

Kreĭn-Višik-Birman self-adjoint extension theory revisited

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Abstract. The core results of the so-called Kreĭn-Višik-Birman theory of self-adjoint extensions of semi-bounded symmetric operators are reproduced, both in their original and in a more modern formulation, within a comprehensive discussion that includes missing details, elucidative steps, and intermediate results of independent interest.

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1. Introduction

This work has a two-fold purpose. On the one hand it aims at reproducing in their *original form* the key results of the so-called Kreĭn-Višik-Birman theory of self-adjoint extensions of semi-bounded symmetric operators, providing an expanded discussion, including missing details and supplementary formulas, of the original works, that up to a large extent are written in a rather compact style and are available in Russian only. On the other hand, the goal is to give evidence of how the original results can be equivalently re-written into what is now the more modern formulation of the theory, as it can be found in the (relatively limited) literature in English language on the subject, formulation which is derived by alternatives means, typically boundary triplets techniques.

The whole field is nowadays undoubtedly classical, and in fact to some extent even superseded by more modern mathematical techniques. Let us then give evidence in this Introduction of the context and of the degree of novelty of this work.

Self-adjointness and self-adjoint extension theory constitute a well-established branch of functional analysis and operator theory, with deep-rooted motivations and applications, among others, in the boundary value problems for partial differential equations and in the mathematical methods for quantum mechanics and quantum field theory. At the highest level of generality, it is von Neumann’s celebrated theory of self-adjoint extensions that provides, very elegantly, the complete solution to the problem of finding self-adjoint operator(s) that extend a given densely defined symmetric operator S on a given Hilbert space \mathcal{H} . As well known, the whole family of such extensions is naturally indexed by all the unitary maps U between the subspaces $\ker(S^* - z)$ and $\ker(S^* - \bar{z})$ of \mathcal{H} for a fixed $z \in \mathbb{C} \setminus \mathbb{R}$, the condition that such subspaces be isomorphic being necessary and sufficient for the problem to have a solution; each extension S_U is determined by an explicit constructive recipe, given U and the above subspaces.

A relevant special case is when S is semi-bounded – one customarily assumes it to be bounded *below*, and so shall we henceforth – which is in fact a typical situation in the quest for stable quantum mechanical Hamiltonians. In this case $\ker(S^* - z)$ and $\ker(S^* - \bar{z})$ are necessarily isomorphic, which guarantees the existence of self-adjoint extensions. Among them, a canonical

form construction (independent of von Neumann’s theory) shows that there exists a distinguished one, the Friedrichs extension S_F , whose bottom coincides with the one of S , which is characterised by being the only self-adjoint extension whose domain is entirely contained in the form domain of S , and which has the property to be the largest among all self-adjoint extensions of S , in the sense of the operator ordering “ \geq ” for self-adjoint operators.

The first systematic extension theory for semi-bounded operators is due to Kreĭn. Kreĭn’s theory shows that all self-adjoint extensions of S , whose bottom is above a prescribed reference level $m \in \mathbb{R}$, are naturally ordered, in the sense of “ \geq ”, between the Friedrichs extension from above (the “rigid” (жесткое) extension, in Kreĭn’s terminology), and a unique lowest extension S_N from below, whose bottom is not less than the chosen m , the so-called Kreĭn-von Neumann extension (the “soft” (мягкое) extension). In short: $S_F \geq \tilde{S} \geq S_N$ for any such extension \tilde{S} . (Let us refer to Appendix A for a more detailed summary of von Neumann’s and Kreĭn’s extension theory, or to modern overviews such as [52, Chapter X] and [56, Chapter 13].)

By the Kreĭn-Višik-Birman (KVB) theory (where the order here reflects the chronological appearance of the seminal works of Kreĭn [30], Višik [62], and Birman [8]), one means a development of Kreĭn’s original theory, in the form of an *explicit* and *extremely convenient* classification of all self-adjoint extensions of a given semi-bounded and densely defined symmetric operator S , both in the operator sense and in the quadratic form sense.

As the distinction “Kreĭn vs KVB” may appear a somewhat artificial retrospective, let us emphasize the following. In Kreĭn’s original work [30] each extension of S is proved to be bijectively associated with a self-adjoint extension, with unit norm, of the Kreĭn transform $(S - \mathbb{1})(S + \mathbb{1})^{-1}$ of S . This way, a difficult self-adjoint extension problem (extension of S) is shown to be equivalent to an easier one (extension of the Kreĭn transform of S), yet no general parametrisation of the extensions of S is given. The KVB theory provides in addition a parametrisation of the extensions, labelling each of them in the form S_B where B runs over all self-adjoint operators acting on Hilbert subspaces of $\ker(S^* + \lambda\mathbb{1})$, for some large enough $\lambda \geq 0$.

The KVB theory has a number of features that make it in many respects more informative as compared to von Neumann’s. First and most importantly, the KVB parametrisation $B \leftrightarrow S_B$ identifies special subclasses of extensions of S , such as those whose bottom is above a prescribed level, in terms of a corresponding subclass of parameters B . In particular, both the Friedrichs extension S_F and the Kreĭn-von Neumann extension S_N of S relative to a given reference lower bound can be selected a priori, meaning that the special parameter B that identifies S_F or S_N is explicitly known. In contrast, the parametrisation $U \leftrightarrow S_U$ based on unitaries U provided by von Neumann’s theory does not identify a priori the particular U that gives S_F or S_N . An amount of further relevant information concerning each extension, including invertibility, semi-boundedness, and special features of its negative spectrum (finiteness, multiplicity, accumulation points) turn out to be

controlled by the the analogous properties of the extension parameter. Furthermore, the KVB extension theory has a natural and explicit re-formulation in terms of quadratic forms, an obviously missing feature in von Neumann’s theory. On this last point, it is worth emphasizing that whereas the KVB classification of the extensions as *operators* is completely general, the classification in terms of the corresponding *quadratic forms* only applies to the family of *semi-bounded* self-adjoint extensions of S , while unbounded below extensions (if any) escape this part of the theory.¹

For several historical and scientific reasons (a fact that itself would indeed deserve a separate study) the mathematical literature in English language on the KVB theory is considerably more limited as compared to von Neumann’s theory. Over the decades the tendency has been in general to re-derive and discuss the main results through routes and with notation and “mathematical flavour” that differ from the original formulation.

At the price of an unavoidable oversimplification, we can say that while in the applications to quantum mechanics von Neumann’s theory has achieved a dominant role, and is nowadays a textbooks standard, on a more abstract mathematical level the original results of Kreĭn, Viřik, and Birman, and their applications to boundary value problems for elliptic PDE, have eventually found a natural evolution and generalisation within the modern theory of boundary triplets. Thus, in modern terms the deficiency space $\ker(S^* + \lambda\mathbb{1})$ is referred to as a *boundary value space*, this space is then equipped with a *boundary triplet structure*, and the extensions of S are parametrised by *linear relations* on the boundary space, with a distinguished position for the Friedrichs and the Kreĭn-von Neumann extensions that are intrinsically encoded in the choice of the boundary triplet.

However, this work is *neither* meant *nor* going to move from the point of view of the boundary triplet theory, which is surely a beautiful and prolific scheme within which one can indeed retrieve the old results of Kreĭn, Viřik, and Birman – in fact, the latter approach is already available in the literature: for example a recent, concise, and relatively complete survey of the re-derivation of Kreĭn, Viřik, and Birman from the boundary triplet theory may be found in [56, Chapters 13 and 14], and in the references therein.

Our perspective, instead, is primarily motivated by the use of the KVB theory in the rigorous construction of quantum Hamiltonians of particle systems with contact interactions and, more generally, in the extension theory of quantum Hamiltonians of few-body and many-body systems where the

¹If the subspaces $\ker(S^* - z\mathbb{1})$ and $\ker(S^* - \bar{z}\mathbb{1})$ have the same *finite* dimension, it is easy to conclude that all self-adjoint extensions of S are bounded below, see, e.g., the Proposition on page 179 of [52]; if their common dimension is *infinite* instead, S may also admit self-adjoint extensions that are unbounded below. The occurrence of such unbounded below extensions may be presented as a mere “academic exercise” about operators on an infinite orthogonal sum of Hilbert spaces (see [52, Chapter 10], Problem 26) but in fact examples are known where they arise as quantum Hamiltonians of physical relevance – see, e.g., the possibility of unbounded below self-adjoint extensions for particle Hamiltonians with point interaction [48, 47, 35, 36, 14, 37].

interaction is singular enough so as to make perturbative techniques inapplicable, and hence to give rise to a multiplicity of self-adjoint realisations to qualify and classify. This is a realm where customarily the largest part of the mathematics is worked out by means of the ‘dominant’ extension theory a la von Neumann, or by the theory of quadratic forms on Hilbert space, and to a lesser extent by means of tools from non-standard analysis or boundary triplets. However, results from Kreĭn and Birman have been known since long to bring in this context complementary or also new information: one paradigmatic instance is the study of particle Hamiltonians of contact interaction carried on by trailblazers such as Berezin, Faddeev, and above all Minlos and his school [48, 41, 45] – an ample historical survey of which is in [37, Section 2], further references being provided here at the end of Section 4. In the above-mentioned contexts, as we shall elaborate further later, comprehensive references in the literature are, and have been over the decades, quite limited in number and scope (as discussed in Section 4), due also to the circumstance that most of the original sources were available in Russian only.

The last considerations constitute our motivations for the present note, the object of which is therefore: first, to provide an exhaustive recapitulation of the KVB theory and of its ‘elementary’ derivation in the original operator-theoretic framework, thus with no reference to more modern superstructures such as boundary triplets; second, to reproduce, neatly and directly from the original formulation, the ‘modern’ version of the main results of the theory, that is, the version appearing essentially in all the (western) literature *after* Kreĭn, Višik, and Birman, and derived therein through more involved and more general schemes.

To this aim, in Section 2 we devote a careful effort to replicate the original results of the KVB theory, in order to make it accessible in its full rigour (and in English language) with respect to its initial version, that is, by filling certain gaps of the original proofs, supplementing the material with non-ambiguous notation and elucidative steps, producing and highlighting intermediate results that have their own independent interest. In a way, and this is our first novelty, the outcome is a complete and self-consistent “reading guide” for the original results and for the route to demonstrate them, together with a clean presentation of all the main statements that are mostly referred to in the applications, significantly Theorem 2.2 (together with the special cases (2.4) and (2.6)), Theorem 2.12, Theorem 2.15, Theorem 2.17, and Proposition 2.19.

Mirror to that, in Section 3 we reproduce an alternative, equivalent version of the main results of the KVB theory. These statements are actually those by which (part of) the KVB theory has been presented, re-derived, discussed, and applied in the subsequent literature in English language. Typically this was done by means of modern boundary-triplet-based extension techniques, whereas the novelty here is to derive such results directly from the original ones, with the minimum amount of operator theory (the key is

the inversion mechanism of our Proposition 3.1). Thus, Section 3 has the two-fold feature of proving the equivalence between “modern” and “original” formulations and of providing another reference scheme of all main results, significantly Theorem 3.4, Theorem 3.5, Theorem 3.6, Proposition 3.7, Theorem 3.9, and Proposition 3.10.

In Section 4 we place the KVB theory into a concise historical perspective of motivations, further developments, and applications.

In Section 5 we complete the main core of the theory with results that characterise relevant properties of the extensions, such as invertibility, semi-boundedness, and other special features of the negative discrete spectrum, in terms of the corresponding properties of the extension parameter.

In Section 6 we discuss, within the KVB formalism, the structure of resolvents of self-adjoint extensions, in the form of Kreĭn-like resolvent formulas. The results emerging from Sections 5 and 6 corroborates the picture that the KVB extension parametrisation is in many fundamental aspects more informative than von Neumann’s parametrisation.

