 2.4] using a general commutator expansion due to Golénia and Jecko [GoJe].

Proof. Since $s > 1/2$ the function f is bounded. We assume, without loss of generality, $6\gamma < 1$ and $0 < \varepsilon \leq 1$. To simplify notations we set $g(\tau) = \langle\tau\rangle^{-s}$ and $f_\varepsilon = f(\varepsilon A)$, $g_\varepsilon = g(\varepsilon A)$. Assume that we have proved that:

$$[S, \mathrm{i}f_\varepsilon] = g_\varepsilon^2\varepsilon S' + g_\varepsilon O(\varepsilon^\alpha)g_\varepsilon. \tag{6.15}$$

If $\beta = \alpha - 1$ then $S' \in C^\beta(A)$ hence from Prop. 6.6 we get $[g_\varepsilon, S'] = g_\varepsilon O(\varepsilon^\beta)g_\varepsilon$. By using $g_\varepsilon^2 S' = g_\varepsilon S' g_\varepsilon + g_\varepsilon[g_\varepsilon, S']$ we then obtain (6.14). Thus it remains to prove (6.15).

As before, we first include ε in A, so we take $\varepsilon = 1$, and then discuss the dependence on ε. Obviously:

$$f(\mathcal{A}_r) - f(\mathcal{A}_\ell) = \int \mathrm{e}^{\mathrm{i}t\mathcal{A}_\ell} \frac{1}{\mathrm{i}t}\big(\mathrm{e}^{\mathrm{i}t\mathcal{A}} - 1\big)\widehat{f}'(t)dt = \int \mathrm{e}^{\mathrm{i}t\mathcal{A}_\ell}\mathcal{A}E(t\mathcal{A})\widehat{f}'(t)dt \tag{6.16}$$

$$= \Big(f'(\mathcal{A}_\ell) + \int \mathrm{e}^{\mathrm{i}t\mathcal{A}_\ell}F(t\mathcal{A})\widehat{f}'(t)dt\Big)\mathcal{A}. \tag{6.17}$$

Thus if S is a bounded operator of class $C^1(A)$ we get the first order commutator expansion with remainder

$$[S, \mathrm{i}f(A)] = f'(A)S' + \mathcal{R}(S') \quad \text{with} \quad \mathcal{R} = \int \mathrm{e}^{\mathrm{i}t\mathcal{A}_\ell}F(t\mathcal{A})\widehat{f}'(t)dt. \tag{6.18}$$

We have $\|\mathrm{e}^{\mathrm{i}t\mathcal{A}_\ell}\| \leq M\mathrm{e}^{\gamma|t|}$ and $\|F(t\mathcal{A})\| \leq C\mathrm{e}^{2\gamma|t|}$ by Lemma 6.1. On the other hand, $\widehat{f}'$ decays like $\mathrm{e}^{-|t|/2}$, so there is no convergence problem at infinity and the integral defining $\mathcal{R}(S')$ is norm convergent. Then

$$[S, \mathrm{i}f(\varepsilon A)] = \varepsilon f'(\varepsilon A)S' + \varepsilon\mathcal{R}^\varepsilon(S') \quad \text{with} \quad \mathcal{R}^\varepsilon = \int \mathrm{e}^{\mathrm{i}\varepsilon t\mathcal{A}_\ell}F(\varepsilon t\mathcal{A})\widehat{f}'(t)dt \tag{6.19}$$

and (6.15) follows if we prove that (recall that $\beta = \alpha - 1 > \frac{1}{2}$):

$$\|\langle \varepsilon A\rangle^s \mathcal{R}^\varepsilon(T)\langle \varepsilon A\rangle^s\| \leq C\varepsilon^\beta,\ T \in C^\beta(A),\ \frac{1}{2} < s < \beta, \tag{6.20}$$

We shall in fact prove a stronger estimate, namely

$$\|(1 - \mathrm{i}\varepsilon A)\mathcal{R}^\varepsilon(T)\langle \varepsilon A\rangle^s\| \leq C\varepsilon^\beta. \tag{6.21}$$

We set $\psi(t) := \widehat{f}'(t) = G_{2s}(t)$ and recall from Lemma 5.7 (4) that since $2s > 1$:

$$\mathrm{e}^{c|t|}\psi', \mathrm{e}^{c|t|}\delta^{(k)}\psi \in L^1(\mathbb{R}),\ 0 \leq c < \frac{1}{2},\ k \in \mathbb{N}. \tag{6.22}$$

Using $\mathcal{A}_\ell = \mathcal{A}_r - \mathcal{A}$ we get:

$$\begin{aligned}(1 - \mathrm{i}\varepsilon\mathcal{A}_\ell)\mathcal{R}^\varepsilon &= \mathcal{R}^\varepsilon - \int \left(\frac{d}{dt}\mathrm{e}^{\mathrm{i}\varepsilon t\mathcal{A}_\ell}\right) F(\varepsilon t\mathcal{A})\psi(t)dt \\ &= \int \mathrm{e}^{\mathrm{i}\varepsilon t\mathcal{A}_\ell}\left(F(\varepsilon t\mathcal{A})\big(t\psi(t)\big) + \widetilde{\psi}(t)\big) + \widetilde{F}(\varepsilon t\mathcal{A})\psi(t)\right)\frac{dt}{t} \\ &= \int \mathrm{e}^{\mathrm{i}\varepsilon t\mathcal{A}_r}\big(F_1(\varepsilon t\mathcal{A})\psi_1(t) + F_2(\varepsilon t\mathcal{A})\psi(t)\big)\frac{dt}{t}\end{aligned}$$

where $F_1(\tau) = \mathrm{e}^{-\mathrm{i}\tau}F(\tau), F_2(\tau) = \mathrm{e}^{-\mathrm{i}\tau}\widetilde{F}(\tau)$, and $\psi_1(t) = \big(t\psi(t) + \widetilde{\psi}(t)\big)$. By taking into account the explicit expressions given in (6.13) for $F, \widetilde{F}$ we obtain $F_1(\tau) = F(-\tau) + (1 - \mathrm{e}^{-\mathrm{i}\tau})$ and $F_2(\tau) = -F(-\tau)$. In order to justify the integration by parts argument we have used the estimates on ψ recalled in (6.22).

Thus we see that $(1 - i\varepsilon\mathcal{A}_\ell)\mathcal{R}^\varepsilon$ is a linear combination of terms of the form $\mathcal{J}_\varepsilon = \int \mathrm{e}^{\mathrm{i}\varepsilon t\mathcal{A}_r}K(\varepsilon t\mathcal{A})\zeta(t)\frac{dt}{t}$ with $K(\tau)$ equal to one of the functions $F(-\tau)$ or $1 - \mathrm{e}^{-\mathrm{i}\tau}$ and $\zeta(t)$ either $\psi(t)$, or $t\psi(t)$, or $\delta\psi(t)$.

In all three cases the function ζ verifies $|\zeta(t)| + |\delta\zeta(t)| \leq C_\mu\mathrm{e}^{-\mu|t|}$ for any $\mu < 1/2$, and $K(\tau)$ satisfies the conditions in Lemma 6.3. We now apply Lemma 6.3 where $m > 0$ may be taken as small as we wish. This proves (6.21) and completes the proof of the proposition. □

7. Boundary values of resolvents

In this section we prove the main result of this paper, described in Thm. 7.9. We show that if H is a self-adjoint operator on a Krein space $\mathcal{K}$, satisfying a positive commutator estimate in the Krein sense on some interval, then weighted resolvent estimates near the real axis (analogous to the well-known Hilbert space case) hold on this interval.

7.1. **Putnam argument and beyond.** To get a better perspective on the positive commutator methods we make some preliminary comments in the context of a theorem due to Putnam, see [P1] or [P2, Thm. 2.2.4]. *In this subsection we assume that $\mathcal{H}$ is a Hilbert space and H is a self-adjoint operator on it.* We denote $\mathbb{1}_J(H)$ the spectral projections of H and set $R(z) = (H - z)^{-1}$.

Putnam discovered that if one may construct a (bounded) self-adjoint operator B such that $[H, \mathrm{i}B] \geq 0$ (in form sense) then H has a rich absolutely continuous spectrum. We recall here his argument [P2, p. 20]. This is the proof of the implication (7.1) $\Rightarrow$ (7.2) below and is very simple but gives only an estimate on the imaginary part of the resolvent $\mathrm{Im}R(z)$ for $z = \lambda + \mathrm{i}\mu, \mu \downarrow 0$. Next we explain how to modify it such as to control the whole resolvent $R(z)$.

Proposition 7.1. *Let $B = B^*$ and C be bounded operators and let us consider the following assertions:*

$$CC^* \leq [H, \mathrm{i}B] \quad \text{as quadratic forms on } \mathrm{Dom}H, \tag{7.1}$$

$$C^*\mathbb{1}_J(H)C \leq \|B\||J| \quad \text{for any Borel set } J, \tag{7.2}$$

$$C^*\big(\mathrm{Im}R(z)\big)C \leq \pi\|B\| \quad \text{for all } z \text{ with } \mathrm{Im}z > 0, \tag{7.3}$$

where $|J|$ is the Lebesgue measure of J. Then we have (7.1) $\Rightarrow$ (7.2)$\Leftrightarrow$ (7.3).

Proof. If J an interval with midpoint λ then

$$\mathbb{1}_J(H)CC^*\mathbb{1}_J(H) \leq \mathbb{1}_J(H)[H - \lambda, \mathrm{i}B]\mathbb{1}_J(H) = 2\mathrm{Re}\,(\mathbb{1}_J(H)(H - \lambda)\mathrm{i}B\mathbb{1}_J(H))$$

hence for any $u \in \mathcal{H}$ we have

$$\begin{aligned}\|C^*\mathbb{1}_J(H)u\|^2 &\leq 2\mathrm{Re}\langle(H - \lambda)\mathbb{1}_J(H)u|\mathrm{i}B\mathbb{1}_J(H))u\rangle \\ &\leq |J|\|\mathbb{1}_J(H)u\|\|B\mathbb{1}_J(H))u\| \leq |J|\|B\|\|\mathbb{1}_J(H)u\|^2.\end{aligned}$$

This is equivalent to

$$\mathbb{1}_J(H)CC^*\mathbb{1}_J(H) \leq \|B\||J|\mathbb{1}_J(H) \leq \|B\||J|,$$

hence $\|C^*\mathbb{1}_J(H)\|^2 \leq \|B\||J|$. Obviously, if (7.2) holds for intervals then it holds for any Borel set. Note also that (7.2) can be stated as $\|\mathbb{1}_J(H)C\| \leq \|B\|^{1/2}|J|^{1/2}$.

Now we prove (7.3) $\Leftrightarrow$ (7.2). If E_u is the measure $E_u(J) = \langle u|\mathbb{1}_J(H)u\rangle$ then

$$\frac{1}{\pi}\mathrm{Im}\langle u|R(\lambda + \mathrm{i}\mu)u\rangle = \frac{1}{\pi}\int \frac{\mu}{(x - \lambda)^2 + \mu^2} dE_u(x).$$

Now clearly $\mathrm{Im}\langle u|R(z)u\rangle \leq \pi M$ holds for all z with $\mathrm{Im}z > 0$ if and only if E_u is an absolutely continuous measure with derivative $E_u'(\lambda) \leq M$ for a.e. λ. □

Remark 7.2. The relation (7.3) says that the imaginary part of the holomorphic function $C^*R(z)C$ in $\mathrm{Im}z > 0$ is bounded, and this is equivalent to the boundedness of the boundary value $C^*\big(\mathrm{Im}R(\lambda + i0)\big)C$. Unfortunately, from the boundedness of the imaginary part of a function holomorphic in the upper half-plane it is not possible to deduce the boundedness of the real part, hence of the function, because the Hilbert transform is not bounded in $L^\infty(\mathbb{R})$. However, if $C^*\big(\mathrm{Im}R(\lambda + i0)\big)C$ is

a Hölder continuous function of λ on a real open set J, then $C^*R(z)C$ extends to a Hölder continuous function on the union of the upper half-plane and J.

We now modify Putnam's argument such as to estimate $C^*R(z)C$ and not only the imaginary part. This is related to the *energy estimate* as presented in [Ge].

Proposition 7.3. *Let $B = B^*$ and C, D be bounded operators with $BC = CD$ and*

$$CC^* \leq [H, \mathrm{i}B] \quad \text{as quadratic forms on } \mathrm{Dom}H. \tag{7.4}$$

Then we have

$$\|C^*R(z)C\| \leq 2(\|B\| + \|D\|) \quad \text{if } \mathrm{Im}z \neq 0. \tag{7.5}$$

A bounded operator D such that $BC = CD$ exists if and only if B leaves the range of C invariant.

Proof. Let $\mathrm{Im}z > 0$ and $b = -\|B\|$ (if $\mathrm{Im}z < 0$ let $b = \|B\|$). Denote $R = R(z)$ and $L = C^*RC$. Then

$$\begin{aligned}
L^*L &= C^*R^*CC^*RC \leq C^*R^*[H, \mathrm{i}B]RC = C^*R^*[H - z, \mathrm{i}(B + b)]RC \\
&= C^*R^*(H - z)\mathrm{i}(B + b)RC - C^*R^*\mathrm{i}(B + b)(H - z)RC \\
&= C^*\mathrm{i}(B + b)RC + C^*R^*(\overline{z} - z)\mathrm{i}(B + b)RC - C^*R^*\mathrm{i}(B + b)C \\
&= 2\mathrm{Im}\big(C^*R^*(B + b)C\big) + C^*R^*(2\mathrm{Im}z)(B + b)RC \\
&= 2\mathrm{Im}\big(C^*R^*C(D + b)\big) + C^*R^*(2\mathrm{Im}z)(B + b)RC.
\end{aligned}$$

Since $(2\mathrm{Im}z)(B + b) \leq 0$ we get with $\alpha = \|L\|/\|D + b\|$:

$$L^*L \leq 2\mathrm{Im}\big(L(D+b)\big) \leq \alpha L^*L + \alpha^{-1}(D+b)^2 \leq \alpha\|L\|^2 + \alpha^{-1}\|D+b\|^2 = 2\|L\|\|D+b\|$$

which is better than (7.5). For the last assertion note that by the closed graph theorem we may take $D = C_0^{-1}BC$ with $C_0 = C|(\mathrm{Ker}\, C)^\perp$, cf. [Do, Thm. 1]. □

Prop. 7.3 and ideas from [Ge] give the following extension of Mourre's theorem [M2].

Theorem 7.4. *Let A be a self-adjoint operator on the Hilbert space $\mathcal{H}$ such that H is of class $C^\alpha(A)$ for some $\alpha > 3/2$ and let I be a real bounded open interval such that*

$$E(I)[H, \mathrm{i}A]E(I) \geq aE(I)$$

for some number $a > 0$. Then for each compact interval $J \subset I$ and each $s > 1/2$ there is a number C such that

$$\|\langle A\rangle^{-s}R(z)\langle A\rangle^{-s}\| \leq C \quad \text{if } \mathrm{Re}z \in J \text{ and } \mathrm{Im}z \neq 0. \tag{7.6}$$

If some $\phi \in C_0^\infty(\mathbb{R})$ with $\phi(\lambda) = \lambda$ near I is fixed, then C depends only on a and on an upper bound for the $C^\alpha(A)$ norm of $\phi(H)$.