Last, in Section 7 we show how the general formulas of the KVB theory apply to simple examples in which the extension problem by means of von Neumann’s theory is already well known, so as to make the comparison between the two approaches evident.

For reference and comparison purposes, in the final Appendix we organised an exhaustive summary of von Neumann’s and of Kreĭn’s self-adjoint extension theories, with special emphasis on the two “distinguished” extensions, the Friedrichs and the Kreĭn-von Neumann one.

Notation. Essentially all the notation adopted here is standard, let us only emphasize the following. Concerning the various sums of spaces that will occur, we shall denote by $\dot{+}$ the direct sum of vector spaces, by \oplus the direct orthogonal sum of *closed* Hilbert subspaces of the same underlying Hilbert space \mathcal{H} (the space where the initial symmetric and densely defined operator is taken), and by \boxplus the direct sum of subspaces of \mathcal{H} that are orthogonal to each other but are not a priori all closed. For any given symmetric operator S with domain $\mathcal{D}(S)$, we shall denote by $m(S)$ the “bottom” of S , i.e., its greatest lower bound

$$m(S) := \inf_{\substack{f \in \mathcal{D}(S) \\ f \neq 0}} \frac{\langle f, Sf \rangle}{\|f\|^2}. \quad (1.1)$$

S being semi-bounded means therefore $m(S) > -\infty$. Let us also adopt the customary convention to distinguish the *operator* domain and the *form* domain of any given densely defined and symmetric operator S by means of the notation $\mathcal{D}(S)$ vs $\mathcal{D}[S]$. To avoid ambiguities, V^\perp will always denote the orthogonal complement of a subspace V of \mathcal{H} *with respect to \mathcal{H} itself*: when interested in the orthogonal complement of V within a closed subspace K of \mathcal{H} we shall keep the extended notation $V^\perp \cap K$. Analogously, the closure \bar{V} of the considered subspaces will be always meant with respect to the norm-topology of the underlying Hilbert space \mathcal{H} . As no particular ambiguity arises

in our formulas when referring to the identity operator, we shall use the symbol $\mathbb{1}$ for it irrespectively of the subspace of \mathcal{H} it acts on. As for the spectral measure of a self-adjoint operator A we shall use the standard notation $dE^{(A)}$ (see, e.g., [56, Chapters 4 and 5]). As customary, $\sigma(T)$ and $\rho(T)$ shall denote, respectively, the spectrum and the resolvent set of an operator T on Hilbert space.

2. Fundamental results in the KVB theory: original version.

In this Section we reproduce, through an expanded and more detailed discussion, the pillars of the KVB theory for self-adjoint extensions of bounded below symmetric operator, in the form they were established in the original works Kreĭn [30], Višik [62], and Birman [8]. The main statements are Lemma 2.1, Theorem 2.2, Remark 2.3, Theorem 2.12, Theorem 2.15, Theorem 2.17, and Proposition 2.19 below. The notation, when applicable, is kept on purpose the same as that of those works.

2.1. General assumptions. Choice of a reference lower bound.

In the following we shall assume that S is a semi-bounded (below), not necessarily closed, densely defined symmetric operator acting on a Hilbert space \mathcal{H} . Unlike the early developments of the theory (Kreĭn's theory), no restriction is imposed to the magnitude of the deficiency indices $\dim \ker(S^* \pm i)$ of S : in particular, they can also be infinite.

It is not restrictive to assume further

$$m(S) > 0, \tag{2.1}$$

for in the general case one applies the discussion that follows to the strictly positive operator $S + \lambda\mathbb{1}$, $\lambda > -m(S)$, and then re-express trivially the final results in terms of the original S .

Associated to S are two canonical, distinguished self-adjoint extensions, the well-known *Friedrichs* extension S_F and *Kreĭn-von Neumann* extension S_N . Whereas a complete summary of the construction and of the properties of such extensions is presented in Appendix A.2, which we will be making reference to whenever in the following we shall need a particular attribute of S_F or S_N for the proofs, let us recall here their distinguishing features.

The extension S_F is semi-bounded and with the same bottom $m(S_F) = m(S)$ of S . Its quadratic form is precisely the closure of the (closable) quadratic form associated with S . In fact, S_F is the restriction of S^* to the domain $\mathcal{D}[S] \cap \mathcal{D}(S^*)$. Among all self-adjoint extensions of S , S_F is *the only one* whose operator domain is contained in $\mathcal{D}[S]$, and moreover S_F is larger than any other semi-bounded extension \tilde{S} of S , in the sense of the ordering $S_F \geq \tilde{S}$ (which, in particular, means $\mathcal{D}[S_F] \subset \mathcal{D}[\tilde{S}]$).

Thus, *the choice* $m(S) > 0$ *implies that the Friedrichs extension* S_F *of* S *is invertible with bounded inverse defined everywhere on* \mathcal{H} : this will allow S_F^{-1} to enter directly the discussion. In the general case in which S_F is not necessarily invertible, the role of S_F^{-1} can be naturally replaced in many

respects (but not all) by the inverse \tilde{S}^{-1} of any a priori known self-adjoint extension \tilde{S} of S , which thus takes the role of given “datum” of the theory. As an example see the role played by the Friedrichs extension in the proofs of Lemma 2.14 and Theorems 2.15, 2.17.

With the choice $m(S) > 0$, the level 0 becomes naturally the reference value with respect to which to express the other distinguished (canonically given) extension of S , the Kreĭn-von Neumann extension S_N . It is qualified among all other positive self-adjoint extensions \tilde{S} of S by being the unique smallest, in the sense $\tilde{S} \geq S_N$.

We underline that unlike Kreĭn’s original theory and many of the recent presentations of the KVB theory, the discussion here is *not* going to be restricted to the positive self-adjoint extensions of S . On the contrary, we shall present the full theory that includes also those extensions, if any, with finite negative bottom, or even unbounded below.

2.2. Adjoint of a semi-bounded symmetric operator. Regular and singular part.

The first step of the theory is to describe the structure of the *domain of the adjoint* S^* of S . Recall that a characterisation of $\mathcal{D}(S^*)$ is already given by von Neumann’s formula

$$\mathcal{D}(S^*) = \mathcal{D}(\bar{S}) \dot{+} \ker(S^* - z\mathbb{1}) \dot{+} \ker(S^* - \bar{z}\mathbb{1}) \quad \text{for } z \in \mathbb{C} \setminus \mathbb{R}, \quad (2.2)$$

which is valid, more generally, for any densely defined S . The KVB theory works with a “real” version of (2.2), with $z = 0$ and with the space

$$U := \ker S^* \quad (2.3)$$

instead of the two deficiency spaces $\ker(S^* - z\mathbb{1})$ and $\ker(S^* - \bar{z}\mathbb{1})$. With a self-explanatory nomenclature, U shall henceforth be referred to as *the* deficiency space of S , with no restriction on $\dim U$.

The result consists of a decomposition of $\mathcal{D}(S^*)$ first proved by Kreĭn (see also Remark A.11) and a further refinement, initially due to Viřik, to which Birman gave later an alternative proof.

Lemma 2.1 (Kreĭn decomposition formula for $\mathcal{D}(S^*)$). *For a densely defined symmetric operator S with positive bottom,*

$$\mathcal{D}(S^*) = \mathcal{D}(S_F) \dot{+} \ker S^*. \quad (2.4)$$

Proof. $\mathcal{D}(S^*) \supset \mathcal{D}(S_F) + \ker S^*$ because each summand is a subspace of $\mathcal{D}(S^*)$. As for the opposite inclusion, one can always decompose an arbitrary $g \in \mathcal{D}(S^*)$ as $g = S_F^{-1}S^*g + (g - S_F^{-1}S^*g)$, where $S_F^{-1}S^*g \in \mathcal{D}(S_F)$, and where $g - S_F^{-1}S^*g \in \ker S^*$, because $S^*(g - S_F^{-1}S^*g) = S^*g - S^*g = 0$. Last, the sum in the r.h.s. of (2.4) is direct because any $g \in \mathcal{D}(S_F) \cap \ker S^*$ is necessarily in $\ker S_F$ ($S_Fg = S^*g = 0$), and from $0 < m(S) = m(S_F)$ one has $\ker S_F = \{0\}$. \square

Theorem 2.2 (Višik-Birman decomposition formula for $\mathcal{D}(S^*)$). *For a densely defined symmetric operator S with positive bottom,*

$$\mathcal{D}(S^*) = \mathcal{D}(\overline{S}) \dot{+} S_F^{-1} \ker S^* \dot{+} \ker S^* . \quad (2.5)$$

Proof. Let $U = \ker S^*$. As in the proof of Lemma 2.1, $\mathcal{D}(S^*) \supset \mathcal{D}(\overline{S}) \dot{+} S_F^{-1}U \dot{+} U$ is obvious and conversely any $g \in \mathcal{D}(S^*)$ can be written as $g = S_F^{-1}S^*g + u$ for some $u \in U = \ker S^*$. In turn, owing to $\mathcal{H} = \overline{\text{ran } S} \oplus \ker S^*$, one writes $S^*g = h_0 + \tilde{u}$, and hence $S_F^{-1}S^*g = S_F^{-1}h_0 + S_F^{-1}\tilde{u}$, for some $\tilde{u} \in U$ and $h_0 = \lim_{n \rightarrow \infty} S\varphi_n$ for some sequence $(\varphi_n)_n$ in $\mathcal{D}(S)$. From $\varphi_n = S_F^{-1}S\varphi_n \rightarrow S_F^{-1}h_0$ and $S\varphi_n \rightarrow h_0$ as $n \rightarrow \infty$, and from the closability of S , one deduces that $f := S_F^{-1}h_0 \in \mathcal{D}(\overline{S})$. Therefore, $g = f + S_F^{-1}\tilde{u} + u$, which proves $\mathcal{D}(S^*) \subset \mathcal{D}(\overline{S}) + S_F^{-1}U + U$. Last, one concludes that the sum in (2.5) is direct as follows: if $g = f + S_F^{-1}\tilde{u} + u = 0$, then $0 = S^*g = \overline{S}f + \tilde{u}$, which forces $\overline{S}f = \tilde{u} = 0$ because $\overline{S}f \perp \tilde{u}$; then also $f = S_F^{-1}\overline{S}f = 0$ and, from $g = 0$, also $u = 0$. \square

Remark 2.3. The argument of the proof above can be repeated to conclude

$$\mathcal{D}(S_F) = \mathcal{D}(\overline{S}) \dot{+} S_F^{-1} \ker S^* . \quad (2.6)$$

and hence

$$\mathcal{D}(S_F) \cap \ker S^* = \{0\} . \quad (2.7)$$

Indeed, while it is obvious that the r.h.s. of (2.6) is contained in the l.h.s., conversely one takes a generic $g \in \mathcal{D}(S_F)$ and decomposes $S_F g = h_0 + \tilde{u}$ with $h_0 \in \overline{\text{ran } S}$ and $\tilde{u} \in U$ as above, whence, by the same argument, $g = S_F^{-1}h_0 + S_F^{-1}\tilde{u}$ with $S_F^{-1}h_0 \in \mathcal{D}(\overline{S})$.

Remark 2.4. Precisely as in the remark above, one also concludes that

$$\mathcal{D}(\tilde{S}) = \mathcal{D}(\overline{S}) \dot{+} \tilde{S}^{-1} \ker S^* \quad (2.8)$$

for any self-adjoint extension \tilde{S} of S that is invertible everywhere on \mathcal{H} .