We sketch only the main idea of the proof to explain the rôle of Prop. 7.3; details are given in a more general context in Subsect. 7.3. Note that it suffices to prove $\sup_{z\notin\mathbb{R}} \|\langle A\rangle^{-s}R(z)\xi(H)^2\langle A\rangle^{-s}\| \leq C$ if $\xi \in C_0^\infty(I)$ real. Clearly one may replace here A by εA with $\varepsilon > 0$. Let f be a function with $f'(\tau) = \langle\tau\rangle^{-2s}$. Then (7.4) is satisfied by $B = \frac{2}{a\varepsilon}\xi(H)f(\varepsilon A)\xi(H)$ and $C = \xi(H)\langle\varepsilon A\rangle^{-s}$ if ε is small and $1/2 < s < 1$.

Remark 7.5. In [M2] it is assumed that $\alpha = 2$ and $\mathrm{e}^{\mathrm{i}tA}\mathrm{Dom}H = \mathrm{Dom}H$ for all t. The extension from $C^2(A)$ to $C^\alpha(A)$ with $\alpha > 3/2$ is not really significant in applications ($\alpha > 1$ is the natural condition and such an improvement would be practically relevant). We included, however, this generalization because it is rather surprising that the method of [Ge] allows one to pass from the class $C^2(A)$ to the

class $C^\alpha(A)$ with $\alpha > 3/2$ without any change in the strategy of the proof. Indeed, the case $\alpha > 1$ as treated in [ABG] requires a rather substantial modification of the "method of differential inequalities" of Mourre, while here the restriction $\alpha > 3/2$ comes only from the proof of (6.14).

7.2. **Positive commutators in Krein spaces.** We now extend the techniques and results of Subsect. 7.1 to the Krein space setting. We begin with a Putnam type assertion.

Proposition 7.6. *Let H be a self-adjoint operator with $\rho(H) \neq \emptyset$ on the $K-$space $\mathcal{H}$. Let Π be a positive projection which commutes with H and let B, C, D be bounded operators such that*

(1) $B = B^*,\ C = \Pi C$,

(2) $BC = CD$,

(3) $CC^* \leq \Pi[H, \mathrm{i}B]\Pi$ *as quadratic forms on* $\mathrm{Dom}H$.

Then the operator $L(z) = C^*R(z)C$ satisfies

$$\langle L(z)u|L(z)u\rangle \leq c(\|B\| + \|D\|)\|L(z)u\|\|u\| \quad \textit{for}\ \ u \in \mathcal{H},\ z \in \rho(H),$$

where c depends only on H and Π.

Proof. Set $R = R(z)$, $L = L(z)$ and assume that $\mathrm{Im}z \geq 0$ (the proof is similar $\mathrm{Im}z \leq 0$). Note that if $z \in \rho(H)$ then $\overline{z} \in \rho(H)$ and $R^* = (H - \overline{z})^{-1}$. For $b \in \mathbb{R}$ we have:

$$\begin{aligned} R^*[H, \mathrm{i}B]R &= R^*[H - z, \mathrm{i}(B + b)]R = \mathrm{i}(B + b)R - R^*\mathrm{i}(B + b) + (2\mathrm{Im}z)R^*(B + b)R \\ &= 2\mathrm{Im}\big(R^*(B + b)\big) + (2\mathrm{Im}z)R^*(B + b)R. \end{aligned}$$

Since $(B + b)C = C(D + b)$ we get

$$C^*R^*[H, \mathrm{i}B]RC = 2\mathrm{Im}\big(C^*R^*C(D + b)\big) + (2\mathrm{Im}z)C^*R^*(B + b)RC. \tag{7.7}$$

Since $C = \Pi C$ and Π commutes with H we have

$$C^*R^*(B + b)RC = C^*R^*\Pi(B + b)\Pi RC.$$

Using (3.1) we may choose $b = -\|B\|_\Pi$ such that $(2\mathrm{Im}z)C^*R^*(B+b)RC \leq 0$, hence from (7.7) we get:

$$C^*R^*[H, \mathrm{i}B]RC \leq 2\mathrm{Im}\big(L^*(D + b)\big).$$

Now observe that $C^*R^*[H, \mathrm{i}B]RC = C^*R^*\Pi[H, \mathrm{i}B]\Pi RC$ hence from hypothesis (3), we get

$$L^*L = C^*R^*CC^*RC \leq 2\mathrm{Im}\big(L^*(D + b)\big).$$

This yields for $u \in \mathcal{H}$, with a constant m depending only on $\mathcal{H}$:

$$\langle Lu|Lu\rangle \leq 2\mathrm{Im}\langle Lu|(D + b)u\rangle \leq m\|Lu\|\|(D + b)u\| \leq m\|Lu\|(\|D\| + \|B\|_\Pi)\|u\|,$$

using that $b = -\|B\|_\Pi$. Since $\|B\|_\Pi \leq d\|B\|$, for some constant d depending only on Π, this gives the required estimate for $c = \max(m, md)$. □

Remark 7.7. If $\mathcal{H}$ is a Krein space then there is a bounded operator D such that hypothesis (2) in Prop. 7.6 is satisfied if and only if B leaves the range of C invariant, cf. [Do, Thm. 1]. Indeed, since $\mathcal{H}$ is Hilbertizable, we may choose a closed subspace $\mathcal{K}$ in $\mathcal{H}$ such that $\mathcal{H} = \mathrm{Ker}\, C \oplus \mathcal{K}$; then take $D = C_0^{-1}BC$ where $C_0 = C|\mathcal{K}$.

Corollary 7.8. *Let $\mathcal{H}$ be a Krein space and Π a positive projection which commutes with H. Assume that B, C are bounded operators with $B = B^*, C = \Pi C$, and such that B leaves invariant the range of C. If the inequality $\Pi[H, iB]\Pi \geq CC^*$ holds in quadratic form sense on $\mathrm{Dom}H$ and if we set $L(z) = C^*R(z)C$ then $\langle L(z)u|L(z)u\rangle \leq c\|L(z)u\|\|u\|\ \forall u \in \mathcal{H}$, where the number c depends only on Π, B, C.*

7.3. **Boundary value estimates.** We refer to Definition 2.2 for the open real set $\beta(H)$ on which H admits a smooth functional calculus. For example, if H is a definitizable operator on a Krein space then by Proposition 4.15 we have $\beta(H) = \mathbb{R}$.

The following theorem is the main result of our work.

Theorem 7.9. *Let $\mathcal{H}$ be a Krein space and A the generator of a C_0-group on $\mathcal{H}$ such that the Krein structure is of class $C^1(A)$. Let H be a self-adjoint operator on $\mathcal{H}$ and Π a positive projection which commutes with H such that the following conditions are satisfied:*

(1) H is of class $C^\alpha(A)$ for some $\alpha > 3/2$, in particular $H' = [H, \mathrm{i}A]$ is well defined;
(2) there is $\varphi \in C_0^\infty(\beta(H))$ real with $\varphi(\lambda) = 1$ on a neighborhood of a compact interval J such that $\varphi(H)\Pi = \varphi(H)$ and:

$$\varphi(H)(\mathrm{Re}H')\varphi(H) \geq a\varphi(H)^2,\ a > 0. \tag{7.8}$$

Then if $s > 1/2$ and $\varepsilon > 0$ is small enough, we have

$$\sup_{J \pm \mathrm{i}]0,\nu]} \|\langle \varepsilon A\rangle^{-s} R(z) \langle \varepsilon A\rangle^{-s}\| < \infty,\ \text{for some } \nu > 0. \tag{7.9}$$

Even though our framework is much more general than the familiar Hilbertian one, we will adopt the usual terminology and call an estimate like (7.8) a *Mourre estimate*.

Remark 7.10. In applications one often assumes that H admits a Borel functional calculus on an interval $I \supset J$ and that $\Pi = \mathbb{1}_I(H)$. If $\mathbb{1}_I(H) \leq 0$ then the assumption (7.8) should be replaced by

$$\varphi(H)(\mathrm{Re}H')\varphi(H) \leq a\varphi^2(H),\ a > 0.$$

Multiplying the Krein structure by -1 one is then reduced to the situation of the theorem.

Proof. Let I be a neighborhood of J on which $\varphi(\lambda) = 1$. We notice that it suffices to show

$$\sup_{z \notin \mathbb{R}} \|\langle \varepsilon A\rangle^{-s} R(z) \xi(H)^2 \langle \varepsilon A\rangle^{-s}\| < \infty$$

for each real $\xi \in C_0^\infty(I)$. Indeed, if $\mathrm{Re}z \in J$ and we choose ξ such that $0 \leq \xi \leq 1$ and $\xi(\lambda) = 1$ when λ is at distance less then ν of J, then $R(z) = R(z)\xi(H)^2 + R(z)(1 - \xi(H)^2)$ and $\|R(z)(1 - \xi(H)^2)\| \leq \nu^{-k}$ for some finite number k.

Clearly we may assume $s < \beta = \alpha - 1 < 1$. We shall use the notations introduced in the proof of Prop. 6.7: $g(\tau) = \langle \tau\rangle^{-s}$, f is a function such that $f' = g^2$, and $g_\varepsilon = g(\varepsilon A), f_\varepsilon = f(\varepsilon A)$. Note that f_ε is a bounded operator by Prop. 5.9. For Greek letters ξ, η, etc, we often adopt the abbreviations $\eta \equiv \eta(H), \xi = \xi(H)$, etc.

If $X_\varepsilon, Y_\varepsilon$ are bounded operators defined for small ε we write $X_\varepsilon \sim Y_\varepsilon$ if $X_\varepsilon - Y_\varepsilon = g_\varepsilon O(\varepsilon^\beta) g_\varepsilon^*$ and $X_\varepsilon \prec Y_\varepsilon$ if $X_\varepsilon - Y_\varepsilon \leq g_\varepsilon O(\varepsilon^\beta) g_\varepsilon^*$. For example, Prop. 5.15 gives $g_\varepsilon \sim g_\varepsilon^*$ and from Prop. 6.6 we obtain $\xi g_\varepsilon \sim g_\varepsilon \xi$ if $\xi \in C_0^\infty(\beta(S))$.

Fix $\phi \in C_0^\infty(\mathbb{R})$ real such that $\phi(\lambda) = 1$ on a neighborhood of the support of φ and set $S = \phi(H)$. Then S is a bounded symmetric operator of class $C^\alpha(A)$ and we

have $\eta S'\eta = \eta H'\eta$ for all $\eta \in C_0^\infty(I)$. From Prop. 6.7 we get $[S, \mathrm{i}\varepsilon^{-1} f_\varepsilon] \sim g_\varepsilon S' g_\varepsilon^*$, hence if we denote $F_\varepsilon = \varepsilon^{-1}\mathrm{Re} f_\varepsilon$ we obtain:

$$[S, \mathrm{i}F_\varepsilon] \sim g_\varepsilon(\mathrm{Re}S')g_\varepsilon^*.$$

Then if $\eta \in C_0^\infty(I)$ we get:

$$\begin{aligned}[S, \mathrm{i}\eta F_\varepsilon \eta] &\sim \eta g_\varepsilon(\mathrm{Re}S')g_\varepsilon^*\eta \sim g_\varepsilon\eta(\mathrm{Re}S')\eta g_\varepsilon^* \\ &= g_\varepsilon\eta(\mathrm{Re}H')\eta g_\varepsilon^* \succ a g_\varepsilon\eta^2 g_\varepsilon^* \sim a\eta g_\varepsilon g_\varepsilon^*\eta.\end{aligned}$$

If η is chosen such that $\xi\eta = \xi$ then we get finally

$$[S, \mathrm{i}\xi F_\varepsilon \xi] \geq \frac{a}{2}\xi g_\varepsilon g_\varepsilon^* \xi$$

for ε small enough.

In Prop. 7.6 we take $B = \xi F_\varepsilon \xi$ and $C = \xi g_\varepsilon$. Observe that $\xi\Pi = \xi\varphi\Pi = \xi\varphi = \xi$ hence, by taking adjoints, $\Pi\xi = \xi\Pi = \xi$. To find D we note that $BC = CD$ means $\xi F_\varepsilon \xi^2 g_\varepsilon = \xi g_\varepsilon D$ hence follows from $F_\varepsilon\xi^2 g_\varepsilon = g_\varepsilon D$ so it suffices to take $D = g_\varepsilon^{-1} F_\varepsilon \xi^2 g_\varepsilon$. This is a bounded operator because ξ is of class $C^1(A)$ and $0 < s < 1$, so $F_\varepsilon\xi^2$ leaves invariant the range of g_ε. Now we apply Prop. 7.6 and obtain

$$\begin{aligned}\langle L_\varepsilon u | L_\varepsilon u\rangle \leq\ & K(\|B_\varepsilon\| + \|D_\varepsilon\|)\|L_\varepsilon u\|\|u\| \\ \leq\ & \delta\|L_\varepsilon u\|^2 + (4\delta)^{-1}(\|B_\varepsilon\| + \|D_\varepsilon\|)^2\|u\|^2,\ u \in \mathcal{H},\end{aligned}$$

for some $\delta > 0$, where we have indicated the dependence in ε for clarity, in particular $L_\varepsilon = g_\varepsilon^*\xi^2 R g_\varepsilon$. We write this as

$$\langle L_\varepsilon u | L_\varepsilon u\rangle \leq \delta\|L_\varepsilon u\|^2 + c\|u\|^2,$$

where $c = c(\delta, \varepsilon)$. With the notation $\eta_\perp = 1 - \eta$ we have $\xi\eta_\perp = 0$ hence

$$\eta_\perp L_\varepsilon = \eta_\perp g_\varepsilon^*\xi^2 R g_\varepsilon = [g_\varepsilon^*, \eta]\xi^2 R g_\varepsilon = g_\varepsilon^* O(\varepsilon) g_\varepsilon^* \xi^2 R g_\varepsilon = O(\varepsilon)L_\varepsilon.$$

Thus we have $\eta L_\varepsilon = L_\varepsilon - \eta^\perp L_\varepsilon = L_\varepsilon + O(\varepsilon)L_\varepsilon$. Since the projection Π is positive, there is a constant N such that $N^{-1}\|v\|^2 \leq \langle v|v\rangle$ for $v \in \Pi\mathcal{H}$. Thus from $\eta = \Pi\eta$ we get:

$$\begin{aligned}N^{-1}\|\eta L_\varepsilon u\|^2 &\leq \langle \eta L_\varepsilon u | \eta L_\varepsilon u\rangle = \langle L_\varepsilon u + O(\varepsilon)L_\varepsilon u | L_\varepsilon u + O(\varepsilon)L_\varepsilon u\rangle \\ &\leq \langle L_\varepsilon u | L_\varepsilon u\rangle + O(\varepsilon)\|L_\varepsilon u\|^2 \leq (\delta + O(\varepsilon))\|L_\varepsilon u\|^2 + c(\delta, \varepsilon)\|u\|^2.\end{aligned}$$

But $L_\varepsilon = \eta L_\varepsilon + O(\varepsilon)L_\varepsilon$ hence $(1 - O(\varepsilon))\|L_\varepsilon u\| \leq \|\eta L_\varepsilon u\|$. Inserting this above we get for ε small enough the estimate

$$\|L_\varepsilon u\|^2 \leq 2N(\delta + O(\varepsilon))\|L_\varepsilon u\|^2 + 2Nc(\delta, \varepsilon)\|u\|^2.$$

Finally, taking both δ and ε small we obtain $\|L_\varepsilon u\| \leq C\|u\|$ for some constant C. Thus $\|g_\varepsilon^*\xi^2 R g_\varepsilon u\| \leq C\|u\|$ and (5.22) gives $\|g_\varepsilon\xi^2 R g_\varepsilon u\| \leq C\|u\|$. □

Remark 7.11. We were forced to ask $\mathcal{H}$ to be a Krein space, and not an arbitrary $K-$space, only because of hilbertizability assumption in Prop. 5.9.