Remark 2.5. Since S is closable and injective ($m(S) > 0$), then as well known

$$\overline{\text{ran } S} = \text{ran } \overline{S} . \quad (2.9)$$

Thus, in the above proof one could claim immediately that $h_0 = \overline{S}f$ for some $f \in \mathcal{D}(\overline{S})$, whence $S_F^{-1}h_0 = S_F^{-1}\overline{S}f = f \in \mathcal{D}(\overline{S})$.

Remark 2.6. In view of the applications in which S and S_F are differential operators on an L^2 -space and hence $\mathcal{D}(S_F)$ indicates an amount of regularity of its elements, it is convenient to regard $\mathcal{D}(S_F) = \mathcal{D}(\overline{S}) \dot{+} S_F^{-1}U$ in (2.5) as the “regular component” and, in contrast, $U = \ker S^*$ as the “singular component” of the domain of S^* .

Remark 2.7. In all the previous formulas the assumption $m(S) > 0$ only played a role to guarantee the existence of the everywhere defined and bounded operator S_F^{-1} . It is straightforward to adapt the arguments above to prove

the following: if S is a symmetric and densely defined operator on \mathcal{H} and \tilde{S} is a self-adjoint extension of S , then for any $z \in \rho(\tilde{S})$ (the resolvent set of \tilde{S})

$$\mathcal{D}(S^*) = \mathcal{D}(\overline{S}) \dot{+} (\tilde{S} - z\mathbb{1})^{-1} \ker(S^* - \bar{z}\mathbb{1}) \dot{+} \ker(S^* - z\mathbb{1}) \quad (2.10)$$

$$\mathcal{D}(S^*) = \mathcal{D}(\tilde{S}) \dot{+} \ker(S^* - z\mathbb{1}) \quad (2.11)$$

$$\mathcal{D}(\tilde{S}) = \mathcal{D}(\overline{S}) \dot{+} (\tilde{S} - z\mathbb{1})^{-1} \ker(S^* - \bar{z}\mathbb{1}). \quad (2.12)$$

2.3. Višik's B operator.

To a generic self-adjoint extension of S one associates, canonically with respect to the decomposition (2.5), a self-adjoint operator B acting on a Hilbert subspace of $\ker S^*$. This “*Višik's B operator*” defined in (2.22) below (introduced first by Višik in [62]) turns out to be a convenient label to index the self-adjoint extensions of S : this is going to be done in formula (2.23) proved in the end of this Subsection.

Let \tilde{S} be a self-adjoint extension of S . Correspondingly, let U_0 and U_1 be the two closed subspaces of $U = \ker S^*$ (and hence of \mathcal{H}), and let \mathcal{H}_+ be the closed subspace of \mathcal{H} , uniquely associated to \tilde{S} by means of the definitions

$$U_0 := \ker \tilde{S}, \quad U = U_0 \oplus U_1, \quad \mathcal{H}_+ := \overline{\text{ran} \tilde{S}} \oplus U_1. \quad (2.13)$$

Thus,

$$\mathcal{H} = \overline{\text{ran} \tilde{S}} \oplus \ker S^* = \overline{\text{ran} \tilde{S}} \oplus U_1 \oplus U_0 = \mathcal{H}_+ \oplus \ker \tilde{S}. \quad (2.14)$$

Let $P_+ : \mathcal{H} \rightarrow \mathcal{H}$ be the orthogonal projection onto \mathcal{H}_+ .

The operator \tilde{S} has the following properties.

Lemma 2.8.

- (i) $\overline{\text{ran} \tilde{S}} \oplus U_1 = \mathcal{H}_+ = \overline{\text{ran} \tilde{S}}$, i.e., $\text{ran} \tilde{S}$ is dense in \mathcal{H}_+
- (ii) $\ker \tilde{S} = (\mathbb{1} - P_+) \mathcal{D}(\tilde{S})$
- (iii) $\mathcal{D}(\tilde{S}) = (\mathcal{D}(\tilde{S}) \cap \mathcal{H}_+) \boxplus \ker \tilde{S} = P_+ \mathcal{D}(\tilde{S}) \boxplus \ker \tilde{S}$ and also $\mathcal{D}(\tilde{S}) \cap \mathcal{H}_+ = P_+ \mathcal{D}(\tilde{S})$
- (iv) $\mathcal{D}(\tilde{S}) \cap \mathcal{H}_+$ is dense in \mathcal{H}_+
- (v) \tilde{S} maps $\mathcal{D}(\tilde{S}) \cap \mathcal{H}_+$ into \mathcal{H}_+
- (vi) $\text{ran} \tilde{S} = \text{ran} \overline{S} \boxplus \tilde{U}_1$ where \tilde{U}_1 is a dense subspace of U_1 uniquely identified by \tilde{S} .

Proof. (i) follows by (2.14), because $\overline{\text{ran} \tilde{S}}$ is the orthogonal complement to $\ker \tilde{S}$ in \mathcal{H} (owing to the self-adjointness of \tilde{S}). In (ii) the “ \supset ” inclusion is obvious and conversely, if $u_0 \in \ker \tilde{S} \subset \mathcal{D}(\tilde{S})$, then $u_0 = (\mathbb{1} - P_+)u_0 \in (\mathbb{1} - P_+) \mathcal{D}(\tilde{S})$. To establish (iii), decompose a generic $g \in \mathcal{D}(\tilde{S})$ as $g = f_+ + u_0$ for some $f_+ \in \mathcal{H}_+$ and $u_0 \in U_0 = \ker \tilde{S}$ (using $\mathcal{H} = \mathcal{H}_+ \oplus \ker \tilde{S}$): since $f_+ = g - u_0 \in \mathcal{D}(\tilde{S})$, then $f_+ \in \mathcal{D}(\tilde{S}) \cap \mathcal{H}_+$ and therefore $\mathcal{D}(\tilde{S}) \subset (\mathcal{D}(\tilde{S}) \cap \mathcal{H}_+) \boxplus \ker \tilde{S}$. The opposite inclusion is obvious, thus $\mathcal{D}(\tilde{S}) = (\mathcal{D}(\tilde{S}) \cap \mathcal{H}_+) \boxplus \ker \tilde{S}$. It remains to prove that $\mathcal{D}(\tilde{S}) \cap \mathcal{H}_+ = P_+ \mathcal{D}(\tilde{S})$: the inclusion $\mathcal{D}(\tilde{S}) \cap \mathcal{H}_+ \subset P_+ \mathcal{D}(\tilde{S})$ is obvious, as for the converse, if $h = P_+ g \in P_+ \mathcal{D}(\tilde{S})$ for some $g \in \mathcal{D}(\tilde{S})$, decompose $g = f_+ + u_0$ in view of $\mathcal{D}(\tilde{S}) = (\mathcal{D}(\tilde{S}) \cap \mathcal{H}_+) \boxplus \ker \tilde{S}$, then $h =$

$P_+g = f_+ \in \mathcal{D}(\tilde{S}) \cap \mathcal{H}_+$, which completes the proof. To establish (iv), for fixed arbitrary $h_+ \in \mathcal{H}_+$ let $(f_n)_{n \in \mathbb{N}}$ be a sequence in $\mathcal{D}(\tilde{S})$ of approximants of h_+ (indeed $\mathcal{D}(\tilde{S})$ is dense in \mathcal{H}): then, as $n \rightarrow \infty$, $f_n \rightarrow h_+$ implies $P_+f_n \rightarrow h_+$. (v) is an immediate consequence of (i), because \tilde{S} maps $\mathcal{D}(\tilde{S}) \cap \mathcal{H}_+$ into $\text{ran} \tilde{S}$. Last, let us prove (vi). Recall that $\overline{\text{ran} \tilde{S}} = \text{ran} \bar{S}$, because S is closable and injective ($m(S) > 0$). Set $\tilde{U}_1 := \{u_g \in U_1 \mid \tilde{S}g = \bar{S}f_g + u_g \text{ for } g \in \mathcal{D}(\tilde{S})\}$, where $f_g \in \mathcal{D}(\tilde{S})$ and $u_g \in U_1$ are uniquely determined by the given $g \in \mathcal{D}(\tilde{S})$ through (i) and the decomposition $\overline{\text{ran} \tilde{S}} = \mathcal{H}_+ = \text{ran} \bar{S} \oplus U_1$. The inclusions $\text{ran} \tilde{S} \subset \text{ran} \bar{S} \boxplus \tilde{U}_1$ and $\text{ran} \tilde{S} \supset \text{ran} \bar{S}$ are obvious, furthermore $\text{ran} \tilde{S} \supset \tilde{U}_1$ because each $\tilde{u}_1 \in \tilde{U}_1$ is by definition the difference of two elements in $\text{ran} \tilde{S}$. Thus, $\text{ran} \tilde{S} = \text{ran} \bar{S} \boxplus \tilde{U}_1$. It remains to prove the density of \tilde{U}_1 in U_1 . Given an arbitrary $u_1 \in U_1 \subset \mathcal{H}_+$ and a sequence $(\tilde{S}g_n)_{n \in \mathbb{N}} \in \text{ran} \tilde{S}$ of approximants of u_1 (owing to the density of $\text{ran} \tilde{S}$ in \mathcal{H}_+), decompose $\tilde{S}g_n = \bar{S}f_n + \tilde{u}_n$, for some $f_n \in \mathcal{D}(\tilde{S})$ and $\tilde{u}_n \in \tilde{U}_1$, in view of $\text{ran} \tilde{S} = \text{ran} \bar{S} \boxplus \tilde{U}_1$: denoting by $P_1 : \mathcal{H}_+ \rightarrow \mathcal{H}_+$ the orthogonal projection onto U_1 , one has $u_1 = P_1 u_1 = P_1 \lim_n (\bar{S}f_n + \tilde{u}_n) = \lim_n \tilde{u}_n$, which shows that $(\tilde{u}_n)_{n \in \mathbb{N}}$ is a sequence in \tilde{U}_1 of approximants of u_1 . \square

Since \tilde{S} maps $\mathcal{D}(\tilde{S}) \cap \mathcal{H}_+$ into \mathcal{H}_+ and trivially U_0 into itself, and since P_+ maps $\mathcal{D}(\tilde{S})$ into itself (Lemma 2.8(iii)), then \mathcal{H}_+ and U_0 are reducing subspaces for \tilde{S} (see, e.g., [56, Prop. 1.15]). The non-trivial (i.e., non-zero) part of \tilde{S} in this reduction is the operator

$$\tilde{S}_+ := \tilde{S} \upharpoonright \mathcal{D}(\tilde{S}_+), \quad \mathcal{D}(\tilde{S}_+) := \mathcal{D}(\tilde{S}) \cap \overline{\text{ran} \tilde{S}} = P_+ \mathcal{D}(\tilde{S}), \quad (2.15)$$

which is therefore a densely defined, injective, and self-adjoint operator on the Hilbert space \mathcal{H}_+ . Explicitly,

$$\begin{aligned} \text{ran} \tilde{S} &= \{\tilde{S}g \mid g \in \mathcal{D}(\tilde{S})\} = \{\tilde{S}P_+g \mid g \in \mathcal{D}(\tilde{S})\} \\ \tilde{S}_+P_+g &= \tilde{S}P_+g \quad \forall g \in \mathcal{D}(\tilde{S}) \\ \text{ran} \tilde{S}_+ &= \text{ran} \tilde{S}. \end{aligned} \quad (2.16)$$

The inverse of \tilde{S}_+ (on \mathcal{H}_+) is the self-adjoint operator \tilde{S}_+^{-1} with

$$\begin{aligned} \mathcal{D}(\tilde{S}_+^{-1}) &= \text{ran} \tilde{S}, \\ \tilde{S}_+^{-1}(\tilde{S}P_+g) &= P_+g \quad \forall g \in \mathcal{D}(\tilde{S}) \end{aligned} \quad (2.17)$$

and hence

$$\text{ran}(\tilde{S}_+^{-1}) = \tilde{S}_+^{-1} \text{ran} \tilde{S} = P_+ \mathcal{D}(\tilde{S}) \quad (2.18)$$

$$\tilde{S}_+^{-1} \text{ran} \bar{S} = P_+ \mathcal{D}(\bar{S}). \quad (2.19)$$

((2.19) follows from $\tilde{S}_+^{-1}(\tilde{S}P_+f) = P_+f$ in (2.17), letting now f run on $\mathcal{D}(\bar{S})$ only: the r.h.s. gives $P_+ \mathcal{D}(\bar{S})$, in the l.h.s. one uses that $\tilde{S}P_+f = \tilde{S}f = \bar{S}f$ $\forall f \in \mathcal{D}(\bar{S})$ and hence $\{\tilde{S}P_+f \mid f \in \mathcal{D}(\bar{S})\} = \text{ran} \bar{S}$.)

Furthermore, by setting

$$\begin{aligned}\mathcal{D}(\mathcal{S}^{-1}) &:= \mathcal{D}(\tilde{S}_+^{-1}) \boxplus U_0 = \text{ran}\tilde{S} \boxplus \ker\tilde{S} \\ \mathcal{S}^{-1}\tilde{S}g &:= \tilde{S}_+^{-1}\tilde{S}g = g \quad \forall g \in \mathcal{D}(\tilde{S}) \\ \mathcal{S}^{-1} \upharpoonright \ker\tilde{S} &:= \mathbb{O},\end{aligned}\tag{2.20}$$

one defines a self-adjoint operator \mathcal{S}^{-1} on the whole \mathcal{H} , with reducing subspaces $\mathcal{H}_+ = \overline{\text{ran}\tilde{S}}$ and $U_0 = \ker\tilde{S}$.

Two further useful properties are the following.

Lemma 2.9.

- (i) $\mathcal{D}(\bar{S}) + U_0 = P_+\mathcal{D}(\bar{S}) \boxplus U_0$
- (ii) $P_+\mathcal{D}(\tilde{S}) = P_+\mathcal{D}(\bar{S}) + \mathcal{S}^{-1}\tilde{U}_1$.

Proof. The inclusion $\mathcal{D}(\bar{S}) + U_0 \subset P_+\mathcal{D}(\bar{S}) \boxplus U_0$ in (i) follows from the fact that each summand in the l.h.s. belongs to the sum in the r.h.s., in particular, $\mathcal{D}(\bar{S}) \subset P_+\mathcal{D}(\bar{S}) + (\mathbb{1} - P_+)\mathcal{D}(\bar{S})$. Conversely, given a generic $h = P_+f \in P_+\mathcal{D}(\bar{S})$ for some $f \in \mathcal{D}(\bar{S})$ and $u_0 \in U_0$, then $h + u_0 = f + u'_0$ with $u'_0 := u_0 - (\mathbb{1} - P_+)f \in U_0$, which proves the inclusion $\mathcal{D}(\bar{S}) + U_0 \supset P_+\mathcal{D}(\bar{S}) \boxplus U_0$. (ii) follows by applying \mathcal{S}^{-1} to the decomposition $\text{ran}\tilde{S} = \text{ran}\bar{S} \boxplus \tilde{U}_1$ of Lemma 2.8(vi), for on the l.h.s. one gets $\mathcal{S}^{-1}\text{ran}\tilde{S} = P_+\mathcal{D}(\tilde{S})$, owing to (2.20), whereas on the r.h.s. one gets $\mathcal{S}^{-1}\text{ran}\bar{S} = P_+\mathcal{D}(\bar{S})$, owing to (2.19). \square

Summarising so far, the given operator S and the given self-adjoint extension \tilde{S} determine canonically (and, in fact, constructively) the closed subspace U_1 of $\ker S^*$, the dense subspace \tilde{U}_1 in U_1 , the closed subspace $\mathcal{H}_+ = \overline{\text{ran}\tilde{S}} = \text{ran}\bar{S} \oplus U_1$ of \mathcal{H} (equivalently, the orthogonal projection P_+ onto \mathcal{H}_+), and the self-adjoint operator \mathcal{S}^{-1} on \mathcal{H} , with the properties discussed above. In terms of these data, one defines

$$\begin{aligned}\mathcal{B} &:= \mathcal{S}^{-1} - P_+S_F^{-1}P_+ \\ \mathcal{D}(\mathcal{B}) &:= \mathcal{D}(\mathcal{S}^{-1}) = \text{ran}\tilde{S} \boxplus \ker\tilde{S},\end{aligned}\tag{2.21}$$

a self-adjoint operator on \mathcal{H} with the following properties.

Lemma 2.10.

- (i) \mathcal{B} is self-adjoint on \mathcal{H} and it is bounded if and only if the inverse of $\tilde{S} \upharpoonright (\mathcal{D}(\tilde{S}) \cap \text{ran}\tilde{S})$ (i.e., \tilde{S}_+^{-1}) is bounded as an operator on \mathcal{H}_+ .
- (ii) With respect to the decomposition (2.14) $\mathcal{H} = \text{ran}\bar{S} \oplus U_1 \oplus U_0$, one has $\mathcal{D}(\mathcal{B}) = \text{ran}\bar{S} \boxplus \tilde{U}_1 \boxplus U_0$, $\mathcal{B}\text{ran}\bar{S} = \{0\}$, $\mathcal{B}\tilde{U}_1 \subset U_1$, and $\mathcal{B}U_0 = \{0\}$.

Proof. (i) is obvious from the definition of \mathcal{B} and of \mathcal{S}^{-1} : the former is bounded if and only if the latter is. As for (ii), $\mathcal{D}(\mathcal{B}) = \text{ran}\tilde{S} \boxplus \ker\tilde{S} = \text{ran}\bar{S} \boxplus \tilde{U}_1 \boxplus U_0$ follows from (2.21) and Lemma 2.8(vi). Moreover, $\mathcal{B}U_0 = \{0\}$ is obvious from (2.20) and (2.21). To see that $\mathcal{B}\text{ran}\bar{S} = \{0\}$ let $f \in \mathcal{D}(\bar{S})$, then $\mathcal{B}\bar{S}f = \mathcal{S}^{-1}\bar{S}f - P_+S_F^{-1}\bar{S}f = \tilde{S}_+^{-1}\bar{S}f - P_+f = P_+f - P_+f = 0$,

where we used (2.21) and $\text{ran}\bar{S} \subset \mathcal{H}_+$ in the first equality, (2.20) in the second equality, and (2.19) in the third equality. In view of the decomposition $\mathcal{H} = \text{ran}\bar{S} \oplus U_1 \oplus U_0$, $\mathcal{D}(\mathcal{B}) = \text{ran}\bar{S} \boxplus \tilde{U}_1 \boxplus U_0$, the self-adjointness of \mathcal{B} and the fact that $\mathcal{B} \text{ran}\bar{S} = \{0\}$ and $\mathcal{B} U_0 = \{0\}$ imply necessarily $\mathcal{B} \tilde{U}_1 \subset U_1$. \square

As a direct consequence of Lemma 2.10 above, the restriction of \mathcal{B} to \tilde{U}_1 , i.e., the operator

$$B := (\mathcal{S}^{-1} - P_+ S_F^{-1} P_+) \upharpoonright \mathcal{D}(B), \quad \mathcal{D}(B) := \tilde{U}_1 \quad (2.22)$$

is a self-adjoint operator on the Hilbert space U_1 (with dense domain \tilde{U}_1), which itself is canonically determined by \tilde{S} . The interest towards this operator B is due the following fundamental property.

Proposition 2.11 (*B-decomposition formula*).

$$\mathcal{D}(\tilde{S}) = \mathcal{D}(\bar{S}) \dot{+} (S_F^{-1} + B)\tilde{U}_1 \dot{+} U_0 \quad (2.23)$$

Proof. One has

$$\begin{aligned} \mathcal{D}(\tilde{S}) &= P_+ \mathcal{D}(\tilde{S}) + U_0 && \text{(Lemma 2.8(iii))} \\ &= P_+ \mathcal{D}(\bar{S}) + \mathcal{S}^{-1} \tilde{U}_1 + U_0 && \text{(Lemma 2.9(ii))} \\ &= \mathcal{D}(\bar{S}) + \mathcal{S}^{-1} \tilde{U}_1 + U_0 && \text{(Lemma 2.9(i))} \\ &= \mathcal{D}(\bar{S}) + (P_+ S_F^{-1} P_+ + B)\tilde{U}_1 + U_0 && \text{(by (2.22))} \\ &= \mathcal{D}(\bar{S}) + (P_+ S_F^{-1} + B)\tilde{U}_1 + U_0 && (\tilde{U}_1 \subset \mathcal{H}_+) \\ &= \mathcal{D}(\bar{S}) + P_+(S_F^{-1} + B)\tilde{U}_1 + U_0 && (B\tilde{U}_1 \subset U_1 \subset \mathcal{H}_+, \text{ Lemma 2.10(ii)}). \end{aligned}$$

This identity, together with

$$P_+(S_F^{-1} + B)\tilde{U}_1 + U_0 = (S_F^{-1} + B)\tilde{U}_1 + U_0 \quad (*)$$

yields $\mathcal{D}(\tilde{S}) = \mathcal{D}(\bar{S}) + (S_F^{-1} + B)\tilde{U}_1 + U_0$, and this sum is direct because if $\mathcal{D}(\tilde{S}) \ni g = f + (S_F^{-1} + B)\tilde{u}_1 + u_0 = f + S_F^{-1}\tilde{u}_1 + (B\tilde{u}_1 + u_0)$ then, according to (2.5) and (2.13), $g = 0$ implies $f = 0$, $\tilde{u}_1 = 0$ and $u_0 = 0$. Thus, in order to prove (2.23) it only remains to prove (*). For the inclusion $P_+(S_F^{-1} + B)\tilde{U}_1 + U_0 \subset (S_F^{-1} + B)\tilde{U}_1 + U_0$ pick $\psi := P_+(S_F^{-1} + B)\tilde{u}_1 + u_0$ for generic $\tilde{u}_1 \in \tilde{U}_1$ and $u_0 \in U_0$. From (2.22), from the fact that $\tilde{u}_1 = P_+\tilde{u}_1$, and from $P_+\mathcal{S}^{-1}\tilde{u}_1 = \mathcal{S}^{-1}\tilde{u}_1$ (which follows from (2.20)), one has

$$P_+(S_F^{-1} + B)\tilde{u}_1 = P_+ S_F^{-1} P_+ \tilde{u}_1 + P_+ \mathcal{S}^{-1} \tilde{u}_1 - P_+ S_F^{-1} P_+ \tilde{u}_1 = \mathcal{S}^{-1} \tilde{u}_1$$

as well as

$$(S_F^{-1} + B)\tilde{u}_1 = (S_F^{-1}\tilde{u}_1 - P_+ S_F^{-1}\tilde{u}_1) + \mathcal{S}^{-1}\tilde{u}_1 = u'_0 + \mathcal{S}^{-1}\tilde{u}_1,$$

where $u'_0 := S_F^{-1}\tilde{u}_1 - P_+ S_F^{-1}\tilde{u}_1 \in \mathcal{H} \ominus \mathcal{H}_+ = U_0$; therefore,

$$\begin{aligned} \psi &= P_+(S_F^{-1} + B)\tilde{u}_1 + u_0 = \mathcal{S}^{-1}\tilde{u}_1 + u_0 \\ &= u'_0 + \mathcal{S}^{-1}\tilde{u}_1 + u_0 - u'_0 = (S_F^{-1} + B)\tilde{u}_1 + (u_0 - u'_0), \end{aligned}$$

which proves that $\psi \in (S_F^{-1} + B)\tilde{U}_1 + U_0$. The opposite inclusion to establish (*), that is, $P_+(S_F^{-1} + B)\tilde{U}_1 + U_0 \supset (S_F^{-1} + B)\tilde{U}_1 + U_0$, is proved repeating the same argument in reverse order. \square

2.4. Classification of all self-adjoint extensions: operator formulation.

After characterising the structure (2.5) of $\mathcal{D}(S^*)$ and providing the decomposition (2.23) of $\mathcal{D}(\tilde{S})$ for a generic self-adjoint extension \tilde{S} in terms of its B -operator, the next fundamental result in the KVB theory is the fact that the B -decomposition actually classifies *all* self-adjoint extensions of S .