7.4. **Virial theorem.** In order to check the positive commutator estimate (7.8), one needs to extend to K-spaces some facts related to the *virial theorem*. We do this in this subsection. Let H be a self-adjoint operator in a $K-$space with a not empty resolvent set. *In all this subsection we fix an open real set I on which H admits a C^0-functional calculus.*

Then, as shown in Thm. 2.4, the calculus extends to a bounded Borel functional calculus on I, so $\varphi(H)$ is well defined if φ is a bounded Borel function on I.

Lemma 7.12. *If $\lambda \in I$ then $\mathbb{1}_{\{\lambda\}}(H)$ is the orthogonal projection onto* $\mathrm{Ker}\,(H - \lambda)$.

Proof. $\mathbb{1}_{\{\lambda\}}(H)$ is a projection because $\mathbb{1}^2_{\{\lambda\}} = \mathbb{1}_{\{\lambda\}}$. Recall that r_z for $z \in \rho(H)$ is the function $r_z(x) = (x-z)^{-1}$. Then $r_z(H) = R(z)$ and clearly $\mathrm{Ker}\,(H-\lambda)$ is exactly the set of vectors $u \in \mathcal{H}$ such that $r_z(H)u = r_z(\lambda)u$. Since the Borel functional calculus is multiplicative we have

$$r_z(H)\mathbb{1}_{\{\lambda\}}(H) = \mathbb{1}_{\{\lambda\}}(H)r_z(H) = (\mathbb{1}_{\{\lambda\}}r_z)(H) = (\mathbb{1}_{\{\lambda\}}r_z(\lambda))(H) = r_z(\lambda)\mathbb{1}_{\{\lambda\}}(H).$$

Thus $\mathbb{1}_{\{\lambda\}}(H)\mathcal{H} \subset \mathrm{Ker}\,(H-\lambda)$. Reciprocally, if $u \in \mathrm{Ker}\,(H-\lambda)$ then $r_z(H)u = r_z(\lambda)u$ hence $\varphi(H)u = \varphi(\lambda)u$ for any rational function with poles only in the resolvent set of H. From (2.4) for example, we then get $\varphi(H)u = \varphi(\lambda)u$ for any $\varphi \in C^\infty_0(I)$, and finally by taking limits we get it for any bounded Borel function on I. In particular $\mathbb{1}_{\{\lambda\}}(H)u = u$. □

Now let A be the generator of a C^0-group such that H is of class $C^1(A)$. If we interpret $H' = [H, iA]$ as a sesquilinear form on $\mathrm{Dom}H$, then we have the following *virial theorem*.

Lemma 7.13. *For any $\lambda \in I$ we have $\mathbb{1}_{\{\lambda\}}(H)H'\mathbb{1}_{\{\lambda\}}(H) = 0$.*

Proof. Let $z \in \rho(H)$ and $R = (z-H)^{-1}$. Then $R' \equiv [R, \mathrm{i}A] = RH'R$ and for any bounded Borel φ with support in I we get $\varphi(H)H'\varphi(H) = \varphi_z(H)R'\varphi_z(H)$ with $\varphi_z(x) = \varphi(x)(z-x)$. Thus we have:

$$\mathbb{1}_{\{\lambda\}}(H)H'\mathbb{1}_{\{\lambda\}}(H) = (z-\lambda)^2\mathbb{1}_{\{\lambda\}}(H)R'\mathbb{1}_{\{\lambda\}}(H) = (z-\lambda)^2 \lim_{\tau\to 0} \mathbb{1}_{\{\lambda\}}(H)[R, A_\tau]\mathbb{1}_{\{\lambda\}}(H)$$

where $A_\tau = (\mathrm{e}^{\mathrm{i}\tau A} - 1)/\tau$. Since

$$\begin{aligned} &\mathbb{1}_{\{\lambda\}}(H)[R, A_\tau]\mathbb{1}_{\{\lambda\}}(H) = \mathbb{1}_{\{\lambda\}}(H)RA_\tau\mathbb{1}_{\{\lambda\}}(H) - \mathbb{1}_{\{\lambda\}}(H)A_\tau R\mathbb{1}_{\{\lambda\}}(H) \\ = \;& \mathbb{1}_{\{\lambda\}}(H)(z-\lambda)A_\tau\mathbb{1}_{\{\lambda\}}(H) - \mathbb{1}_{\{\lambda\}}(H)A_\tau(z-\lambda)\mathbb{1}_{\{\lambda\}}(H) = 0, \end{aligned}$$

we get the required result. □

Corollary 7.14. *Let H be a self-adjoint operator on the Krein space $\mathcal{H}$ and let $I \subset \beta(H)$. Assume that for some $J \subset I$ we have $\mathbb{1}_J(H) \geq 0$ and that there is a number $a > 0$ and a compact operator K such that*

$$\mathbb{1}_J(H)H'\mathbb{1}_J(H) \geq a\mathbb{1}_J(H) + K.$$

Then the point spectrum of H in J is finite and consists of eigenvalues of finite multiplicity. Moreover, if $\lambda \in J$ is not an eigenvalue of H and $b < a$ then there is a compact neighborhood I of λ in J such that

$$\mathbb{1}_I(H)H'\mathbb{1}_I(H) \geq b\mathbb{1}_I(H).$$

Proof. The range of $\mathbb{1}_J(H)$ is a Hilbert space (for the induced Krein structure) stable under H, so the usual proof (see e.g. [M2]) applies. □

We shall need one more technical fact for applications in Section 8. We write $S \simeq T$ if S, T are operators and $S - T$ is compact. Recall that $C^\alpha(A) \subset C^1_{\mathrm{u}}(A)$ for $\alpha > 1$.

Lemma 7.15. *Assume $H \in C^1_{\mathrm{u}}(A)$. Let H_0 be a second operator (not necessarily self-adjoint) of class $C^1_{\mathrm{u}}(A)$ such that $(H-z)^{-1} \simeq (H_0-z)^{-1}$ for some $z \in \rho(H) \cap \rho(H_0)$. If H_0 admits a smooth functional calculus on J then for any $\varphi \in C^\infty_0(J)$ we have $\varphi(H)H'\varphi(H) \simeq \varphi(H_0)H_0'\varphi(H_0)$.*

Proof. Let $R = (z-H)^{-1}, R_0 = (z-H_0)^{-1}$, and φ_z as above. Then

$$\varphi(H)H'\varphi(H) - \varphi(H_0)H_0'\varphi(H_0) = \varphi_z(H)R'\varphi_z(H) - \varphi_z(H_0)R_0'\varphi_z(H_0).$$

The operator $R' - R_0'$ is compact as norm limit of compact operators, using that $H, H_0 \in C^1_{\mathrm{u}}(A)$, and $\varphi_z(H) - \varphi_z(H_0)$ is compact by a standard argument. □

8. Klein-Gordon operators

In this section we discuss various Krein spaces and operators on them associated to the following *abstract Klein-Gordon equation*:

$$\partial_t^2\phi(t) - 2\mathrm{i}k\partial_t\phi(t) + h\phi(t) = 0, \tag{8.1}$$

where $\phi : \mathbb{R} \to \mathcal{H}$, $\mathcal{H}$ is a Hilbert space and h, k are self-adjoint, resp. symmetric operators on $\mathcal{H}$.

We first introduce an abstract setting which allows one to treat in a unified way the *charge* and *energy* versions of the Klein-Gordon operators. We then study in details the functional calculus of the *free* Klein-Gordon operators, which corresponds to the case $k = 0$ in (8.1). Finally we introduce some abstract conditions under which a Mourre estimate can be shown for the charge Klein-Gordon operator. This section is somewhat complementary to our paper [GGH1], where resolvent estimates for energy Klein-Gordon operators are obtained, although the method to obtain a Mourre estimate is quite different.

8.1. **Notations.** We need some new notations and terminology.

Linear operators

We write $f : X \tilde{\to} Y$ if X, Y are sets and $f : X \to Y$ is bijective. If X, Y, Z are Banach spaces with $X \subset Y \subset Z$ continuously and densely then to each continuous operator $S : X \to Z$ we associate a densely defined operator $\widehat{S}$ acting in Y, namely the restriction of S to the domain $\mathrm{Dom}\widehat{S} = S^{-1}(Y)$. We say that $\widehat{S}$ is the operator induced by S in Y and use the same notation for S and $\widehat{S}$ unless this abuse of notations leads to confusions.

Scale of Sobolev spaces

Let $\mathcal{H}$ be a Hilbert space with norm $\|\cdot\|$ and scalar product $(\cdot|\cdot)$. We identify $\mathcal{H}$ with its adjoint space $\mathcal{H}^* = \mathcal{H}$ via the Riesz isomorphism. Let h be a selfadjoint operator on $\mathcal{H}$.

We can associate to it the *non-homogeneous Sobolev spaces*

$$\langle h\rangle^{-s}\mathcal{H} := \mathrm{Dom}|h|^s,\ \langle h\rangle^{s}\mathcal{H} := (\langle h\rangle^{-s}\mathcal{H})^*,\ s \geq 0.$$

The spaces $\langle h\rangle^{-s}\mathcal{H}$ are equipped with the graph norm $\|\langle h\rangle^s u\|$. We will use the notation

$$(u|v),\ u \in \langle h\rangle^{-s}\mathcal{H},\ v \in \langle h\rangle^{s}\mathcal{H},\ s \geq 0,$$

to denote the duality bracket between $\langle h\rangle^{-s}\mathcal{H}$ and $\langle h\rangle^{s}\mathcal{H}$.

8.2. **Quadratic pencils.** We fix a Hilbert space $\mathcal{H}$ with $\mathcal{H}^* = \mathcal{H}$ and consider two operators h, k such that:

$$\text{(A1)}\quad \begin{cases} h \text{ is self-adjoint on } \mathcal{H}, \\ k \in B(\langle h\rangle^{-\frac{1}{2}}\mathcal{H}, \mathcal{H}) \text{ is symmetric.} \end{cases}$$

The unique continuous extension of $k : \mathcal{H} \to \langle h\rangle^{\frac{1}{2}}\mathcal{H}$ will still be denoted by k.

We set also:

$$\begin{aligned} &h_0 := h + k^2 : \langle h\rangle^{-\frac{1}{2}}\mathcal{H} \to \langle h\rangle^{\frac{1}{2}}\mathcal{H}, \\ &p(z) = h + z(2k - z) = h_0 - (k - z)^2 : \langle h\rangle^{-\frac{1}{2}}\mathcal{H} \to \langle h\rangle^{\frac{1}{2}}\mathcal{H} \text{ for } z \in \mathbb{C}. \end{aligned}$$

The map $z \mapsto p(z)$ is called a *quadratic pencil*.

Note that formally $\phi(t) = \mathrm{e}^{\mathrm{i}zt}\phi$ solves the Klein-Gordon equation (8.1) iff $p(z)\phi = 0$.

Obviously $p(z)$ is also a well defined operator in $B(\langle h\rangle^{-1}\mathcal{H},\mathcal{H})$ and $B(\mathcal{H},\langle h\rangle\mathcal{H})$. Moreover, *the domain in $\mathcal{H}$ of the operator $p(z):\langle h\rangle^{-\frac12}\mathcal{H}\to\langle h\rangle^{\frac12}\mathcal{H}$ is precisely $\langle h\rangle^{-1}\mathcal{H}$, i.e. $\langle h\rangle^{-1}\mathcal{H}=p(z)^{-1}\mathcal{H}$.* Indeed, for $u\in\langle h\rangle^{-\frac12}\mathcal{H}$ we have $p(z)u=hu+z(2k-z)u$ and the last term belongs to $\mathcal{H}$, hence $p(z)u\in\mathcal{H}$ if and only if $hu\in\mathcal{H}$.

Clearly $p(z)^*=p(\overline{z})$ in $B(\langle h\rangle^{-\frac12}\mathcal{H},\langle h\rangle^{\frac12}\mathcal{H})$. We shall prove below that this relation also holds for the operators in $\mathcal{H}$ induced by $p(z)$ and $p(\overline{z})$.

Lemma 8.1. *Assume (A1). Then the operator induced by $p(z)$ in $\mathcal{H}$ is a closed operator and its Hilbert space adjoint is the operator induced by $p(\overline{z})$ in $\mathcal{H}$. In other terms, the relation $p(z)^*=p(\overline{z})$ also holds in the sense of closed operators in $\mathcal{H}$. The following six conditions are equivalent:*

(1) $p(z):\langle h\rangle^{-1}\mathcal{H}\tilde{\to}\mathcal{H}$; *(2)* $p(\overline{z}):\langle h\rangle^{-1}\mathcal{H}\tilde{\to}\mathcal{H}$;
(3) $p(z):\mathcal{H}\tilde{\to}\langle h\rangle\mathcal{H}$; *(4)* $p(\overline{z}):\mathcal{H}\tilde{\to}\langle h\rangle\mathcal{H}$;
(5) $p(z):\langle h\rangle^{-\frac12}\mathcal{H}\to\langle h\rangle^{\frac12}\mathcal{H}$; *(6)* $p(\overline{z}):\langle h\rangle^{-\frac12}\mathcal{H}\to\langle h\rangle^{\frac12}\mathcal{H}$.

In particular, the set

$$\rho(h,k):=\{z\in\mathbb{C}\mid p(z):\langle h\rangle^{-\frac12}\mathcal{H}\tilde{\to}\langle h\rangle^{\frac12}\mathcal{H}\}=\{z\in\mathbb{C}\mid p(z):\langle h\rangle^{-1}\mathcal{H}\tilde{\to}\mathcal{H}\}\tag{8.2}$$

is invariant under conjugation.

Proof. If we set $\ell=\zeta(2k-\zeta)\in B(\langle h\rangle^{-\frac12}\mathcal{H},\mathcal{H})$ then $\ell:\langle h\rangle^{-\frac12}\mathcal{H}\to\mathcal{H}$ and its adjoint in $\mathcal{H}$ satisfies $\ell^*\supset\overline{\zeta}(2k-\overline{\zeta})\in B(\langle h\rangle^{-\frac12}\mathcal{H},\mathcal{H})$. In particular, ℓ and ℓ^* are h-bounded with relative bound zero, hence there is a real number n such that $\|\ell(h+\mathrm{i}n)^{-1}\|<1$ and $\|\ell^*(h-\mathrm{i}n)^{-1}\|<1$. From $h+\ell+\mathrm{i}n=\big(1+\ell(h+\mathrm{i}n)^{-1}\big)(h+\mathrm{i}n)$ it follows that $h+\ell+\mathrm{i}n:\mathcal{H}^1\tilde{\to}\mathcal{H}$ from which we get that $(h+\ell+\mathrm{i}n)^*$ is a bijection from its domain onto $\mathcal{H}$, see e.g. [We, Thms. 4.17, 5.12].