Theorem 2.12 (Viřik-Birman representation theorem). *Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$). There is a one-to-one correspondence between the family of the self-adjoint extensions of S on \mathcal{H} and the family of the self-adjoint operators on Hilbert subspaces of $\ker S^*$, that is, the collection of triples (U_1, \tilde{U}_1, B) , where U_1 is a closed subspace of $\ker S^*$, \tilde{U}_1 is a dense subspace of U_1 , and B is a self-adjoint operator on the Hilbert space U_1 with domain $\mathcal{D}(B) = \tilde{U}_1$. For each such triple, let U_0 be the closed subspace of $\ker S^*$ defined by $\ker S^* = U_0 \oplus U_1$. Then, in this correspondence $S_B \leftrightarrow B$, each self-adjoint extension S_B of S is given by*

$$\begin{aligned} S_B &= S^* \upharpoonright \mathcal{D}(S_B) \\ \mathcal{D}(S_B) &= \mathcal{D}(\tilde{S}) \dot{+} (S_F^{-1} + B)\tilde{U}_1 \dot{+} U_0. \end{aligned} \tag{2.24}$$

Proof. The fact that *each* self-adjoint extension of S is precisely of the form S_B is the content of Proposition 2.11, where B is Viřik’s B operator associated to the considered self-adjoint extension. Conversely, one has to prove that each operator on \mathcal{H} of the form S_B above is a self-adjoint extension of S , and that the correspondence $S_B \leftrightarrow B$ is one-to-one.

Fixed (U_1, \tilde{U}_1, B) as in the statement, let us consider the corresponding S_B . One sees from (2.24) that S_B is densely defined ($\mathcal{D}(S_B) \supset \mathcal{D}(S)$) and it is an operator extension of S ($S_B f = \overline{S} f$ for all $f \in \mathcal{D}(\tilde{S})$). In fact, S_B is a *symmetric* extension: for two generic elements of $\mathcal{D}(S_B)$ one has

$$\begin{aligned} \langle f' + (S_F^{-1} + B)\tilde{u}'_1 + u'_0, S_B(f + (S_F^{-1} + B)\tilde{u}_1 + u_0) \rangle &= \\ &= \langle f', \overline{S} f \rangle + \langle f', \tilde{u}_1 \rangle + \langle S_F^{-1} \tilde{u}'_1, \overline{S} f \rangle + \langle S_F^{-1} \tilde{u}'_1, \tilde{u}_1 \rangle + \langle B\tilde{u}'_1, \tilde{u}_1 \rangle \\ &= \langle \overline{S} f, f' \rangle + \langle \overline{S} f', S_F^{-1} \tilde{u}_1 \rangle + \langle \tilde{u}'_1, f \rangle + \langle \tilde{u}'_1, S_F^{-1} \tilde{u}_1 \rangle + \langle \tilde{u}'_1, B\tilde{u}_1 \rangle \\ &= \langle S_B(f' + (S_F^{-1} + B)\tilde{u}'_1 + u'_0), f + (S_F^{-1} + B)\tilde{u}_1 + u_0 \rangle \end{aligned}$$

(where in the first step we used that $\langle B\tilde{u}'_1, \overline{S} f \rangle = \langle S^* B\tilde{u}'_1, f \rangle = 0$, $\langle u'_0, \overline{S} f \rangle = \langle S^* u'_0, f \rangle = 0$, $\langle u'_0, \tilde{u}_1 \rangle = 0$, in the second step we used the symmetry of \overline{S} , the self-adjointness of S_F^{-1} and B , and the properties of the adjoint S^* , and in the last step we used that $\langle \overline{S} f', B\tilde{u}_1 \rangle = \langle f', S^* B\tilde{u}_1 \rangle = 0$, $\langle \overline{S} f', u_0 \rangle = \langle f', S^* u_0 \rangle = 0$, $\langle \tilde{u}'_1, u_0 \rangle = 0$). Therefore, $S \subset S_B \subset S_B^* \subset S^*$ and in order to show that $S_B = S_B^*$ it suffices to prove that $\mathcal{D}(S_B) \supset \mathcal{D}(S_B^*)$.

Let us then pick $h \in \mathcal{D}(S_B^*)$, generic. Since $S_B^* \subset S^*$, one has $h = \varphi + S_F^{-1} \bar{v} + v$ by (2.5) for some $\varphi \in \mathcal{D}(\tilde{S})$ and $v, \bar{v} \in U = \ker S^*$, and

$S_B^*h = \overline{S}\varphi + \bar{v}$. Actually $\bar{v} \in U_1$, because $U = U_0 \oplus U_1$ and $\langle \bar{v}, u_0 \rangle = \langle S_B^*h, u_0 \rangle - \langle \overline{S}\varphi, u_0 \rangle = \langle h, S_B u_0 \rangle - \langle \varphi, S^*u_0 \rangle = \langle h - \varphi, S^*u_0 \rangle = 0 \quad \forall u_0 \in U_0$. Thus, representing $v = v_0 + v_1$, $v_0 \in U_0$, $v_1 \in U_1$, one writes

$$h = \varphi + S_F^{-1}\bar{v} + v = \varphi + (S_F^{-1}\bar{v} + v_1) + v_0.$$

In order to recognise this vector to belong to $\mathcal{D}(S_B)$, let us exploit the identity $\langle h, S_B k \rangle = \langle S_B^*h, k \rangle$, valid $\forall k \in \mathcal{D}(S_B)$, for the k 's of the special form $k = f + (S_F^{-1} + B)\tilde{u}_1$, $f \in \mathcal{D}(\overline{S})$, $\tilde{u}_1 \in \mathcal{D}(B)$. In this case

$$\begin{aligned} \langle h, S_B k \rangle &= \langle (\varphi + S_F^{-1}\bar{v}) + v_1 + v_0, S^*(f + S_F^{-1}\tilde{u}_1 + B\tilde{u}_1) \rangle \\ &= \langle (\varphi + S_F^{-1}\bar{v}), S^*(f + S_F^{-1}\tilde{u}_1) \rangle + \langle v_1 + v_0, \overline{S}f + \tilde{u}_1 \rangle \\ &= \langle (\varphi + S_F^{-1}\bar{v}), S_F(f + S_F^{-1}\tilde{u}_1) \rangle + \langle v_1, \tilde{u}_1 \rangle \end{aligned}$$

(indeed, $S_B B\tilde{u}_1 = S^*B\tilde{u}_1 = 0$, $\varphi + S_F^{-1}\bar{v} \in \mathcal{D}(S_F)$, $f + S_F^{-1}\tilde{u}_1 \in \mathcal{D}(S_F)$, $\langle v_1 + v_0, \overline{S}f \rangle = \langle S^*(v_1 + v_0), f \rangle = 0$, and $\langle v_0, \tilde{u}_1 \rangle = 0$) and

$$\begin{aligned} \langle S_B^*h, k \rangle &= \langle \overline{S}\varphi + \bar{v}, (f + S_F^{-1}\tilde{u}_1) + B\tilde{u}_1 \rangle \\ &= \langle S_F(\varphi + S_F^{-1}\bar{v}), (f + S_F^{-1}\tilde{u}_1) \rangle + \langle \bar{v}, B\tilde{u}_1 \rangle \end{aligned}$$

(indeed, $\langle \overline{S}\varphi, B\tilde{u}_1 \rangle = \varphi, S^*B\tilde{u}_1 = 0$). Equating these two expressions and using the self-adjointness of S_F yields

$$\langle v_1, \tilde{u}_1 \rangle = \langle \bar{v}, B\tilde{u}_1 \rangle \quad \forall \tilde{u}_1 \in \mathcal{D}(B)$$

which implies, owing to the self-adjointness of B , $\bar{v} \in \mathcal{D}(B)$ and $B\bar{v} = v_1$. Thus, the above decomposition for h reads now

$$h = \varphi + (S_F^{-1} + B)\bar{v} + v_0$$

for some $\bar{v} \in \mathcal{D}(B) = \tilde{U}_1$ and $v_0 \in U_0$, thus proving that $h \in \mathcal{D}(S_B)$.

Last, one proves that the operator B in the decomposition (2.24) is unique and therefore the correspondence between self-adjoint extensions of S and operators of the form S_B is one-to-one. Indeed, if

$$\mathcal{D}(S_B) = \mathcal{D}(\overline{S}) \dot{+} (S_F^{-1} + B)\tilde{U}_1 \dot{+} U_0 = \mathcal{D}(\overline{S}) \dot{+} (S_F^{-1} + B')\tilde{U}'_1 \dot{+} U'_0$$

where $\ker S^* = U_0 \oplus U_1 = U'_0 \oplus U'_1$ and where B and B' are self-adjoint operators, respectively on the Hilbert spaces U_1 and U'_1 , with domain, respectively, \tilde{U}_1 and \tilde{U}'_1 , then the action of S_B on an arbitrary element $g \in \mathcal{D}(S_B)$ gives, in terms of the decomposition $g = f + (S_F^{-1} + B)\tilde{u}_1 + u_0 = f' + (S_F^{-1} + B')\tilde{u}'_1 + u'_0$, $S_B g = \overline{S}f + \tilde{u}_1 = \overline{S}f' + \tilde{u}'_1$; each sum belongs to the orthogonal sum $\mathcal{H} = \overline{\text{ran}}\overline{S} \oplus \ker S^*$, whence $\tilde{u}_1 = \tilde{u}'_1$ and, by injectivity of S , $f = f'$ (whence also $u_0 = u'_0$); thus, $\tilde{U}_1 = \tilde{U}'_1$ and, after taking the closure $U_1 = U'_1$ and $U_0 = U'_0$; this also implies $B\tilde{u}_1 = B'\tilde{u}_1$, whence $B = B'$. \square

2.5. Characterisation of semi-bounded extensions: operator version.

A further relevant feature of the KVB theory is that the general classification (2.24) of Theorem 2.12 allows to identify special subclasses of self-adjoint extensions of S , significantly those that are bounded below, or in particular positive or also strictly positive, in terms of suitable subclasses of the corresponding B -operators in the representation (2.24).

In this respect, the convenient characterisation is expressed in terms of the inverse of B , more precisely of the self-adjoint operator B_\star^{-1} on the Hilbert space

$$\mathcal{H}_B := \overline{\text{ran}B} \oplus \ker S_B, \tag{2.25}$$

which is a Hilbert subspace of $\ker S^*$ (recall the notation $\ker S_B \equiv U_0$, $\ker S^* \equiv U$, and observe that $\text{ran}B \oplus \ker S_B \subset U_1 \oplus U_0 = U = \ker S^*$), defined by

$$\begin{aligned} \mathcal{D}(B_\star^{-1}) &:= \text{ran}B \boxplus \ker S_B \\ B_\star^{-1} \upharpoonright \text{ran}B &:= B^{-1} \\ B_\star^{-1} \upharpoonright \ker S_B &:= \mathbb{0}. \end{aligned} \tag{2.26}$$

It is fair to refer to B_\star^{-1} as “*Birman’s operator*”, for it is Birman who first determined and exploited its properties (Lemma 2.14 and Theorem 2.15 below).