Clearly $(h+\ell+\mathrm{i}n)^*\supset h+\ell^*-\mathrm{i}n$, and an argument similar to that already used implies $h+\ell^*-\mathrm{i}n:\langle h\rangle^{-1}\mathcal{H}\tilde{\to}\mathcal{H}$. Thus $(h+\ell)^*=h+\ell^*$ which means $p(\zeta)^*=p(\overline{\zeta})$.

Now the equivalence $p(\zeta):\langle h\rangle^{-1}\mathcal{H}\tilde{\to}\mathcal{H}\Leftrightarrow p(\overline{\zeta}):\langle h\rangle^{-1}\mathcal{H}\tilde{\to}\mathcal{H}$ is immediate (see again [We]). If these relations hold, then $p(\zeta):\mathcal{H}\tilde{\to}\langle h\rangle^1\mathcal{H}$ because this operator is the adjoint of $p(\overline{\zeta}):\langle h\rangle^{-1}\mathcal{H}\tilde{\to}\mathcal{H}$, and then by interpolation we obtain $p(\zeta):\langle h\rangle^{-\frac12}\mathcal{H}\tilde{\to}\langle h\rangle^{\frac12}\mathcal{H}$ hence $p(\overline{\zeta}):\langle h\rangle^{-\frac12}\mathcal{H}\tilde{\to}\langle h\rangle^{\frac12}\mathcal{H}$. Reciprocally, if $p(\zeta):\langle h\rangle^{-\frac12}\mathcal{H}\tilde{\to}\langle h\rangle^{\frac12}\mathcal{H}$ then $p(\zeta):\langle h\rangle^{-1}\mathcal{H}\tilde{\to}\mathcal{H}$ because the domain of the operator in $\mathcal{H}$ associated to $p(\zeta):\langle h\rangle^{-\frac12}\mathcal{H}\to\langle h\rangle^{\frac12}\mathcal{H}$ is $\langle h\rangle^{-1}\mathcal{H}$. □

In the sequel we will assume

(A2) $\quad\rho(h,k)\neq\emptyset$.

Let us state an easy lemma which allows to check (A2).

Lemma 8.2. *If (A1) holds and h is bounded below, then there is $c_0>0$ such that*

$$\{z\ :|\mathrm{Im}z|>|\mathrm{Re}z|+c_0\}\subset\rho(h,k).$$

Proof. Consider $p(z)$ as a linear operator on $\mathcal{H}$ with domain $\langle h\rangle^{-1}\mathcal{H}$. Let c be such that $h+c^2\geq1$ and $\delta=\|k(h+c^2)^{-\frac12}\|$. For $z=a+\mathrm{i}b$, $\alpha>0$:

$$\begin{aligned}\mathrm{Re}p(z)=&\ h+b^2-a^2+2ka\\ \geq&\ h+c^2+b^2-a^2-c^2-\alpha a^2-\alpha^{-1}k^2\\ \geq&\ (1-\alpha^{-1}\delta^2)(h+c^2)+b^2-a^2-c^2-\alpha a^2\end{aligned}$$

For $\alpha=\delta^2$ this yields

$$\mathrm{Re}p(z)\geq b^2-(1+\delta^2)a^2-c^2\geq c_1>0,$$

if $|b| > |a| + c_0$ for $c_0 > 0$. If we set $p := p(z)$ then for all $u \in \langle h\rangle^{-1}\mathcal{H}$ we shall have $c_1\|u\|^2 \leq \mathrm{Re}(u|pu) \leq \|u\|\|pu\|$ hence $c_1\|u\| \leq \|pu\|$ and similarly $c_1\|u\| \leq \|p^*u\|$. Since p is closed this implies $p : \langle h\rangle^{-1}\mathcal{H} \tilde{\to} \mathcal{H}$. □

8.3. **Spaces.** The following two spaces play a fundamental role in what follows:

$$\mathcal{E} := \langle h\rangle^{-\frac{1}{2}}\mathcal{H} \oplus \mathcal{H} \quad \text{and} \quad \mathcal{E}^* := \mathcal{H} \oplus \langle h\rangle^{\frac{1}{2}}\mathcal{H}. \tag{8.3}$$

One often calls $\mathcal{E}$ the *energy space*. Observe that $\mathcal{E} \subset \mathcal{E}^*$. As decided in Subsect. 2.1, the space $\mathcal{E}^*$ is identified with the adjoint space of $\mathcal{E}$ with the help of the sesquilinear form:

$$\langle u|v\rangle = (u_0|v_1) + (u_1|v_0), \quad \text{for } u = \left(\begin{smallmatrix} u_0 \\ u_1 \end{smallmatrix}\right) \in \mathcal{E},\ v = \left(\begin{smallmatrix} v_0 \\ v_1 \end{smallmatrix}\right) \in \mathcal{E}^*, \tag{8.4}$$

usually called the *charge*.

We identify $\mathcal{E}^{**} = \mathcal{E}$ as in the Hilbert space case by setting $\langle v|u\rangle = \overline{\langle u|v\rangle}$. This allows us to speak about symmetric or positive operators $S : \mathcal{E} \to \mathcal{E}^*$.

Observe that we have dense and continuous embeddings $\mathcal{E} \subset \mathcal{H} \oplus \mathcal{H} \subset \mathcal{E}^*$ and the identification of $\mathcal{E}^*$ with the adjoint of $\mathcal{E}$ is determined by the Krein structure of $\mathcal{H} \oplus \mathcal{H}$ exactly as in the case of Friedrichs couples in the category of Hilbert spaces. Note however that $\mathcal{H} \oplus \mathcal{H}$ is not an interpolation space between $\mathcal{E}$ and $\mathcal{E}^*$ if $\mathcal{H}$ is infinite dimensional (see below). In any case, by complex interpolation we get for any $0 \leq \sigma \leq 1$:

$$[\mathcal{E}, \mathcal{E}^*]_\sigma = \langle h\rangle^{(\sigma-1)/2}\mathcal{H} \oplus \langle h\rangle^{\sigma/2}\mathcal{H}, \tag{8.5}$$

so we cannot obtain $\mathcal{H} \oplus \mathcal{H}$ in this way. We define the *charge space of order* θ for $0 \leq \theta \leq 1/2$ by

$$\mathcal{K}_\theta = \langle h\rangle^{-\theta}\mathcal{H} \oplus \langle h\rangle^{\theta}\mathcal{H}. \tag{8.6}$$

Then $\mathcal{E} \subset \mathcal{K}_\theta \subset \mathcal{E}^*$ strictly and two such spaces are not comparable (if $\mathcal{H}$ is infinite dimensional, which is implicitly assumed in all this work). Observe that the middle space defined by complex interpolation

$$[\mathcal{E}, \mathcal{E}^*]_{1/2} = \langle h\rangle^{-1/4}\mathcal{H} \oplus \langle h\rangle^{1/4}\mathcal{H} \tag{8.7}$$

equals $\mathcal{K}_{1/4}$ and we shall see that it plays a remarkable role in the theory. If $\theta \neq 1/4$ then $\mathcal{K}_\theta$ is not an interpolation space between $\mathcal{E}$ and $\mathcal{E}^*$: in Remark 8.14 we give examples of bounded operators on $\mathcal{E}^*$ which leave $\mathcal{E}$ invariant but not $\mathcal{K}_\theta$ if $\theta \neq 1/4$.

Since $(\langle h\rangle^{-\theta}\mathcal{H})^* = \langle h\rangle^{\theta}\mathcal{H}$, the spaces $(\mathcal{K}_\theta, \langle\cdot|\cdot\rangle)$ are examples of Krein spaces as in Subsect. 3.4.

Below, when we speak of self-adjointness of operators in $\mathcal{K}_\theta$, we refer to this Krein structure.

Since $\mathcal{E} \subset \mathcal{E}^*$, the sesquilinear form $\langle\cdot|\cdot\rangle$ restricts to a hermitian form on $\mathcal{E}$. Note however that $(\mathcal{E}, \langle\cdot|\cdot\rangle)$ is *not* a Krein space, since $\langle\cdot|\cdot\rangle$ is not non-degenerate on $\mathcal{E}$.

8.4. **Operators.** It is easy to extend the relations from Subsect. 3.4 to the present setting. For example, since we think of elements of $\mathcal{E}$ as column matrices, we may represent operators $\mathcal{E} \to \mathcal{E}^*$ as matrices of operators:

$$S = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \text{ with } \begin{cases} a \in B(\langle h\rangle^{-\frac{1}{2}}\mathcal{H}, \mathcal{H}),\ b \in B(\mathcal{H}), \\ c \in B(\langle h\rangle^{-\frac{1}{2}}\mathcal{H}, \langle h\rangle^{\frac{1}{2}}\mathcal{H}),\ d \in B(\mathcal{H}, \langle h\rangle^{\frac{1}{2}}\mathcal{H}). \end{cases}$$

A computation gives $S^* = \left(\begin{smallmatrix} d^* & b^* \\ c^* & a^* \end{smallmatrix}\right)$ hence S is symmetric if and only if

$$S = \begin{pmatrix} a & b \\ c & a^* \end{pmatrix} \text{ with } \begin{cases} a \in B(\langle h\rangle^{-\frac{1}{2}}\mathcal{H}, \mathcal{H}),\ b = b^* \in B(\mathcal{H}), \\ c = c^* \in B(\langle h\rangle^{-\frac{1}{2}}\mathcal{H}, \langle h\rangle^{\frac{1}{2}}\mathcal{H}),\ d \in B(\mathcal{H}, \langle h\rangle^{\frac{1}{2}}\mathcal{H}). \end{cases} \tag{8.8}$$

Lemma 3.6 also has a natural version in the present context.

We may view any $S \in B(\mathcal{E}, \mathcal{E}^*)$ as operator on $\mathcal{E}^*$ with domain $\mathcal{E}$, hence its resolvent set and spectrum are well defined. More precisely, the *resolvent set* $\rho(S)$ of S is the set of $z \in \mathbb{C}$ such that $S - z : \mathcal{E} \to \mathcal{E}^*$ is bijective and the *spectrum* of S is $\sigma(S) = \mathbb{C} \setminus \rho(S)$.

8.5. **Klein-Gordon operators.** The *Klein-Gordon operator* is the continuous map $\hat{K} : \mathcal{E} \to \mathcal{E}^*$ defined by

$$\hat{K} = \begin{pmatrix} k & 1 \\ h_0 & k \end{pmatrix} \quad \text{hence} \quad \hat{K} \begin{pmatrix} u_0 \\ u_1 \end{pmatrix} = \begin{pmatrix} ku_0 + u_1 \\ h_0 u_0 + k u_1 \end{pmatrix}. \tag{8.9}$$

Formally we see that if $\phi(t)$ is a solution of (8.1) and we set

$$f(t) = \begin{pmatrix} \phi(t) \\ \mathrm{i}^{-1}\partial_t \phi(t) - k\phi(t) \end{pmatrix}, \tag{8.10}$$

then $f(t) = \mathrm{e}^{\mathrm{i}t\hat{K}} f(0)$, hence $\hat{K}$ (or more precisely some of its restrictions) is the generator of the group associated to (8.1) for the parametrization (8.10) of Cauchy data. The choice (8.10) is natural when one wants to emphasize the *symplectic aspect* of the Klein-Gordon equation (8.1).

From (8.8) it follows that $\hat{K}$ is a symmetric operator and that for all $u \in \mathcal{E}$:

$$\langle u | \hat{K} u \rangle = (u_0 | h_0 u_0) + \|u_1\|^2 + 2\mathrm{Re}(ku_0 | u_1) = (u_0 | h u_0) + \|ku_0 + u_1\|^2. \tag{8.11}$$

Note that we may, and we shall, think of $\hat{K}$ as closed densely defined operator in $\mathcal{E}^*$. There is no a priori given Krein structure on $\mathcal{E}^*$ but various charge and energy Klein-Gordon operators will be obtained as operators induced by $\hat{K}$ in Krein spaces continuously embedded in $\mathcal{E}^*$.

Proposition 8.3. *Assume (A1). Then $\rho(\hat{K}) = \rho(h, k)$ and if $z \in \rho(\hat{K})$ we have:*

$$(\hat{K} - z)^{-1} =: R_{\hat{K}}(z) = \begin{pmatrix} p(z)^{-1}(z-k) & p(z)^{-1} \\ 1 + (z-k)p(z)^{-1}(z-k) & (z-k)p(z)^{-1} \end{pmatrix}. \tag{8.12}$$

Proof. We shall prove that $\hat{K} - z : \mathcal{E} \tilde{\to} \mathcal{E}^* \Leftrightarrow p(z) : \langle h \rangle^{-\frac{1}{2}} \mathcal{H} \tilde{\to} \langle h \rangle^{\frac{1}{2}} \mathcal{H}$ and if these conditions are satisfied then we shall justify the formally obvious relation (8.12). Assume first $p(z) : \langle h \rangle^{-\frac{1}{2}} \mathcal{H} \tilde{\to} \langle h \rangle^{\frac{1}{2}} \mathcal{H}$. Set $q = p(z)^{-1}$, $\ell = k - z$, and let G be the right hand of (8.12), so that

$$G = \begin{pmatrix} -q\ell & q \\ 1 + \ell q \ell & -\ell q \end{pmatrix} \quad \text{and} \quad G \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} -q(\ell a - b) \\ a + \ell q (\ell a - b) \end{pmatrix}. \tag{8.13}$$

This clearly defines a continuous operator $\mathcal{E}^* \to \mathcal{E}$ and a simple computation gives $(\hat{K} - z)G = 1$ on $\mathcal{E}^*$ and $G(\hat{K} - z) = 1$ on $\mathcal{E}$. So G is the inverse of $\hat{K} - z : \mathcal{E} \to \mathcal{E}^*$.

Reciprocally, assume that $\hat{K} - z : \mathcal{E} \tilde{\to} \mathcal{E}^*$. If $u_0 \in \langle h \rangle^{-\frac{1}{2}} \mathcal{H}$ and $u_1 = -\ell u_0$ then $u_1 \in \mathcal{H}$ and $h_0 u_0 + \ell u_1 = (h_0 - \ell^2) u_0 = p(z) u_0$ hence $(\hat{K} - z)\left(\begin{smallmatrix} u_0 \\ u_1 \end{smallmatrix}\right) = \left(\begin{smallmatrix} 0 \\ p(z)u_0 \end{smallmatrix}\right)$. Thus if $p(z)u_0 = 0$ then $(\hat{K} - z)\left(\begin{smallmatrix} u_0 \\ u_1 \end{smallmatrix}\right) = 0$ and so $u_0 = 0$. Hence $p(z) : \langle h \rangle^{-\frac{1}{2}} \mathcal{H} \to \langle h \rangle^{\frac{1}{2}} \mathcal{H}$ is injective. Now let $v_1 \in \langle h \rangle^{\frac{1}{2}} \mathcal{H}$. Since $(\hat{K} - z)\mathcal{E} = \mathcal{E}^*$ and $\left(\begin{smallmatrix} 0 \\ v_1 \end{smallmatrix}\right) \in \mathcal{E}^*$, there are $u_0 \in \langle h \rangle^{-\frac{1}{2}} \mathcal{H}$ and $u_1 \in \mathcal{H}$ such that $(\hat{K} - z)\left(\begin{smallmatrix} u_0 \\ u_1 \end{smallmatrix}\right) = \left(\begin{smallmatrix} 0 \\ v_1 \end{smallmatrix}\right)$, or $\ell u_0 + u_1 = 0$ and $h_0 u_0 + \ell u_1 = v_1$, hence $p(z) u_0 = v_1$. This proves that $p(z)\langle h \rangle^{-\frac{1}{2}} \mathcal{H} = \langle h \rangle^{\frac{1}{2}} \mathcal{H}$ and so $p(z) : \langle h \rangle^{-\frac{1}{2}} \mathcal{H} \tilde{\to} \langle h \rangle^{\frac{1}{2}} \mathcal{H}$. □

We now realize the Klein-Gordon operator as a closed densely defined operator in other Banach spaces.