For reference purposes, in (2.26) we intentionally kept Birman’s original notation [8]. A more precise definition of the operator B_\star^{-1} is the following

$$\begin{aligned} \mathcal{H}_B &:= \overline{\text{ran}B} \oplus (\ker S^* \cap \mathcal{D}(B)^\perp) \\ &= \overline{\text{ran}B} \oplus (\ker S^* \ominus \overline{\mathcal{D}(B)}) = \overline{\mathcal{D}(B_\star^{-1})} \\ \mathcal{D}(B_\star^{-1}) &:= \text{ran}B \boxplus (\ker S^* \cap \mathcal{D}(B)^\perp) \\ \mathcal{D}(B_\star^{-1})Bz &:= \mathcal{D}(B) \cap \overline{\text{ran}B} \\ \mathcal{D}(B_\star^{-1})u_0 &:= 0 \quad \forall u_0 \in \ker S^* \cap \mathcal{D}(B)^\perp \end{aligned} \tag{2.27}$$

where we used the decompositions $U_1 = \overline{\mathcal{D}(B)} = \overline{\text{ran}B} \oplus \ker B$ and $\tilde{U}_1 = \mathcal{D}(B) = (\mathcal{D}(B) \cap \overline{\text{ran}B}) \boxplus \ker B$. Thus, the action of B_\star^{-1} on a generic element $B\tilde{u}_1 \in \text{ran}B$ is given, in view of the decomposition $\tilde{u}_1 = z + z_0$ for some $z \in \mathcal{D}(B) \cap \overline{\text{ran}B}$ and $z_0 \in \ker B$, by $B_\star^{-1}B\tilde{u}_1 = z$.

Remark 2.13. One has

$$\mathcal{D}(S_B) \subset \mathcal{D}(S_F) \dot{+} \mathcal{D}(B_\star^{-1}). \tag{2.28}$$

Indeed, according to (2.24), any $g \in \mathcal{D}(S_B)$ decomposes for some $f_0 \in \mathcal{D}(\overline{S})$, $\tilde{u}_1 \in \tilde{U}_1 = \mathcal{D}(B)$, $u_0 \in U_0 = \ker S^* \cap \mathcal{D}(B)^\perp$ as $g = f_0 + (S_F^{-1} + B)\tilde{u}_1 + u_0 = f + v$, where $f := f_0 + S_F^{-1}\tilde{u}_1 \in \mathcal{D}(S_F)$ and (by (2.27)) $v := B\tilde{u}_1 + u_0 \in \mathcal{D}(B_\star^{-1})$. The sum in the r.h.s. of (2.28) is direct because if $v \in \mathcal{D}(S_F) \cap \mathcal{D}(B_\star^{-1})$, then $v \in \ker S^*$ by definition (2.26) and hence $\|v\|^2 = \langle S_F S_F^{-1} v, v \rangle = \langle S_F^{-1} v, S_F v \rangle = \langle S_F^{-1} v, S^* v \rangle = 0$. Observe, conversely, that inclusion is generically strict. Indeed, for a generic $h \in \mathcal{D}(S_F) \dot{+} \mathcal{D}(B_\star^{-1})$ one writes, according

to (2.6) and (2.27), $h = (f_0 + S_F^{-1}\tilde{u}_1 + B\tilde{u}_1 + u_0) + S_F^{-1}(u - \tilde{u}_1)$ for some $f_0 \in \mathcal{D}(\bar{S})$, $\tilde{u}_1 \in \mathcal{D}(B)$, $u_0 \in \ker S^* \cap \mathcal{D}(B)^\perp$, $u \in \ker S^*$, and this is not enough to use (2.24) and deduce that $h \in \mathcal{D}(S_B)$.

Lemma 2.14.

- (i) *If, with respect to the notation of (2.24) and (2.27), S_B is a self-adjoint extension of a given densely defined symmetric operator S with positive bottom ($m(S) > 0$), then*

$$\mathcal{D}(B_\star^{-1}) \subset \mathcal{D}[S_B] \cap \ker S^*. \quad (2.29)$$

- (ii) *If in addition S_B is bounded below, then*

$$S_B[v_1, v_2] = \langle v_1, B_\star^{-1}v_2 \rangle \quad \forall v_1, v_2 \in \mathcal{D}(B_\star^{-1}). \quad (2.30)$$

Proof. The fact that $\mathcal{D}(B_\star^{-1}) \subset \ker S^*$ is stated in the definition (2.26). To prove that $\mathcal{D}(B_\star^{-1}) \subset \mathcal{D}[S_B]$, decompose an arbitrary $v \in \mathcal{D}(B_\star^{-1})$, according to (2.27), as $v = B\tilde{u}_1 + u_0$ for some $\tilde{u}_1 \in \mathcal{D}(B) \setminus \ker B \subset \tilde{U}_1$ and $u_0 \in U_0 = \ker S_B$. From $v = ((S_F^{-1} + B)\tilde{u}_1 + u_0) - S_F^{-1}\tilde{u}_1$ one can then regard v as the difference between an element in $\mathcal{D}(S_B)$, according to (2.24), and an element in $\mathcal{D}(S_F)$. Since $\mathcal{D}(S_B) \subset \mathcal{D}[S_B]$ and $\mathcal{D}(S_F) \subset \mathcal{D}[S_F] \subset \mathcal{D}[S_B]$ (the Friedrichs extension has the smallest form domain among all semi-bounded extensions, Theorem A.2(vii)), then $v \in \mathcal{D}[S_B]$, which proves $\mathcal{D}(B_\star^{-1}) \subset \mathcal{D}[S_B]$ and completes the proof of (2.29). To prove (2.30), consider again an arbitrary $v = B\tilde{u}_1 + u_0$ in $\mathcal{D}(B_\star^{-1})$ as above: for $f := S_F^{-1}\tilde{u}_1 \in \mathcal{D}(S_F)$ and $g := f + v = S_F^{-1}\tilde{u}_1 + B\tilde{u}_1 + u_0 \in \mathcal{D}(S_B)$, one has $S_B g = \tilde{u}_1 = S_F f$, $B_\star^{-1}v = \tilde{u}_1$, and

$$\begin{aligned} S_B[g, g] &= \langle g, S_B g \rangle = \langle f + v, \tilde{u}_1 \rangle = \langle f, S_F f \rangle + \langle v, \tilde{u}_1 \rangle \\ &= S_F[f, f] + \langle v, B_\star^{-1}v \rangle. \end{aligned}$$

All this is still valid *irrespective of the semi-boundedness* of S_B . On the other hand, if S_B is bounded below, then a central result in Kreĭn's theory of self-adjoint extensions (see (A.22) quoted in Appendix A) states that $S_B[f, v] = 0$ for any $f \in \mathcal{D}[S_F]$ and any $v \in \mathcal{D}[S_B] \cap \ker S^*$ (which is what holds for f and v in the present case, owing to (i)), whence

$$S_B[g, g] = S_F[f, f] + S_B[v, v].$$

Thus, by comparison, $S_B[v, v] = \langle v, B_\star^{-1}v \rangle \forall v \in \mathcal{D}(B_\star^{-1})$. (2.30) then follows by polarisation. \square

Theorem 2.15 (Characterisation of semi-bounded extensions). *Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$). If, with respect to the notation of (2.24) and (2.27), S_B is a self-adjoint extension of S , and if $\alpha < m(S)$, then*

$$\begin{aligned} \langle g, S_B g \rangle &\geq \alpha \|g\|^2 \quad \forall g \in \mathcal{D}(S_B) \\ &\Downarrow \\ \langle v, B_\star^{-1}v \rangle &\geq \alpha \|v\|^2 + \alpha^2 \langle v, (S_F - \alpha \mathbb{1})^{-1}v \rangle \quad \forall v \in \mathcal{D}(B_\star^{-1}). \end{aligned} \quad (2.31)$$

As an immediate consequence, $m(B_\star^{-1}) \geq m(S_B)$ for any semi-bounded S_B . In particular, positivity or strict positivity of the bottom of S_B is equivalent to the same property for B_\star^{-1} , that is,

$$\begin{aligned} m(S_B) \geq 0 &\Leftrightarrow m(B_\star^{-1}) \geq 0 \\ m(S_B) > 0 &\Leftrightarrow m(B_\star^{-1}) > 0. \end{aligned} \quad (2.32)$$

Moreover, if $m(B_\star^{-1}) > -m(S)$, then

$$m(B_\star^{-1}) \geq m(S_B) \geq \frac{m(S) m(B_\star^{-1})}{m(S) + m(B_\star^{-1})}. \quad (2.33)$$

Proof. Let us start with the proof of (2.31). Observe that the fact that S_B is bounded below by α is equivalently expressed as $S_B[g] \geq \alpha \|g\|^2 \forall g \in \mathcal{D}[S_B]$. For generic $f \in \mathcal{D}(S_F)$ and $v \in \mathcal{D}(B_\star^{-1})$, one has that $g := f + v \in \mathcal{D}[S_B]$ and $S_B[v] = \langle v, B_\star^{-1}v \rangle$ (Lemma 2.14). On the other hand, since $v \in \mathcal{D}[S_B] \cap \ker S^*$ (Lemma 2.14), then $S_B[f, v] = 0$ (owing to (A.22)). Therefore, $S_B[g] = S_B[f + v] = S_F[f] + S_B[v] = \langle f, S_F f \rangle + \langle v, B_\star^{-1}v \rangle$. Thus, the assumption that S_B is bounded below by α reads, for all such g 's,

$$\langle f, S_F f \rangle + \langle v, B_\star^{-1}v \rangle \geq \alpha (\langle f, f \rangle + \langle f, v \rangle + \langle v, f \rangle + \langle v, v \rangle) \quad (i)$$

whence also, replacing $f \mapsto \lambda f$, $v \mapsto \mu v$,

$$\begin{aligned} (\langle f, S_F f \rangle - \alpha \|f\|^2) |\lambda|^2 - \alpha \langle f, v \rangle \lambda \bar{\mu} - \alpha \langle v, f \rangle \bar{\lambda} \mu \\ + (\langle v, B_\star^{-1}v \rangle - \alpha \|v\|^2) |\mu|^2 \geq 0 \quad \forall \lambda, \mu \in \mathbb{C}. \end{aligned} \quad (ii)$$

Since $\alpha < m(S)$, and hence $\langle f, S_F f \rangle - \alpha \|f\|^2 > 0$, inequality (ii) holds true if and only if

$$\alpha^2 |\langle f, v \rangle|^2 \leq (\langle v, B_\star^{-1}v \rangle - \alpha \|v\|^2) (\langle f, S_F f \rangle - \alpha \|f\|^2) \quad (iii)$$

for arbitrary $f \in \mathcal{D}(S_F)$ and $v \in \mathcal{D}(B_\star^{-1})$, which is therefore a necessary condition for S_B to be bounded below by α . Condition (iii) is in fact also sufficient. To see this, decompose an arbitrary $g \in \mathcal{D}(S_B)$ as $g = f + v$ for some $f \in \mathcal{D}(S_F)$ and $v \in \mathcal{D}(B_\star^{-1})$ (which is always possible, as observed in Remark 2.13) and apply (iii) to this case: one then obtains (ii) owing to $\alpha < m(S)$, which in turns yields (i) when $\lambda = \mu = 1$; from (i) one goes back to $S_B[g] \geq \alpha \|g\|^2$ following in reverse order the same steps discussed at the beginning. Thus, (iii) is *equivalent* to the fact that S_B is bounded below by α . By re-writing (iii) as

$$\langle v, B_\star^{-1}v \rangle - \alpha \|v\|^2 \geq \alpha^2 \frac{|\langle f, v \rangle|^2}{\langle f, (S_F - \alpha \mathbb{1})f \rangle}$$

and by the fact that the above inequality is valid for arbitrary $f \in \mathcal{D}(S_F)$ and hence holds true also when the supremum over such f 's is taken, one finds

$$\langle v, B_\star^{-1}v \rangle - \alpha \|v\|^2 \geq \alpha^2 \langle v, (S_F - \alpha \mathbb{1})^{-1}v \rangle$$

by means of a standard operator-theoretic argument applied to the bottom-positive operator $S_F - \alpha \mathbb{1}$ (Lemma 2.16). This completes the proof of (2.31).