Proposition 8.4. *Let $\mathcal{L}$ be a Banach space such that $\mathcal{E} \subset \mathcal{L} \subset \mathcal{E}^*$ continuously and densely.* The operator L induced by $\hat{K}$ in $\mathcal{L}$ *is the restriction of $\hat{K}$ to* $\mathrm{Dom}L = \{u \in \mathcal{E} \mid \hat{K}u \in \mathcal{L}\}$ *considered as operator in $\mathcal{L}$. This is a closed densely defined operator such that $\rho(L) \supset \rho(h,k)$ and $R_L(z) := (L-z)^{-1} = R_{\hat{K}}(z)|\mathcal{L}$ for any $z \in \rho(h,k)$, in particular* $\mathrm{Dom}L = R_{\hat{K}}(z)\mathcal{L}$ *for any such z.*

Proof. If $u \in \mathcal{E} \subset \mathcal{L}$ and $z \in \rho(h,k)$ then $\hat{K}u \in \mathcal{L}$ if and only if $(\hat{K}-z)u \in \mathcal{L}$ hence if and only if $u \in (\hat{K}-z)^{-1}\mathcal{L} = R_{\hat{K}}(z)\mathcal{L}$. Since $R_{\hat{K}}(z)$ is a continuous surjection and $\mathcal{L}$ is dense in $\mathcal{K}^*$, the space $\mathrm{Dom}L$ is dense in $\mathcal{E}$, which is dense in $\mathcal{L}$, hence $\mathrm{Dom}L$ is also dense in $\mathcal{L}$. By the closed graph theorem, the restriction of $R_{\hat{K}}(z)$ to $\mathcal{L}$ is a continuous operator in $\mathcal{L}$, so L is a closed densely defined operator in $\mathcal{L}$. □

Let us now discuss several natural operators obtained from Prop. 8.4 for various choices of $\mathcal{L}$.

The largest possible choice of $\mathcal{L}$ is $\mathcal{L} = \mathcal{E}^*$. In this case the operator L equals $\hat{K}$. When we want to stress that we look at $\hat{K}$ as closed densely defined operator in $\mathcal{E}^*$ we denote it by $K_{\max}$.

We have $\hat{K}^* = \hat{K}$ if we consider $\hat{K}$ as an operator $\mathcal{E} \to \mathcal{E}^*$ but as we shall see below $K_{\min} = K_{\max}^*$ is a quite different object.

The smallest possible choice of $\mathcal{L}$ is $\mathcal{L} = \mathcal{E}$. We shall denote $K_{\min}$ the operator induced by $\hat{K}$ in $\mathcal{E}$. Note that

$$K_{\min} \subset L \subset K_{\max},$$

for any realization L of the Klein-Gordon operator.

In the next proposition we describe explicitly the domain of $K_{\min}$, its resolvent set, and we compute its adjoint. Recall that we identified the adjoint space of $\mathcal{E}$ with $\mathcal{E}^*$ with the help of the sesquilinear form (8.4). In particular, if S is a closed densely defined operator in $\mathcal{E}$ then the domain of S^* is the set of $v \in \mathcal{E}^*$ such that the map $u \mapsto \langle Su|v\rangle$ is continuous for the $\mathcal{E}$-topology and then S^*v is the unique $w \in \mathcal{E}^*$ such that $u \mapsto \langle Su|v\rangle = \langle u|w\rangle$ for all $u \in \mathrm{Dom}S$.

Proposition 8.5. *Assume (A1), (A2). Let $K_{\min}$ be the operator induced by $\hat{K}$ in $\mathcal{E}$. Then $K_{\min}^* = K_{\max}$, $\rho(K_{\min}) = \rho(h,k)$ and*

$$\mathrm{Dom}K_{\min} = \{\left(\begin{smallmatrix} u_0 \\ u_1 \end{smallmatrix}\right) \mid u_0 \in \langle h\rangle^{-1}\mathcal{H},\ u_1 \in \mathcal{H},\ ku_0 + u_1 \in \langle h\rangle^{-\frac{1}{2}}\mathcal{H}\} \tag{8.14}$$

Proof. We denote by $\mathcal{D}$ the right hand of (8.14) and first prove $\mathrm{Dom}K_{\min} = \mathcal{D}$.

We have $u \in \mathrm{Dom}K_{\min}$ if and only if $u \in \mathcal{E}$ and $\hat{K}u \in \mathcal{E}$, i.e. $ku_0 + u_1 \in \langle h\rangle^{-\frac{1}{2}}\mathcal{H}$ and $h_0u_0 + ku_1 \in \mathcal{H}$. These conditions are satisfied if $u \in \mathcal{D}$ because $h_0u_0 + ku_1 = hu_0 + k(ku_0+u_1)$ and $hu_0 \in \mathcal{H}, k(ku_0+u_1) \in \mathcal{H}$. Thus $\mathcal{D} \subset \mathrm{Dom}K_{\min}$. Reciprocally, if $u \in \mathrm{Dom}K_{\min}$ then $hu_0 = h_0u_0 - k^2u_0 = (h_0u_0 + ku_1) - k(ku_0 + u_1)$ belongs to $\mathcal{H}$, hence $u_0 \in \mathcal{H}^1$. This proves that $\mathrm{Dom}K_{\min} \subset \mathcal{D}$ hence (8.14) is true.

Next we prove $K_{\min}^* = K_{\max}$. For any $u \in \mathrm{Dom}K_{\min}$ and $v \in \mathcal{E}^*$ we have

$$\langle Ku|v\rangle = (ku_0 + u_1|v_1) + (h_0u_0 + ku_1|v_0).$$

If $v \in \mathcal{E} = \mathrm{Dom}K_{\max}$ then it is clear that the right hand side is continuous for the $\mathcal{E}$-topology and the right hand side above is just $\langle u|K_{\max}v\rangle$. Therefore $K_{\max} \subset K_{\min}^*$.

Reciprocally, we would like to show that

$$|\langle K_{\min}u|v\rangle| \leq C\|u\|_{\mathcal{E}},\ \forall\ u \in \mathrm{Dom}K_{\min} \tag{8.15}$$

implies $v \in \mathcal{E}$. Fix $z \in \rho(h,k)$ and let $R = R_{\hat{K}}(z)$. Then $(K_{\min} - z)^{-1} = R_{|\mathcal{E}}$ by Prop. 8.4. Note that (8.15) is equivalent to

$$|\langle(\hat{K}-z)u|v\rangle| \leq C'\|u\|_{\mathcal{E}}\ ,\forall\ u \in \mathrm{Dom}K_{\min},$$

for some constant C' and this is equivalent to

$$|\langle w|v\rangle| = |\langle(\hat{K}-z)Rw|v\rangle| \leq C'\|Rw\|_{\mathcal{E}},\ \forall\ w\in\mathcal{E}.$$

But $R:\mathcal{E}^*\to\mathcal{E}$ is continuous, so we obtain $|\langle w|v\rangle|\leq C''\|w\|_{\mathcal{E}^*}$ for all $w\in\mathcal{E}$. Since $\mathcal{E}$ is dense in $\mathcal{E}^*$ we see that $\langle\cdot|v\rangle$ extends to a continuous form on $\mathcal{E}^*$, hence $v\in\mathcal{E}$.

Finally, we have $\rho(K_{\min})=\rho(K_{\max})^*=\rho(h,k)^*=\rho(h,k)$. □

Corollary 8.6. *If (A1) holds and if h is bounded from below then $K_{\min}$ and $K_{\max}$ are generators of C_0-groups.*

Proof. Since $K_{\min}^*=K_{\max}$ it suffices to consider the case of $K_{\min}$. The rest of the proof is a variation on the proof of [K, Thm. 3.2]. First we show that it suffices to assume $h\geq 1$. Indeed, if c is a number such that $h+c\geq 1$ and if we replace everywhere h by $h+c$ then h_0 gets replaced by h_0+c and we have

$$\hat{K}=\begin{pmatrix} k & 1\\ h_0+c & k\end{pmatrix}-\begin{pmatrix} 0 & 0\\ c & 0\end{pmatrix}.$$

Since the last term is a bounded operator, it suffices to show that the first term on the right hand side is a generator of C_0-group. So from now on we may assume $h\geq 1$. Then $0\in\rho(h,k)$ and due to (8.12) we have

$$K_{\min}^{-1}=\begin{pmatrix} -h^{-1}k & h^{-1}\\ 1+kh^{-1}k & -kh^{-1}\end{pmatrix}.$$

We know that this is a bounded operator on $\mathcal{E}$. On the other hand, it is easy to check that the "energy" hermitian form $\langle u|\hat{K}u\rangle=(u_0|hu_0)+\|ku_0+u_1\|^2$ introduced in (8.11) is an admissible scalar product on $\mathcal{E}$, i.e. $\mathcal{E}$ equipped with this form is a Hilbert space. Since $\langle u|\hat{K}K_{\min}^{-1}u\rangle=\langle u|u\rangle\in\mathbb{R}$, the operator $K_{\min}^{-1}$ is symmetric, hence $K_{\min}$ is a self-adjoint operator on this Hilbert space. □

Another case of interest is $\mathcal{L}=\mathcal{K}_\theta$, $0\leq\theta<\frac{1}{2}$, which we now discuss.

Proposition 8.7. *Assume (A1), (A2). Let K_θ be the operator induced by $\hat{K}$ in the space $\mathcal{K}_\theta$ defined in* (8.6)*. Then*

(8.16)

$$\mathrm{Dom}K_\theta=\{\tbinom{u_0}{u_1}\mid u_0\in\langle h\rangle^{-\frac{1}{2}}\mathcal{H},\ u_1\in\mathcal{H},\ ku_0+u_1\in\langle h\rangle^{-\theta}\mathcal{H},\ h_0u_0+ku_1\in\langle h\rangle^{\theta}\mathcal{H}\}.$$

Moreover K_θ is self-adjoint on the Krein space $(\mathcal{K}_\theta,\langle\cdot|\cdot\rangle)$ and $\rho(K_\theta)=\rho(h,k)$.

Proof. If $v_0\in\langle h\rangle^{-\theta}\mathcal{H}$, $v_1\in\langle h\rangle^{\theta}\mathcal{H}$ and $\binom{u_0}{u_1}:=R_{\hat{K}}(z)\binom{v_0}{v_1}$ then, with the notations of the proof of Prop. 8.3, we have $\ell u_0+u_1=v_0$ and $h_0u_0+\ell u_1=v_1$ hence $\binom{u_0}{u_1}$ belongs to the set $\mathcal{D}$ defined by the right hand side of (8.16). Thus $R_{\hat{K}}(z)\mathcal{K}\subset\mathcal{D}$. Reciprocally, if u_0,u_1 are as in (8.16) then $\binom{v_0}{v_1}:=(\hat{K}-z)\binom{u_0}{u_1}$ belongs to $\mathcal{K}_\theta$ and $R_{\hat{K}}(z)\binom{v_0}{v_1}=\binom{u_0}{u_1}$, thus $\mathcal{D}\subset R_{\hat{K}}(z)\mathcal{D}$. This proves (8.16).

To prove the self-adjointness of K_θ it suffices to show $R_{K_\theta}(z)^*=R_{K_\theta}(\overline{z})$ for some $z\in\rho(h,k)$, which is not empty, by (A2). But this is obvious, see the line before (8.8).

Since by Prop. 8.4 we know that $\rho(h,k)\subset\rho(K_\theta)$, it remains to prove that $\rho(K_\theta)\subset\rho(h,k)$. Assume that $K_\theta-z:\mathrm{Dom}K_\theta\tilde{\to}\mathcal{K}_\theta$ and argue as in the proof of Prop. 8.3. We first show that $p(z):\langle h\rangle^{-\frac{1}{2}}\mathcal{H}\to\langle h\rangle^{\frac{1}{2}}\mathcal{H}$ is injective. If $u_0\in\langle h\rangle^{-\frac{1}{2}}\mathcal{H}$ and $p(z)u_0=0$ set $u_1=-\ell u_0$. Then $u_1\in\mathcal{H}$ and

$$h_0u_0+\ell u_1=(h_0-\ell^2)u_0=p(z)u_0=0,$$

hence $(\hat{K}-z)\left(\begin{smallmatrix}u_0\\u_1\end{smallmatrix}\right)=0$. Also:

$$\begin{aligned} ku_0+u_1 &= lu_0+u_1+zu_0=zu_0\in\langle h\rangle^{-\frac{1}{2}}\mathcal{H}\subset\langle h\rangle^{-\theta}\mathcal{H},\\ h_0u_0+ku_1 &= h_0u_0+lu_1+zu_1=zu_1\in\mathcal{H}\subset\langle h\rangle^{-\theta}\mathcal{H}. \end{aligned}$$

Thus $\left(\begin{smallmatrix}u_0\\u_1\end{smallmatrix}\right)\in\mathrm{Dom}K_\theta$ and $(K_\theta-z)\left(\begin{smallmatrix}u_0\\u_1\end{smallmatrix}\right)=0$, so $u_0=0$. This proves the injectivity of $p(z):\langle h\rangle^{-\frac{1}{2}}\mathcal{H}\to\langle h\rangle^{\frac{1}{2}}\mathcal{H}$. In particular, $p(z):\langle h\rangle^{-1}\mathcal{H}\to\mathcal{H}$ is injective.

According to Lemma 8.1, it remains to prove that this map is also surjective. Let $v_1\in\mathcal{H}$. Since $(K_\theta-z)\mathrm{Dom}K_\theta=\mathcal{K}_\theta$ and $\left(\begin{smallmatrix}0\\v_1\end{smallmatrix}\right)\in\mathcal{K}_\theta$, there is $u\in\mathrm{Dom}K_\theta$ such that $(K_\theta-z)u=\left(\begin{smallmatrix}0\\v_1\end{smallmatrix}\right)$, hence $lu_0+u_1=0$ and $h_0u_0+lu_1=v_1$, thus $p(z)u_0=v_1$. But $p(z)=h-z^2+2zk$ hence $hu_0=v_1+z^2u_0-2zku_0\in\mathcal{H}$ so $u_0\in\langle h\rangle^{-1}\mathcal{H}$. Thus $p(z)\langle h\rangle^{-1}\mathcal{H}=\mathcal{H}$. □

Remark 8.8. As explained before, we have $K_{\min}\subset K_\theta\subset K_{\max}$ for any $0\leq\theta\leq\frac{1}{2}$ and the spectrum of all these operators coincide. But for $\theta=1/4$ we have more: from (8.7) it follows that in this case the operator $K_{1/4}$ is obtained by interpolation of order $1/2$ between $K_{\min}$ and $K_{\max}=K_{\min}^*$ (in resolvent sense). In particular, these operators should have similar spectral properties and functional calculus, fact which will be confirmed by later developments.

8.6. **Charge and energy operators.** The self-adjoint operator K_θ in the Krein space $\mathcal{K}_\theta$ will be called *charge Klein-Gordon* operator, although this terminology is often reserved to the case $\theta=1/4$.

If $\phi(t)$ is a solution of (8.1) and we set instead of (8.10):

$$f(t)=\begin{pmatrix}\phi(t)\\ \mathrm{i}^{-1}\partial_t\phi(t)\end{pmatrix}, \tag{8.17}$$

then formally $f(t)=\mathrm{e}^{\mathrm{i}t\hat{H}}f(0)$ for

$$\hat{H}=\begin{pmatrix}0&1\\h&2k\end{pmatrix}.$$

The choice (8.17) of Cauchy data is the standard one in the PDE literature and is convenient when one wants to emphasize the *energy conservation* of the Klein-Gordon equation (8.1).

We now show that the operator $K_{\min}$ is isomorphic to the usual *energy Klein-Gordon* operator H, which is the realization of $\hat{H}$ on $\mathcal{E}$, so we could say that $K_{\min}$ is the *energy Klein-Gordon operator in the charge representation*.

Note first that if $a:\langle h\rangle^{-\frac{1}{2}}\mathcal{H}\to\mathcal{H}$ is a continuous symmetric map then the operator $\Phi(a)=\left(\begin{smallmatrix}1&0\\a&1\end{smallmatrix}\right)$ is a well defined continuous map $\mathcal{E}^*\to\mathcal{E}^*$ which leaves $\mathcal{E}$ invariant. Thus $\Phi(a)$ is an isomorphism $\mathcal{E}^*\to\mathcal{E}^*$ with $\Phi(-a)$ as inverse, which clearly implies that $\Phi(a):\mathcal{E}\to\mathcal{E}$ is also an isomorphism. Observe that $\Phi(a)$ is symmetric when considered as operator $\mathcal{E}\to\mathcal{E}^*$.

Set $\Phi=\Phi(k)$. Then

$$\hat{H}:=\begin{pmatrix}0&1\\h&2k\end{pmatrix}:\mathcal{E}\to\mathcal{E}^*$$

is a continuous (not symmetric) operator and $\Phi\hat{K}=\hat{H}\Phi$.

The usual *energy Klein-Gordon operator* H is the closed operator in $\mathcal{E}$ induced by $\hat{H}$. Clearly

$$\mathrm{Dom}H=\langle h\rangle^{-1}\mathcal{H}\oplus\langle h\rangle^{-\frac{1}{2}}\mathcal{H}\text{ and }\Phi K_{\min}\Phi^{-1}=H,$$

where Φ is considered as an automorphism of $\mathcal{E}$. Thus we immediately get $\rho(H)=\rho(h,k)$ and, more generally, $K_{\min}$ and H have the same spectral properties.

Assume now that $0 \in \rho(h,k)$. According to Lemma 8.1 this is equivalent to $h : \langle h\rangle^{-\frac{1}{2}}\mathcal{H}\tilde{\to}\langle h\rangle^{\frac{1}{2}}\mathcal{H}$ hence $\left(\begin{smallmatrix} 0 & 1 \\ h & 0\end{smallmatrix}\right) : \mathcal{E}\tilde{\to}\mathcal{E}^*$. Then $\mathcal{E}$, equipped with the form

$$\langle u|v\rangle_{\mathcal{E}} = \langle u|\left(\begin{smallmatrix} 0 & 1 \\ h & 0\end{smallmatrix}\right)v\rangle = (u_0|hv_0) + (u_1|v_1) \tag{8.18}$$

is a Krein space. It is easy to check that H is self-adjoint on $(\mathcal{E}, \langle\cdot|\cdot\rangle_{\mathcal{E}})$. Indeed, we have $0 \in \rho(H) = \rho(h,k)$ and $H^{-1} = \left(\begin{smallmatrix} -2h^{-1}k & h^{-1} \\ 1 & 0\end{smallmatrix}\right)$ is a bounded symmetric operator because $\langle u|H^{-1}u\rangle_{\mathcal{E}} = 2\mathrm{Re}(u_0|u_1) - 2(u_0|u_0)$.

This is the usual energy Klein-Gordon setting. We now express it in the charge representation, i.e. in terms of the operator $K_{\min}$. Since $\Phi^{-1} : \mathcal{E} \to \mathcal{E}$ is an isomorphism which intertwines E and $K_{\min}$ we see that the *energy Krein structure* on $\mathcal{E}$ is given by (8.11) and that $K_{\min}$ is self-adjoint for it.

8.7. **Free operators.** We now discuss the *free operators*

$$\hat{K}_0 := \begin{pmatrix} 0 & 1 \\ h_0 & 0\end{pmatrix} : \mathcal{E} \to \mathcal{E}^*,$$

obtained for $k = 0$. In this case $h_0 = h$ and we will formulate the various results below in terms of h_0.

Denote by L_0 any of the operators $K_{0,\min}$ and $K_{0,\theta}$ induced by $\hat{K}_0$ in $\mathcal{E}$ and $\mathcal{K}_\theta$ respectively. Note that the operator $K_{0,\max}$ has the same properties as $K_{0,\min}$ because $K_{0,\max} = (K_{0,\min})^*$.

Lemma 8.9. *Set $\sigma_\pm(h_0) := \sigma(h_0) \cap \mathbb{R}^\pm$ and $R_{h_0}(z) := (h_0 - z)^{-1}$. Then:*

$$\sigma(L_0) = \big(\sigma_+(h_0)^{1/2}\big) \cup \big(-\sigma_+(h_0)^{1/2}\big) \cup \big(\mathrm{i}|\sigma_-(h_0)|^{1/2}\big) \cup \big(-\mathrm{i}|\sigma_-(h_0)|^{1/2}\big), \tag{8.19}$$

$$\begin{aligned} R_{L_0}(z) &= \begin{pmatrix} zR_{h_0}(z^2) & R_{h_0}(z^2) \\ 1 + z^2R_{h_0}(z^2) & zR_{h_0}(z^2)\end{pmatrix} \\ &= \begin{pmatrix} zR_{h_0}(z^2) & R_{h_0}(z^2) \\ h_0R_{h_0}(z^2) & zR_{h_0}(z^2)\end{pmatrix} = (L_0 + z)R_{h_0}(z^2). \end{aligned} \tag{8.20}$$

Proof. By Props. 8.5 and 8.7 we have $\sigma(L_0) = \{z \in \mathbb{C} \ : \ z^2 \in \sigma(h_0)\}$, which implies (8.19). Then (8.20) follows from

$$(L_0 - z)(L_0 + z) = L_0^2 - z^2 = h_0 - z^2,$$

where h_0 is identified with the diagonal matrix having h_0 on the diagonal. □

Remark 8.10. Note that the resolvent of the operator $K_{0,0}$ has a rather unusual behavior: if h_0 is positive and unbounded and if we equip $\mathcal{K}_0 = \mathcal{H} \oplus \mathcal{H}$ with the Hilbert direct sum norm, then (8.20) implies $\|R_{K_{0,0}}(z)\| \geq \|h_0R_{h_0}(z^2)\| \geq 1 \ \forall z$.

We now compute $\varphi(L_0)$ for entire functions φ by using the relations

$$L_0^{2n} = \begin{pmatrix} {h_0}^n & 0 \\ 0 & {h_0}^n\end{pmatrix} \quad \text{and} \quad L_0^{2n+1} = \begin{pmatrix} 0 & {h_0}^n \\ {h_0}^{n+1} & 0\end{pmatrix}, \ n \in \mathbb{N}.$$

If $\varphi(z) = \sum_{n\geq 0} a_n z^n$ and if we define

$$\varphi_{\mathrm{c}}(z) = \frac{1}{2}\big(\varphi(\sqrt{z}) + \varphi(-\sqrt{z})\big) = \textstyle\sum_{n\geq 0} a_{2n}z^n, \tag{8.21}$$

$$\varphi_{\mathrm{s}}(z) = \frac{1}{2\sqrt{z}}\big(\varphi(\sqrt{z}) - \varphi(-\sqrt{z})\big) = \textstyle\sum_{n\geq 0} a_{2n+1}z^n \tag{8.22}$$

then by working with the set of entire vectors of the self-adjoint operator h_0 in $\mathcal{H}$ we obtain

$$\varphi(L_0) = \begin{pmatrix} \varphi_{\mathrm{c}}(h_0) & \varphi_{\mathrm{s}}(h_0) \\ h_0\varphi_{\mathrm{s}}(h_0) & \varphi_{\mathrm{c}}(h_0)\end{pmatrix}. \tag{8.23}$$

For example, if $h_0 = \varepsilon^2$ for some operator ε, not necessarily self-adjoint, then

$$\mathrm{e}^{\mathrm{i}tL_0} = \begin{pmatrix} \cos(t\varepsilon) & \mathrm{i}\varepsilon^{-1}\sin(t\varepsilon) \\ \mathrm{i}\varepsilon\sin(t\varepsilon) & \cos(t\varepsilon) \end{pmatrix}. \tag{8.24}$$

Let us now assume $h_0 = \epsilon^2$ for $\epsilon \geq 0$. Then $\sigma(L_0) = \sigma(\varepsilon) \cup -\sigma(\varepsilon)$ and (8.23) becomes

$$\varphi(L_0) = \begin{pmatrix} \frac{\varphi(\varepsilon)+\varphi(-\varepsilon)}{2} & \frac{\varphi(\varepsilon)-\varphi(-\varepsilon)}{2\varepsilon} \\ \varepsilon\frac{\varphi(\varepsilon)-\varphi(-\varepsilon)}{2} & \frac{\varphi(\varepsilon)+\varphi(-\varepsilon)}{2} \end{pmatrix} = \begin{pmatrix} \varphi_+(\varepsilon) & \varphi_-(\varepsilon)/\varepsilon \\ \varphi_-(\varepsilon)\varepsilon & \varphi_+(\varepsilon) \end{pmatrix} \tag{8.25}$$

where

$$\varphi_\pm(x) = (\varphi(x) \pm \varphi(-x))/2,$$

are the even and odd parts of the function φ. The value of $(\varphi(x) - \varphi(-x))/2x$ at $x = 0$ is $\varphi'(0)$ by definition.

We now discuss bounds for the Borel functional calculus of L_0.

The bounds in the case of $K_{0,\min}$ and $K_{0,\max}$ are of a different nature than those for $K_{0,\theta}$ (unless $\theta = 1/4$). We introduce the following spaces Λ, Λ_θ of bounded Borel functions. Recall that $\varphi_\pm$ denote the even/odd parts of φ.

Definition 8.11. *We denote by Λ, resp. Λ_θ, the spaces of Borel functions $\varphi : \mathbb{R} \to \mathbb{C}$ such that:*

$$\|\varphi\|_\Lambda := \sup_{x\in\mathbb{R}} |\varphi(x)| + \sup_{x\geq 0} |\varphi_-(x)/x| < \infty, \tag{8.26}$$

resp.

$$\|\varphi\|_{\Lambda_\theta} := \|\varphi\|_\Lambda + \sup_{x\geq 0} |\varphi_-(x)/x| + \sup_{x\in\mathbb{R}} |\varphi_-(x)|\langle x\rangle^{|4\theta-1|} < \infty. \tag{8.27}$$

Note that $\Lambda_{1/4} = \Lambda$.

Lemma 8.12. *Assume $h_0 = \epsilon^2$ for some $\epsilon \geq 0$. Then there is a unique linear map $\Lambda \ni \varphi \mapsto \varphi(K_{0,\min}) \in B(\mathcal{E})$ such that $\varphi(K_{0,\min}) = (K_{0,\min} - z)^{-1}$ if $\varphi(x) = (x - z)^{-1}$ with $z \notin \mathbb{R}$ and such that the following continuity property is satisfied:*

if φ_n is a bounded sequence in Λ with $\varphi_n(x) \to \varphi(x)$ for each real x, then $\varphi_n(K_{0,\min}) \to \varphi(K_{0,\min})$ weakly.

The map $\Lambda \ni \varphi \mapsto \varphi(K_{0,\min}) \in B(\mathcal{E})$ is an algebra morphism and (8.25) holds. Moreover:

$$\|\varphi(K_{0,\min})\|_{B(\mathcal{E})} \leq C\|\varphi\|_\Lambda,\ C \geq 0. \tag{8.28}$$

Lemma 8.13. *Assume $h_0 = \epsilon^2$ for some $\epsilon \geq 0$. Then there is a unique linear map $\Lambda_\theta \ni \varphi \mapsto \varphi(K_{0,\theta}) \in B(\mathcal{K}_\theta)$ such that $\varphi(K_{0,\theta}) = (K_{0,\theta} - z)^{-1}$ if $\varphi(x) = (x - z)^{-1}$ with $z \notin \mathbb{R}$ and such that the following continuity property is satisfied:*

if φ_n is a bounded sequence in Λ_θ with $\varphi_n(x) \to \varphi(x)$ for each real x, then $\varphi_n(K_{0,\theta}) \to \varphi(K_{0,\theta})$ weakly.

The map $\Lambda_\theta \ni \varphi \mapsto \varphi(K_{0,\theta}) \in B(\mathcal{K}_\theta)$ is an algebra morphism and (8.25) holds. Moreover:

$$\|\varphi(K_{0,\theta})\|_{B(\mathcal{K}_\theta)} \leq C\|\varphi\|_{\Lambda_\theta},\ C \geq 0. \tag{8.29}$$

Proof of Lemmas 8.12, 8.13. For later use we note the following easy facts:

$$\sup_{x\in\mathbb{R}} |\varphi(x)| \sim \sup_{x\geq 0} |\varphi_+(x)| + \sup_{x\geq 0} |\varphi_-(x)|, \tag{8.30}$$

$$\begin{aligned} & \sup_{x\geq 0} |\langle x\rangle\varphi_-(x)/x| + \sup_{x\geq 0} |x\varphi_-(x)/\langle x\rangle| \\ \sim\ & \sup_{x\geq 0} |\varphi_-(x)| + \sup_{x\geq 0} |\varphi_-(x)/x|, \end{aligned} \tag{8.31}$$

$$
\begin{aligned}
&\sup_{x\geq 0}|\langle x\rangle^{4\theta}\varphi_-(x)/x| + \sup_{x\geq 0}|x\varphi_-(x)/\langle x\rangle^{4\theta}| \\
\sim\ &\sup_{x\geq 0}|\varphi_-(x)| + \sup_{x\geq 0}|\varphi_-(x)\varphi_-(x)/x| + \sup_{x\geq 0}|\langle x\rangle^{|4\theta-1|}\varphi_-(x)|.
\end{aligned} \tag{8.32}
$$

Let us first prove Lemma 8.12. We consider on $\mathcal{E}$ the admissible norm defined by $\|u\|_{\mathcal{E}}^2 = \|\langle\varepsilon\rangle u_0\|^2 + \|u_1\|^2$. The diagonal matrix with coefficients $\langle\varepsilon\rangle$ and 1 is an isometric bijection $\mathcal{E}\to\mathcal{K}_0 = \mathcal{H}\oplus\mathcal{H}$. It follows from (8.25) that if φ is an entire function, bounded on $\mathbb{R}$, the norm of the operator $\varphi(K_{0,\min})$ in $\mathcal{E}$ is equal to the norm in $\mathcal{K}_0$ of the operator

$$
\begin{aligned}
&\begin{pmatrix} \langle\varepsilon\rangle & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \varphi_+(\varepsilon) & \varphi_-(\varepsilon)/\varepsilon \\ \varphi_-(\varepsilon)\varepsilon & \varphi_+(\varepsilon)\end{pmatrix}\begin{pmatrix} \langle\varepsilon\rangle^{-1} & 0 \\ 0 & 1\end{pmatrix} \\
= &\begin{pmatrix} \varphi_+(\varepsilon) & \langle\varepsilon\rangle\varphi_-(\varepsilon)/\varepsilon \\ \varphi_-(\varepsilon)\varepsilon/\langle\varepsilon\rangle & \varphi_+(\varepsilon)\end{pmatrix},
\end{aligned}
$$

with a convention as stated above for $\varphi_-(0)/0$. Hence there is a number $c>0$ such that

$$
c\|\varphi(K_{0,\min})\|_{\mathcal{E}} \leq \sup_{x\geq 0}|\varphi_+(x)| + \sup_{x\geq 0}|\langle x\rangle\varphi_-(x)/x| + \sup_{x\geq 0}|x\varphi_-(x)/\langle x\rangle|. \tag{8.33}
$$

Applying (8.30), (8.31) we obtain (8.28). We extend the functional calculus from entire functions in Λ to Borel functions in Λ in the standard way.