From (2.31) one deduces immediately both the first equivalence of (2.32), by taking $\alpha = 0$, and the implication “ $m(S_B) > 0 \Rightarrow m(B_\star^{-1}) > 0$ ” in the second equivalence of (2.32), because $m(B_\star^{-1}) \geq m(S_B)$. Conversely, if $m(B_\star^{-1}) > 0$, then it follows from (2.26)-(2.27) that B_\star^{-1} has a bounded inverse, that $U_0 = \ker S_B = \{0\}$, and that $B : \mathcal{D}(B) \equiv \tilde{U}_1 \subset U_1 \rightarrow U_1$ is bounded; this, in turn, implies by Lemma 2.10(ii) and by (2.22) that the operator \mathcal{B} defined in (2.21) is bounded, which by Lemma 2.10(i) means that S_B has a bounded inverse (densely defined) on the whole \mathcal{H}_+ and therefore ($\mathcal{H} = \mathcal{H}_+ \oplus U_0$) on the whole \mathcal{H} . This fact excludes that $m(S_B) = 0$, and since $m(B_\star^{-1}) > 0 \Rightarrow m(S_B) \geq 0$ by the first of (2.32), one finally concludes $m(S_B) > 0$, which completes the proof of (2.32).

Last, it only remains to prove $m(S_B) \geq m(S)m(B_\star^{-1})(m(S)+m(B_\star^{-1}))^{-1}$ in (2.33) (assuming $m(B_\star^{-1}) > -m(S)$). In this case, for

$$\alpha := \frac{m(S) m(B_\star^{-1})}{m(S) + m(B_\star^{-1})}$$

one has $\alpha < m(S) = m(S_F)$ and $m(B_\star^{-1}) = \alpha m(S)(m(S) - \alpha)^{-1}$, whence $(m(S) - \alpha)^{-1} \geq (S_F - \alpha)^{-1}$ and

$$\begin{aligned} \langle v, B_\star^{-1}v \rangle &\geq m(B_\star^{-1})\|v\|^2 = \frac{\alpha m(S)}{m(S) - \alpha} \|v\|^2 = \alpha \|v\|^2 + \frac{\alpha^2}{m(S_F) - \alpha} \|v\|^2 \\ &\geq \alpha \|v\|^2 + \alpha^2 \langle v, (S_F - \alpha)^{-1}v \rangle \quad \forall v \in \mathcal{D}(B_\star^{-1}). \end{aligned}$$

Owing to (2.31), the latter inequality is equivalent to $m(S_B) \geq \alpha$, which completes the proof of (2.33). □

Lemma 2.16. *If A is a self-adjoint operator on a Hilbert space \mathcal{H} with positive bottom ($m(A) > 0$), then*

$$\sup_{f \in \mathcal{D}(A)} \frac{|\langle f, h \rangle|^2}{\langle f, Af \rangle} = \langle h, A^{-1}h \rangle \quad \forall h \in \mathcal{H}.$$

Proof. Setting $g := A^{1/2}f$ one has

$$\sup_{f \in \mathcal{D}(A)} \frac{|\langle f, h \rangle|^2}{\langle f, Af \rangle} = \sup_{g \in \mathcal{H}} \frac{|\langle A^{-1/2}g, h \rangle|^2}{\|g\|^2} = \sup_{\|g\|=1} |\langle g, A^{-1/2}h \rangle|^2$$

and since $|\langle g, A^{-1/2}h \rangle|$ attains its maximum for $g = A^{-1/2}h/\|A^{-1/2}h\|$, the conclusion then follows. □

2.6. Characterisation of semi-bounded extensions: form version.

The operator characterisation of the semi-bounded self-adjoint extensions of S provided by Theorem 2.15 has the virtue that it can be directly reformulated in terms of the quadratic form associated with an extension. The result is a very clean expression of $\mathcal{D}[S_B]$ in terms of the intrinsic space $\mathcal{D}[S_F]$ and the additional space $\mathcal{D}[B_\star^{-1}]$, where B (equivalently, B_\star^{-1}) plays the role of the “parameter” of the extension also in the form sense. This is a plus as compared to von Neumann’s characterisation (Theorem A.1), for the latter only classifies the self-adjoint extensions of S by indexing each operator extension

S_U in terms of a unitary U acting between defect subspaces, whereas the quadratic form associated with each S_U has no explicit description in terms of U .

Theorem 2.17 (Characterisation of semi-bounded extensions – form version).

Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$) and, with respect to the notation of (2.24) and (2.27), let S_B be a semi-bounded (not necessarily positive) self-adjoint extension of S . Then

$$\mathcal{D}[B_\star^{-1}] = \mathcal{D}[S_B] \cap \ker S^* \quad (2.34)$$

and

$$\begin{aligned} \mathcal{D}[S_B] &= \mathcal{D}[S_F] \dot{+} \mathcal{D}[B_\star^{-1}] \\ S_B[f + v, f' + v'] &= S_F[f, f'] + B_\star^{-1}[v, v'] \\ \forall f, f' \in \mathcal{D}[S_F], \forall v, v' \in \mathcal{D}[B_\star^{-1}]. \end{aligned} \quad (2.35)$$

As a consequence,

$$S_{B_1} \geq S_{B_2} \quad \Leftrightarrow \quad B_{1\star}^{-1} \geq B_{2\star}^{-1} \quad (2.36)$$

and

$$B_\star^{-1} \geq S_B. \quad (2.37)$$

Remark 2.18. Identity (2.34) is the form version of the inclusion (2.28) for operator domains, the latter holding for a generic (not necessarily semi-bounded) extension S_B . Property (2.35) represents the actual improvement of the KVB theory, as compared to Kreĭn's original theory, as far as the quadratic forms of the extensions are concerned. Recall indeed that Kreĭn's original theory (see Section A.3 and (A.21) in the Appendix) establishes, for a generic *semi-bounded* self-adjoint extension \tilde{S} of a densely defined symmetric operator S with positive bottom, the property

$$\begin{aligned} \mathcal{D}[\tilde{S}] &= \mathcal{D}[S_F] \dot{+} \mathcal{D}[\tilde{S}] \cap \ker S^* \\ \tilde{S}[f + u, f' + u'] &= S_F[f, f'] + \tilde{S}[u, u'] \\ \forall f, f' \in \mathcal{D}[S_F], \forall u, u' \in \mathcal{D}[\tilde{S}] \cap \ker S^*. \end{aligned} \quad (2.38)$$

What the KVB theory does in addition to (2.38), is therefore to characterise the space $\mathcal{D}[\tilde{S}] \cap \ker S^*$ in terms of the parameter B (equivalently, B_\star^{-1}) of each semi-bounded extension.

Proof of Theorem 2.17. Let us fix $\alpha \in \mathbb{R}$ such that $\alpha < m(S_B)$ and $|\alpha| > 1$. To establish the inclusion $\mathcal{D}[B_\star^{-1}] \subset \mathcal{D}[S_B] \cap \ker S^*$ in (2.34) let us exploit the fact that $\mathcal{D}[B_\star^{-1}]$ is the completion of $\mathcal{D}(B_\star^{-1})$ in the norm associated with the scalar product

$$\langle v_1, v_2 \rangle_{B_\star^{-1}} := \langle v_1, B_\star^{-1} v_2 \rangle - \alpha \langle v_1, v_2 \rangle$$

(indeed, owing to Theorem 2.15), $m(B_\star^{-1}) \geq m(S_B) > \alpha$), whereas $\mathcal{D}[S_B]$ is complete in the norm associated with the scalar product

$$\langle v_1, v_2 \rangle_{S_B} := S_B[v_1, v_2] - \alpha \langle v_1, v_2 \rangle.$$

Owing to Lemma 2.14, $\mathcal{D}(B_\star^{-1}) \subset \mathcal{D}[S_B]$ and

$$\|v\|_{B_\star^{-1}}^2 = \langle v, B_\star^{-1}v \rangle - \alpha\|v\|^2 = S_B[v] - \alpha\|v\|^2 = \|v\|_{S_B}^2,$$

thus the $\|\cdot\|_{B_\star^{-1}}$ -completion of $\mathcal{D}(B_\star^{-1})$ does not exceed $\mathcal{D}[S_B]$. On the other hand,

$$\|v\|_{B_\star^{-1}} \geq (m(B_\star^{-1}) - \alpha)\|v\|^2$$

and the r.h.s. above is obviously a norm with respect to which $\ker S^*$ is closed: therefore the $\|\cdot\|_{B_\star^{-1}}$ -completion of $\mathcal{D}(B_\star^{-1})$ does not exceed $\ker S^*$ either. This proves $\mathcal{D}[B_\star^{-1}] \subset \mathcal{D}[S_B] \cap \ker S^*$. For the opposite inclusion, let us preliminarily observe that the assumption $m(S_B) > \alpha$ implies

$$\alpha^2|\langle f, v \rangle|^2 \leq \|f\|_{S_B}^2\|v\|_{S_B}^2 \quad \forall f \in \mathcal{D}(S_F), \forall v \in \mathcal{D}(B_\star^{-1}) \quad (*)$$

(where $\|v\|_{B_\star^{-1}} = \|v\|_{S_B}$ $\forall v \in \mathcal{D}(B_\star^{-1})$ was used), as seen already in the course of the proof of Theorem 2.15, when condition (iii) therein was established. Let us also remark that $\mathcal{D}[S_F]$ is a $\|\cdot\|_{S_B}$ -closed subspace of $\mathcal{D}[S_B]$ (which follows from $\mathcal{D}[S_F] \subset \mathcal{D}[S_B]$, from $S_B[f] = S_F[f]$ $\forall f \in \mathcal{D}[S_F]$, and from $m(S_F) \geq m(S_B) > \alpha$, see Theorem A.2), and so is $\mathcal{D}[B_\star^{-1}]$ (as discussed previously in this proof). Let now $u \in \mathcal{D}[S_B] \cap \ker S^*$, arbitrary, and let $(g_n)_{n \in \mathbb{N}}$ be a sequence in $\mathcal{D}(S_B)$ of approximants of u in the $\|\cdot\|_{S_B}$ -norm. As remarked with (2.28), $g_n = f_n + v_n$ for some $f_n \in \mathcal{D}(S_F)$ and $v_n \in \mathcal{D}(B_\star^{-1})$, which are both vectors in $\mathcal{D}[S_B]$. From this and from (*) above one has

$$\begin{aligned} \|g_n - g_m\|_{S_B}^2 &\geq \|f_n - f_m\|_{S_B}^2 - 2|\langle f_n - f_m, v_n - v_m \rangle_{S_B}| + \|v_n - v_m\|_{S_B}^2 \\ &\geq \|f_n - f_m\|_{S_B}^2 - \frac{2}{\alpha^2}\|f_n - f_m\|_{S_B}\|v_n - v_m\|_{S_B} + \|v_n - v_m\|_{S_B}^2 \\ &\geq (1 - \alpha^{-2})(\|f_n - f_m\|_{S_B}^2 + \|v_n - v_m\|_{B_\star^{-1}}^2). \end{aligned}$$