To prove Lemma 8.13 we argue similarly, introducing the compatible norm $\|u\|_{\mathcal{K}_\theta}^2 = \|\langle\varepsilon\rangle^{2\theta}u_0\|^2 + \|\langle\varepsilon\rangle^{-2\theta}u_1\|^2$ on $\mathcal{K}_\theta$. The diagonal matrix with coefficients $\langle\varepsilon\rangle^{2\theta}$ and $\langle\varepsilon\rangle^{-2\theta}$ is an isometric bijection $\mathcal{K}_\theta\to\mathcal{K}_0$. Hence the norm of $\varphi(K_{0,\theta})$ in $\mathcal{K}$ is equal to the norm in $\mathcal{K}_0$ of the operator

$$
\begin{aligned}
&\begin{pmatrix} \langle\varepsilon\rangle^{2\theta} & 0 \\ 0 & \langle\varepsilon\rangle^{-2\theta} \end{pmatrix}\begin{pmatrix} \varphi_+(\varepsilon) & \varphi_-(\varepsilon)/\varepsilon \\ \varphi_-(\varepsilon)\varepsilon & \varphi_+(\varepsilon)\end{pmatrix}\begin{pmatrix} \langle\varepsilon\rangle^{-2\theta} & 0 \\ 0 & \langle\varepsilon\rangle^{2\theta}\end{pmatrix} \\
= &\begin{pmatrix} \varphi_+(\varepsilon) & \langle\varepsilon\rangle^{4\theta}\varphi_-(\varepsilon)/\varepsilon \\ \varphi_-(\varepsilon)\varepsilon/\langle\varepsilon\rangle^{4\theta} & \varphi_+(\varepsilon)\end{pmatrix}.
\end{aligned}
$$

Thus there is a number $c>0$ such that

$$
c\|\varphi(K_{0,\theta})\|_{\mathcal{K}} \leq \sup_{x\geq 0}|\varphi_+(x)| + \sup_{x\geq 0}|\varphi_-(x)/x|\langle x\rangle^{4\theta} + \sup_{x\geq 0}|x\varphi_-(x)|/\langle x\rangle^{4\theta}. \tag{8.34}
$$

Using (8.30), (8.32) we obtain (8.29). □

Remark 8.14. If ε is not bounded we see that the lack of regularity at infinity of the function $\varphi(x) = \mathrm{e}^{\mathrm{i}tx}$ makes $\mathrm{e}^{\mathrm{i}tK_{0,\theta}}$ unbounded if $t\neq 0$ and $\theta\neq 1/4$. This fact also allows us to show that the spaces $\mathcal{K}_\theta$ with $\theta\neq 1/4$ are not interpolation spaces between $\mathcal{E}$ and $\mathcal{E}^*$. Indeed, if $t\neq 0$ then $\mathrm{e}^{\mathrm{i}tK_{\max}}$ is bounded in $\mathcal{E}^*$, leaves $\mathcal{E}$ invariant and induces there the bounded operator $\mathrm{e}^{\mathrm{i}tK_{\min}}$. It induces in $\mathcal{K}$ the densely defined operator $\mathrm{e}^{\mathrm{i}tK_{0,\theta}}$ which is unbounded if $\theta\neq 1/4$.

Remark 8.15. One may clearly give sense to the right hand side of (8.25) as a closed densely defined operator for a large class of functions φ and so to give a meaning to $\varphi(L_0)$ as (unbounded) operator. For example, if $\varepsilon>0$ then

$$
\mathbb{1}_{\mathbb{R}^\pm}(L_0) = \frac{1}{2}\begin{pmatrix} 1 & \pm\varepsilon^{-1} \\ \pm\varepsilon & 1\end{pmatrix} =: \Pi_\pm \tag{8.35}
$$

and these are the spectral projections of L_0 corresponding to the half lines $\mathbb{R}^\pm$. By the preceding lemmas or by a simple direct argument the operators $\mathbb{1}_{\mathbb{R}^\pm}(K^0_{\min})$ are bounded operators on $\mathcal{E}$ if and only if $\inf\varepsilon>0$ while the $\mathbb{1}_{\mathbb{R}^\pm}(K_{0,\theta})$ are bounded operators on $\mathcal{K}_\theta$ if and only if $\inf\varepsilon>0$ and $\theta=1/4$. In any case, the $\Pi_\pm$ are projections (i.e. $\Pi_\pm^2=\Pi_\pm$) such that $\Pi_+\Pi_- = \Pi_-\Pi_+ = 0$ and $\Pi_+ + \Pi_- = 1$ at least on dense domains. It is easy to check that $\mathbb{1}_{\mathbb{R}^+}(K_{0,\theta})\geq 0$ and $\mathbb{1}_{\mathbb{R}^-}(K_{0,\theta})\leq 0$ (by Lemma 3.6 in the bounded case and a direct argument in general). The case

of $\Pi_+ = \mathbb{1}_{\mathbb{R}^+}(K_{0,\theta})$ for $\theta \neq 1/4$ (e.g. let $\theta = 0$ and $\inf \varepsilon > 0$) is particularly interesting: this is a positive self-adjoint operator on $\mathcal{K}$ which is an (unbounded) orthogonal projection whose resolvent set is empty. Indeed, for any $z \neq 0, 1$ the operator $z(\Pi_+ - z)^{-1} = (1-z)^{-1}\Pi_+ - 1$ is not bounded.

It is easy to compute the boundary values of the resolvent and the "spectral measure" of L_0. From (8.20) we see that if $\lambda > 0$ then, in the sense of distributions,

$$R_{L_0}(\lambda + \mathrm{i}0) = \begin{pmatrix} \lambda R_{h_0}(\lambda^2 + \mathrm{i}0) & R_{h_0}(\lambda^2 + \mathrm{i}0) \\ h_0 R_{h_0}(\lambda^2 + \mathrm{i}0) & \lambda R_{h_0}(\lambda^2 + \mathrm{i}0) \end{pmatrix}, \tag{8.36}$$

while if $\lambda < 0$ then

$$R_{L_0}(\lambda + \mathrm{i}0) = \begin{pmatrix} \lambda R_{h_0}(\lambda^2 - \mathrm{i}0) & R_{h_0}(\lambda^2 - \mathrm{i}0) \\ h_0 R_{h_0}(\lambda^2 - \mathrm{i}0) & \lambda R_{h_0}(\lambda^2 - \mathrm{i}0) \end{pmatrix}. \tag{8.37}$$

Recall that, if S is a self-adjoint (in the usual sense) operator with resolvent R_S and spectral measure E_S then

$$E'_S(\lambda) = \frac{1}{2\pi\mathrm{i}}\big(R_S(\lambda + \mathrm{i}0) - R_S(\lambda - \mathrm{i}0)\big)$$

by which we mean $\varphi(S) = \int \varphi(\lambda) dE_S(\lambda) = \int \varphi(\lambda) E'_S(\lambda) d\lambda$ where the second equality holds in the sense of distributions for smooth φ. If $S > 0$ (i.e. $S \geq 0$ and is injective) then we get:

$$\begin{aligned} &\int \varphi(\lambda) E'_S(\lambda^2) d\lambda = \int \tfrac{1}{2\lambda^{1/2}} \varphi(\lambda^{1/2}) E'_S(\lambda) d\lambda \\ = \quad &\tfrac{1}{2S^{1/2}} \varphi(S^{1/2}) = \tfrac{1}{2S^{1/2}} \int \varphi(\lambda) E'_{S^{1/2}}(\lambda), \end{aligned}$$

which can be written

$$E'_S(\lambda^2) = \frac{1}{2S^{1/2}} E'_{S^{1/2}}(\lambda) = \frac{1}{2\lambda} E'_{S^{1/2}}(\lambda).$$

By using this in (8.36) and (8.37) we get for $\lambda > 0$:

$$E'_{L_0}(\lambda) = \begin{pmatrix} \lambda E'_{h_0}(\lambda^2) & E'_{h_0}(\lambda^2) \\ h_0 E'_{h_0}(\lambda^2) & \lambda E'_{h_0}(\lambda^2) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} E'_\varepsilon(\lambda) & \varepsilon^{-1} E'_\varepsilon(\lambda) \\ \varepsilon E'_\varepsilon(\lambda) & E'_\varepsilon(\lambda) \end{pmatrix} \tag{8.38}$$

and

$$E'_{L_0}(-\lambda) = -\begin{pmatrix} -\lambda E'_{h_0}(\lambda^2) & E'_{h_0}(\lambda^2) \\ h_0 E'_{h_0}(\lambda^2) & -\lambda E'_{h_0}(\lambda^2) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} E'_\varepsilon(\lambda) & -\varepsilon^{-1} E'_\varepsilon(\lambda) \\ -\varepsilon E'_\varepsilon(\lambda) & E'_\varepsilon(\lambda) \end{pmatrix}. \tag{8.39}$$

8.8. **Conjugate operators for K_θ.** We now construct conjugate operators for the free and total Hamiltonian. The treatment is cleaner for the charge Klein-Gordon operators $K_{0,\theta}$, K_θ because they are self-adjoint for the same Krein structure so we concentrate on this case.

Several types of conjugate operators can be considered in this context, here we shall work only with those of scalar type. To be precise, operators of the form $S = s \oplus s$, i.e. diagonal matrices $S = \left(\begin{smallmatrix} s & 0 \\ 0 & s \end{smallmatrix}\right)$, will be called *scalar operators*. We use the same notation for an operator s in $\langle h \rangle^\theta \mathcal{H}$ which leaves $\langle h \rangle^{-\theta} \mathcal{H}$ invariant and the diagonal operator $S = s \oplus s$ in $\mathcal{K}_\theta$.

We introduce the assumptions:

(E) $\begin{cases} \varepsilon \text{ is a positive self-adjoint operator on } \mathcal{H}, \\ k : \mathrm{Dom}\varepsilon \to \mathcal{H} \text{ is compact and symmetric as operator in } \mathcal{H}. \end{cases}$

(M) $\begin{cases} a \text{ is a self-adjoint operator on } \mathcal{H} \text{ such that } \mathrm{e}^{\mathrm{i}ta}\mathrm{Dom}\varepsilon \subset \mathrm{Dom}\varepsilon \text{ for all } t \in \mathbb{R}, \\ \varepsilon \text{ and } k \text{ considered as operators } \mathrm{Dom}\varepsilon \to \mathcal{H} \text{ are of class } C^1_{\mathrm{u}}(a). \end{cases}$

If (E) holds the quadratic form $\varepsilon^2 - k^2$ on $D(\varepsilon)$ is closed and bounded from below. If h is the associated self-adjoint operator, h is bounded below and its spectrum is discrete below $\inf \varepsilon^2$. As before, we set $h_0 = \varepsilon^2$ and we have $\langle h\rangle^{-1/2}\mathcal{H} = \langle h_0\rangle^{-1/2}\mathcal{H} = \mathrm{Dom}\varepsilon$. This implies $\langle h\rangle^s\mathcal{H} = \langle \epsilon\rangle^{2s}\mathcal{H}$ for $|s| \leq 1/2$.

In particular (A1), (A2) of Sect. 8.2 are satisfied, by Lemma 8.2.

If (M) holds $\mathrm{e}^{\mathrm{i}ta}$ induces a C_0-group in $\mathrm{Dom}\varepsilon$ hence in all $\langle h\rangle^\sigma\mathcal{H}$ with $|\sigma| \leq \frac{1}{2}$. This gives a meaning to the regularity condition on ε and k. As before we use notations like $\varepsilon' := [\varepsilon, \mathrm{i}a]$, etc.

Our purpose is to study the self-adjoint operators

$$K_{0,\theta} = \begin{pmatrix} 0 & 1 \\ \varepsilon^2 & 0 \end{pmatrix} \quad \text{and} \quad K_\theta = \begin{pmatrix} k & 1 \\ \varepsilon^2 & k \end{pmatrix} \tag{8.40}$$

acting in the Krein space $\mathcal{K}_\theta$. The conjugate operator will be

$$A := \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix} = a \oplus a.$$

Clearly A is the generator of the C_0-group of scalar operators $\mathrm{e}^{\mathrm{i}tA} = \mathrm{e}^{\mathrm{i}ta} \oplus \mathrm{e}^{\mathrm{i}ta}$ on $\mathcal{K}_\theta$. More generally:

Lemma 8.16. *Let $A = a \oplus a$. Then $\mathrm{e}^{\mathrm{i}tA} = \mathrm{e}^{\mathrm{i}ta} \oplus \mathrm{e}^{\mathrm{i}ta}$ is a C_0-group on $\mathcal{E}^*$ which leaves invariant the spaces $\mathcal{E}$ and $\mathcal{K}$ and induces C_0-groups on them. The Krein structure of $\mathcal{K}_\theta$ is of class $C^1(A)$.*

In fact $\mathrm{e}^{\mathrm{i}tA}$ is unitary on $\mathcal{K}_\theta$, i.e. we have $\langle \mathrm{e}^{\mathrm{i}tA}u|\mathrm{e}^{\mathrm{i}tA}v\rangle = \langle u|v\rangle$ for all $u, v \in \mathcal{K}_\theta$.

The resolvent of K_θ is the restriction of the resolvent $R_{\hat{K}}(z) : \mathcal{E}^* \to \mathcal{E}$ explicitly described in (8.12) and it is easier to work with $R_{\hat{K}}(z)$. Here and below z is a fixed point in $\rho(h, k) \cap \rho(h_0, 0)$. Note that $\hat{K} - \hat{K}_0 = \left(\begin{smallmatrix} k & 0 \\ 0 & k \end{smallmatrix}\right) : \mathcal{E} \to \mathcal{E}^*$ is compact hence $R_{\hat{K}}(z) - R_{\hat{K}_0}(z) : \mathcal{E}^* \to \mathcal{E}$ is a compact operator too. In particular $R_{K_\theta}(z) - R_{K_{0,\theta}}(z)$ *is a compact operator on $\mathcal{K}_\theta$.*

Lemma 8.17. *K_θ and $K_{0,\theta}$ are of class $C^1_{\mathrm{u}}(A)$.*

Proof. It suffices to prove the stronger property that the map

$$\mathbb{R} \ni t \mapsto \mathrm{e}^{\mathrm{i}tA} R_{\hat{K}}(z) \mathrm{e}^{-\mathrm{i}tA} \in B(\mathcal{E}^*, \mathcal{E})$$

is norm differentiable. If we set $K(t) = \mathrm{e}^{\mathrm{i}tA} K \mathrm{e}^{-\mathrm{i}tA}$, this is clearly equivalent to the norm differentiability of $t \mapsto K(t) \in B(\mathcal{E}, \mathcal{E}^*)$. But this is obvious because if $h_t = \mathrm{e}^{-\mathrm{i}ta} h \mathrm{e}^{\mathrm{i}ta}$ and k_t is defined similarly, then we have $K(t) = \left(\begin{smallmatrix} k_t & 1 \\ h_t & k_t \end{smallmatrix}\right)$ and h_t, k_t clearly are norm differentiable when considered as $B(\langle h\rangle^{-\frac{1}{2}}\mathcal{H}, \langle h\rangle^{\frac{1}{2}}\mathcal{H})$ valued functions. □

We saw before that $K_{0,\theta} \geq 0$ and $\sigma(K_{0,\theta}) = \sigma(\varepsilon) \cup \sigma(-\varepsilon)$. Our first purpose is to construct a such that A be conjugate to $K_{0,\theta}$ on some subsets of its spectrum. Our choice of A does not seem convenient because

$$[K_{0,\theta}, \mathrm{i}A] = \begin{pmatrix} 0 & 0 \\ [\varepsilon^2, \mathrm{i}a] & 0 \end{pmatrix}, \tag{8.41}$$

but the restriction to positive or negative energies of this commutator satisfies the Mourre estimate. It is here that positivity properties of functions of $K_{0,\theta}$ with respect to the Krein structure of $\mathcal{K}_\theta$ will play a role.

Lemma 8.18. *Let $\varphi \in \Lambda_\theta$ with $\varphi \geq 0$. If $\varphi(\lambda) = 0$ for $\lambda \leq 0$ then $\varphi(K_{0,\theta}) \geq 0$. If $\varphi(\lambda) = 0$ for $\lambda \geq 0$ then $\varphi(K_{0,\theta}) \leq 0$.*

Proof. In the first case we obtain from (8.25)

$$\varphi(K_{0,\theta}) = \frac{1}{2}\begin{pmatrix} \varphi(\varepsilon) & \varphi(\varepsilon)/\varepsilon \\ \varepsilon\varphi(\varepsilon) & \varphi(\varepsilon) \end{pmatrix} \tag{8.42}$$

while in the second case we get

$$\varphi(K_{0,\theta}) = \frac{1}{2}\begin{pmatrix} \varphi(-\varepsilon) & -\varphi(-\varepsilon)/\varepsilon \\ -\varepsilon\varphi(-\varepsilon) & \varphi(-\varepsilon) \end{pmatrix} \tag{8.43}$$

and Lemma 3.6 gives the stated results. □

Remark 8.19. By using the "spectral projections" $\Pi_\pm = \mathbb{1}_{\mathbb{R}^\pm}(H_0)$ associated to the intervals $\mathbb{R}^\pm$ discussed in Remark 8.15 we see that the operator H_0 is "scalar" on each of the regions $\lambda > 0$ and $\lambda < 0$ in the following sense: if φ is a bounded function with compact support in one of the regions $\lambda > 0$ or $\lambda < 0$ then

$$H_0\Pi_\pm = \pm\varepsilon\Pi_\pm \quad \text{and} \quad \varphi(H_0) = \varphi(H_0)\Pi_\pm = \varphi(\pm\varepsilon)\Pi_\pm \tag{8.44}$$

This is a simple computation based on (8.42) and (8.43). Note however that the second equality above is also a direct consequence of the first one, i.e. the explicit relations (8.42) and (8.43) are not really needed.

Remark 8.20. If $\inf \varepsilon > 0$ and $\theta = 1/4$ then $\Pi_\pm$ are bounded orthogonal projections on $\mathcal{K}_{1/4}$ with $\Pi_+\Pi_- = \Pi_-\Pi_+ = 0$, $\Pi_+ + \Pi_- = \mathbb{1}$, and $\pm\Pi_\pm \geq 0$. Then $\mathcal{K}_\pm = \pm\Pi_\pm\mathcal{K}_{1/4}$ are Hilbert spaces (the minus sign means that we change the sign of the scalar product), we have $\mathcal{K}_{1/4} = \mathcal{K}_+ \oplus \mathcal{K}_-$ topologically, and the operator $K_{0,1/4}$ leaves $\mathcal{K}_\pm$ invariant and induces there self-adjoint operators in the usual sense. But the operators $\mathrm{e}^{\mathrm{i}tA}$ do note leave invariant this direct sum if the commutator $[K_{0,1/4}, \mathrm{i}A]$ is not trivial.

Lemma 8.21. *Let $\varphi, \psi \in C_0^\infty(]0,\infty[)$ with $\varphi\psi = \varphi$. Then*

$$\varphi(K_{0,\theta}) = \varphi(K_{0,\theta})\psi(\varepsilon) = \psi(\varepsilon)\varphi(K_{0,\theta}),$$

and

$$\varphi(K_{0,\theta})[K_{0,\theta}, \mathrm{i}A]\varphi(K_{0,\theta}) = \varphi(K_{0,\theta})\psi(\varepsilon)\varepsilon'\psi(\varepsilon)\varphi(K_{0,\theta}). \tag{8.45}$$

Proof. Clearly

$$\varphi(K_{0,\theta}) = \varphi(K_{0,\theta})\psi(K_{0,\theta})\Pi_+ = \varphi(K_{0,\theta})\Pi_+\psi(\varepsilon) = \varphi(K_{0,\theta})\psi(\varepsilon).$$

Then the left hand side above is

$$\begin{aligned} & \varphi(K_{0,\theta})K_{0,\theta}\mathrm{i}A\varphi(K_{0,\theta}) - \varphi(K_{0,\theta})\mathrm{i}AK_{0,\theta}\varphi(K_{0,\theta}) \\ = \;& \varphi(K_{0,\theta})\psi(\varepsilon)\varepsilon\mathrm{i}a\psi(\varepsilon)\varphi(K_{0,\theta}) - \varphi(K_{0,\theta})\psi(\varepsilon)\mathrm{i}a\varepsilon\psi(\varepsilon)\varphi(K_{0,\theta}), \end{aligned}$$

which is equal to $\varphi(K_{0,\theta})\psi(\varepsilon)[\varepsilon, \mathrm{i}a]\psi(\varepsilon)\varphi(K_{0,\theta})$. □

Lemma 8.22. *Assume that $\mathbb{1}_U(\varepsilon)\varepsilon'\mathbb{1}_U(\varepsilon) = \phi(\varepsilon)\mathbb{1}_U(\varepsilon)$ for some open set $U \subset \mathbb{R}^+$ and some $\phi \in C_0(]0,\infty[)$. Then*

$$\varphi(K_\theta)K'_\theta\varphi(K_\theta) \simeq \varphi(K_\theta)\phi(K_\theta)\varphi(K_\theta), \;\; \forall \varphi \in C_0^\infty(U).$$

Proof. Due to Lemma 7.15 we have $\varphi(K_\theta)K'_\theta\varphi(K_\theta) \simeq \varphi(K_{0,\theta})K'_{0,\theta}\varphi(K_{0,\theta})$. Let $\psi \in C_0^\infty(U)$ such that $\varphi\psi = \varphi$. Then Lemma 8.21 implies

$$\begin{aligned} & \varphi(K_\theta)K'_\theta\varphi(K_\theta) \simeq \varphi(K_{0,\theta})\psi(\varepsilon)\varepsilon'\psi(\varepsilon)\varphi(K_{0,\theta}) \\ = \;& \varphi(K_{0,\theta})\psi(\varepsilon)\phi(\varepsilon)\psi(\varepsilon)\varphi(K_{0,\theta}) \\ = \;& \varphi(K_{0,\theta})\phi(K_{0,\theta})\varphi(K_{0,\theta}) \\ \simeq \;& \varphi(K_\theta)\phi(K_\theta)\varphi(K_\theta). \;\square \end{aligned}$$

In the next proposition, we prove a Mourre estimate for K_θ, assuming that K_θ is definitizable.

Proposition 8.23. *Assume that (E), (M) are satisfied and that K_θ is definitizable on $\mathcal{K}_\theta$. Let $J \subset]0,+\infty[$ be a compact interval with $\mathbb{1}_J(K_\theta) \geq 0$. Assume finally that*

$$\mathbb{1}_U(\varepsilon)\varepsilon'\mathbb{1}_U(\varepsilon) = \phi(\varepsilon)\mathbb{1}_U(\varepsilon), \tag{8.46}$$

with $U \subset]0,\infty[$ open and some $\phi \in C_0(]0,\infty[)$, $\phi(x) > 0$ on J. Then:

1. *J contains at most a finite number of eigenvalues of K_θ,*
2. *if $\lambda \in J$ is not an eigenvalue of K_θ then there is a number $c > 0$ and a neighborhood I of λ in J such that*

$$\mathbb{1}_I(K_\theta)\mathrm{Re}(K'_\theta)\mathbb{1}_I(K_\theta) \geq c\mathbb{1}_I(K_\theta).$$

Proof. If $\varphi \in C_0^\infty(U)$ then from Lemma 8.22 we get

$$\begin{aligned}\varphi(K_\theta)\mathrm{Re}(K'_\theta)\varphi(K_\theta) &= \mathrm{Re}(\varphi(K_\theta)K'_\theta\varphi(K_\theta))\\ \simeq\ \mathrm{Re}(\varphi(K_\theta)\phi(K_\theta)\varphi(K_\theta)) &= \varphi(K_\theta)\phi(K_\theta)\varphi(K_\theta).\end{aligned}$$

By taking φ equal to 1 on J we get

$$\mathbb{1}_I(K_\theta)\mathrm{Re}(K'_\theta)\mathbb{1}_I(K_\theta) \simeq \phi(K_\theta)\mathbb{1}_J K_\theta) \geq (\inf_J \phi)\mathbb{1}_J(K_\theta).$$

Then we apply the virial theorem proved in Corollary 7.14. □

8.9. **Definitizability of charge Klein-Gordon operators.** In Prop. 8.23 we assumed that K_θ was definitizable. We state here a rather standard result in this direction, see [J2], [LNT2]. Note that the condition $0 \notin \sigma(\varepsilon)$ below can be interpreted as (strict) *positivity of the mass*.

Proposition 8.24. *Assume (A1), (A2) of Sect. 8.2 and $0 \notin \sigma(\varepsilon)$. Then $K_{1/4}$ is definitizable on $(\mathcal{K}_{1/4}, \langle\cdot|\cdot\rangle)$. Moreover the critical points of $K_{1/4}$ are eigenvalues.*

Proof. The result follows directly from [J2], provided we check the hypotheses there. Let us denote for simplicity $\mathcal{K}_{1/4}$, $K_{0,1/4}$ and $K_{1/4}$ simply by $\mathcal{K}$, K_0 and K. Since $0 \notin \sigma(\varepsilon)$, we can equip $\mathcal{K}$ with the Hilbertian scalar product

$$(u|v)_{\mathcal{K}} := (u_0|\varepsilon^{\frac{1}{2}}v_0) + (u_1|\varepsilon^{-\frac{1}{2}}v_1),$$

which induces the same topology on $\mathcal{K}$. K_0 is self-adjoint for $(\cdot|\cdot)_{\mathcal{K}}$, hence has no singular critical points (see [J2] for this notion). Moreover since $|K_0| = \left(\begin{smallmatrix}\varepsilon & 0\\ 0 & \varepsilon\end{smallmatrix}\right)$ the spaces $\mathcal{H}_{\pm 1}$ in [J2, Sect. 1.2] are equal to $\langle K_0\rangle^{\mp\frac{1}{2}}\mathcal{H}$. In particular we have

$$\mathcal{H}_1 = \mathcal{E},\ \mathcal{H}_{-1} = \mathcal{E}^*. \tag{8.47}$$

We have $K = K_0 + V$, for $V = \left(\begin{smallmatrix}k & 0\\ 0 & k\end{smallmatrix}\right)$. By (8.47) we see that $V : \mathcal{H}_1 \to \mathcal{H}_{-1}$ is compact iff $k : \langle\varepsilon\rangle^{-1}\mathcal{H} \to \mathcal{H}$ is compact, which holds by (E2). Therefore we can apply [J2, Thm. 3] to obtain the proposition. □

8.10. **Examples.** We now give some concrete examples. Let us consider the *charged Klein-Gordon equation* on Minkowski space:

$$(\partial_t - \mathrm{i}v(x))^2\phi(t,x) - \Delta_x\phi(t,x) + m^2\phi(t,x) = 0,\ \text{in } \mathbb{R}^{1+d}.$$

It is an example of (8.1) for $\mathcal{H} = L^2(\mathbb{R}^d, dx)$, $k = v(x)$ a real electric potential, and $h = -\Delta_x + m^2 - v^2(x)$, $m > 0$ is the mass of the Klein-Gordon field. Concerning the electric potential we assume

$$v\varepsilon^{-1} \text{ is compact on } L^2(\mathbb{R}^d), \tag{8.48}$$

Let us consider the charge Klein-Gordon operator $K = K_{1/4}$.

We have $h_0 = -\Delta_x + m^2$, $\varepsilon = (-\Delta_x + m^2)^{\frac{1}{2}}$ hence (E) is satisfied and $\varepsilon^{-1}\mathcal{H}$ equals the Sobolev space $H^1(\mathbb{R}^d)$.

As conjugate operator we take

$$a = \frac{1}{2}(f(|p|)p \cdot x + x \cdot pf(|p|)), \text{ with } f \in C_0^\infty(0,\infty),\ p = \mathrm{i}^{-1}\nabla_x.$$

Clearly (M) is satisfied. Moreover $[\varepsilon, \mathrm{i}a] = f(|p|)p^2\varepsilon^{-1}$. This implies that condition (8.46) in Prop. 8.23 is satisfied for all $U \subset \mathbb{R}\backslash\{0\}$.

The operator ε is clearly of class $C^\infty(a)$. If we assume that

$$\langle x\rangle^\alpha v\varepsilon^{-1} \text{ is bounded on } L^2(\mathbb{R}^d), \tag{8.49}$$

then k is of class $C^\alpha_{\mathrm{u}}(a)$. Therefore for $\alpha \geq 1$ condition (M2) is satisfied. Moreover we easily see that K is of class $C^\alpha(A)$. Therefore if (8.49) holds for some $\alpha > 3/2$ we can apply Thm. 7.9. Note that one may add in the standard way a long-range component $v_{\mathrm{l}}(x)$ to $v(x)$, by imposing a decay condition on $\partial_x^\alpha v(x)$ for $|\alpha| \leq 2$.

Note that the operator A, hence the weights $\langle A\rangle^{-s}$ are scalar operators. Again by standard arguments, one obtains finally the following resolvent estimate on K, for I a compact interval disjoint from eigenvalues of $K_{1/4}$:

$$\sup_{z\in I\pm\mathrm{i}]0,\nu]} \|\langle x\rangle^{-s}(K-z)^{-1}\langle x\rangle^{-s}\|_{B(\mathcal{K}_{1/4})} < \infty,\ \forall s > \frac{1}{2}.$$

Note that these estimates are also obtained in [GGH1], by a different method.

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