Since $1 - \alpha^{-2} > 0$, one deduces that both $(f_n)_{n \in \mathbb{N}}$ and $(v_n)_{n \in \mathbb{N}}$ are Cauchy sequences, respectively, in $\mathcal{D}[S_F]$ and $\mathcal{D}[B_\star^{-1}]$, with respect to the topology of the $\|\cdot\|_{S_B}$ -norm, with limits, say, $f_n \rightarrow f \in \mathcal{D}[S_F]$ and $v_n \rightarrow v \in \mathcal{D}[B_\star^{-1}]$ as $n \rightarrow \infty$. Taking $n \rightarrow \infty$ in $g_n = f_n + v_n$ thus yields $u = f + v$. Having proved above that $\mathcal{D}[B_\star^{-1}] \subset \ker S^*$, one therefore concludes $f = u - v \in \ker S^*$, which together with $f \in \mathcal{D}[S_F]$ implies $f = 0$ (indeed $m(S_F) = m(S) > 0$ and hence $\mathcal{D}[S_F] \cap \ker S^* = \{0\}$). Then $u = v \in \mathcal{D}[B_\star^{-1}]$, which complete the proof of $\mathcal{D}[B_\star^{-1}] \supset \mathcal{D}[S_B] \cap \ker S^*$ and establishes finally (2.34). Coming now to the proof of (2.35), the identity $\mathcal{D}[S_B] = \mathcal{D}[S_F] \dot{+} \mathcal{D}[B_\star^{-1}]$ is a direct consequence of (2.34) and of (2.38). Furthermore, owing to the fact that $\mathcal{D}[B_\star^{-1}]$ is closed in $\mathcal{D}[S_B]$, identity (2.30) lifts to $S_B[v_1, v_2] = B_\star^{-1}[v_1, v_2]$ $\forall v_1, v_2 \in \mathcal{D}[B_\star^{-1}]$, which allows do deduce also the second part of (2.35) from (2.38). \square

2.7. Parametrisation of distinguished extensions: S_F and S_N .

One recognises in formulas (2.24) and (2.35) the special parameter B (equivalently, B_\star^{-1}) that selects, among all positive self-adjoint extensions S_B , the Friedrichs extension S_F or the Kreĭn-von Neumann extension S_N . (The characterisation and a survey of the main properties of S_F and S_N can be found,

respectively, in Theorem A.2-A.3 and in Theorems A.6-A.7.) This is another plus with respect to von Neumann’s theory, where S_F or S_N are not identifiable a priori by a special choice of the unitary that labels each extension.

The result can be summarised as follows

$$\text{Friedrichs } (S_F): \quad \begin{array}{l} \mathcal{D}[B_\star^{-1}] = \{0\} \\ \text{“}B_\star^{-1} = \infty\text{”} \end{array} \quad \begin{array}{l} \mathcal{D}(B) = \ker S^* \\ B = \mathbb{O} \end{array} \quad (2.39)$$

$$\text{Kre\u00efn-von Neumann } (S_N): \quad \begin{array}{l} \mathcal{D}[B_\star^{-1}] = \ker S^* \\ B_\star^{-1} = \mathbb{O} \end{array} \quad \begin{array}{l} \mathcal{D}(B) = \{0\} \\ \text{“}B = \infty\text{”} \end{array} \quad (2.40)$$

the details of which are discussed in the following Proposition.

Proposition 2.19. *Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$) and let S_B be a positive self-adjoint extension of S , parametrised by B (equivalently, by B_\star^{-1}) according to Theorems 2.12 and 2.17.*

- (i) S_B is the Friedrichs extension when $\mathcal{D}[B_\star^{-1}] = \{0\}$, equivalently, when $\mathcal{D}(B) = \ker S^*$ and $Bu = 0 \ \forall u \in \ker S^*$.
- (ii) S_B is the Kre\u00efn-von Neumann extension when $\mathcal{D}(B_\star^{-1}) = \mathcal{D}[B_\star^{-1}] = \ker S^*$ and $B_\star^{-1}u = 0 \ \forall u \in \ker S^*$; equivalently, when $\mathcal{D}(B) = \{0\}$.

Proof. Concerning part (i), $\mathcal{D}[B_\star^{-1}] = \{0\}$ follows from (2.35) when $S_B = S_F$. Hence also $\mathcal{D}(B_\star^{-1}) = \{0\}$, which implies $\text{ran} B = \{0\}$ (owing to (2.26)), that is, B is the zero operator on its domain. Comparing (2.6) and (2.24) one therefore has $U_0 = \{0\}$, $\tilde{U}_1 = U_1 = \ker S^*$, and hence $\mathcal{D}(B) = \ker S^*$. As for part (ii), $\mathcal{D}[B_\star^{-1}] = \ker S^*$ follows by comparing (2.35), when $S_B = S_N$, with the property (A.14) of S_N . This, together with $S_N[u] = 0 \ \forall u \in \ker S^*$ (given by (A.13)) and with $B_\star^{-1}[u] = S_B[u] = S_N[u] \ \forall u \in \mathcal{D}[B_\star^{-1}]$ (given by (2.35) when $S_B = S_N$), yields $B_\star^{-1}[u] = 0 \ \forall u \in \mathcal{D}[B_\star^{-1}]$, that is, $B_\star^{-1}[u]$ is the zero operator on its domain and hence $\mathcal{D}(B_\star^{-1}) = \mathcal{D}[B_\star^{-1}] = \ker S^*$. In turn, (A.14) now gives $\mathcal{D}(B_\star^{-1}) = \ker S^* = \ker S_N$, and therefore (2.26) (when $S_B = S_F$) yields $\text{ran} B = \{0\}$. Comparing (A.14) and (2.24) one therefore has $U_0 = \ker S^*$, $\tilde{U}_1 = U_1 = \{0\}$, and hence $\mathcal{D}(B) = \{0\}$. \square

Remark 2.20. The customary convention, adopted in (2.39)-(2.40), to label the Friedrichs extension formally with “ $B_\star^{-1} = \infty$ ” and the Kre\u00efn-von Neumann extension formally with “ $B = \infty$ ” (where it is understood that the considered operator has trivial domain $\{0\}$), is to make the labelling consistent with the ordering (2.36).

Remark 2.21. In the case in which S_F^{-1} is replaced by the inverse \tilde{S}^{-1} of an invertible self-adjoint extension \tilde{S} of S , there is no canonical choice any longer for the parameter B to select the Friedrichs extension S_F . However, it remains true that “ $B = \infty$ ” parametrises the Kre\u00efn-von Neumann extension (S_N) while $B = \mathbb{O}$ parametrises \tilde{S} instead of S_F . This is the case, for example, when one investigates the self-adjoint extensions of the (non semi-bounded) Dirac-Coulomb Hamiltonian [?].

3. Equivalent formulations of the KVB theory

Theorems 2.12, 2.15, and 2.17, and Proposition 2.19 above are *not* in the form they have customarily appeared in the mathematical literature in English language that followed the original works [30], [62], and [8], nor are their proofs. While we defer to the next Section a more detailed comparison with the more recent formulations, let us discuss in this Section a natural alternative parametrisation of the extensions which is equivalent to the original one provided by the original KVB theory.

In fact, this alternative arises naturally when the roles of the parameters B and B_\star^{-1} are interchanged. Both B and B_\star^{-1} are self-adjoint operators acting on Hilbert subspaces of $\ker S^*$. Although these two parameters are not exactly the inverse of each other, the definition of B_\star^{-1} resembles very much an operator inversion. Proposition 3.1 and Remarks 3.2 and 3.3 here below highlight the general properties of such an “inversion” mechanism. This will provide the ground to establish Theorems 3.4, 3.5, and 3.6 as an *equivalent* version, respectively, of Theorems 2.12, 2.15, and 2.17.

Proposition 3.1. *Let \mathcal{K} be a Hilbert space and let $\mathcal{S}(\mathcal{K})$ be the collection of the self-adjoint operators acting on Hilbert subspaces of \mathcal{K} . Given $T \in \mathcal{S}(\mathcal{K})$, let V be the closed subspace of \mathcal{K} which T acts on, with domain $\mathcal{D}(T) \equiv \overline{V}$ dense in V , and let $W := V^\perp$, i.e., $\mathcal{K} = V \oplus W$. Let $\phi(T)$ be the densely defined operator acting on the Hilbert subspace $\overline{\text{ran}T} \oplus W$ of \mathcal{K} defined by*

$$\begin{aligned} \mathcal{D}(\phi(T)) &:= \text{ran}T \boxplus W \\ \phi(T)Tv &:= v \quad \forall v \in \mathcal{D}(T) \cap \ker T \\ \phi(T)w &:= 0 \quad \forall w \in W. \end{aligned} \tag{3.1}$$

Then:

- (i) $\phi(T) \in \mathcal{S}(\mathcal{K})$,
- (ii) the map $\phi : \mathcal{S}(\mathcal{K}) \rightarrow \mathcal{S}(\mathcal{K})$ is a bijection on $\mathcal{S}(\mathcal{K})$,
- (iii) $\phi^2 = \iota$, the identity map on $\mathcal{S}(\mathcal{K})$, that is, $\phi^{-1} = \phi$.

Remark 3.2. In shorts, ϕ provides a transformation of T that is similar to the inversion. More precisely, although T is in general not invertible, $\phi(T)$ inverts T on $\text{ran}T$, while it is the zero operator on the orthogonal complement in \mathcal{K} of the Hilbert subspace where T was acting on. In particular, if T is densely defined in \mathcal{K} itself and invertible, then $\phi(T) = T^{-1}$, that is, ϕ is precisely the inversion transformation.

Remark 3.3. By comparing (2.27) and (3.1) in the special case $\mathcal{K} = \ker S^*$, $T = B$, $V = U_1$, and $W = U_0 = \ker S_B$, one concludes that $B_\star^{-1} = \phi(B)$, that is, the Birman operator B_\star^{-1} is precisely the ϕ -inversion of the Višik operator B .

Proof of Proposition 3.1. The self-adjointness of $\phi(T)$ on the Hilbert space $\overline{\text{ran}T} \oplus W$ is a standard and straightforward consequence of its definition. For the rest of the proof, it obviously suffices to show that $\phi(\phi(T)) = T$ for any $T \in \mathcal{S}(\mathcal{K})$. By definition the operator $\phi(T)$ acts on the Hilbert space

$V' := \overline{\text{ran}T} \oplus W$ with domain $\tilde{V}' := \text{ran}T \boxplus W$ dense in V' . Setting $W' := V'^{\perp}$, in view of the decomposition $\mathcal{K} = V' \oplus W'$ the operator $\phi(\phi(T))$ is therefore determined, by definition, as the operator that acts on the Hilbert subspace $\text{ran}\phi(T) \oplus W'$ of \mathcal{K} according to

$$\begin{aligned} \mathcal{D}(\phi(\phi(T))) &:= \text{ran}\phi(T) \boxplus W' \\ \phi(\phi(T))\phi(T)v' &:= v' \quad \forall v' \in \mathcal{D}(\phi(T)) \setminus \ker\phi(T) \\ \phi(\phi(T))w' &:= 0 \quad \forall w' \in W'. \end{aligned}$$

Since $V = \overline{\text{ran}T} \oplus \ker T$, and hence $\mathcal{K} = \overline{\text{ran}T} \oplus \ker T \oplus W$, then $W' = \ker T$. Thus,

$$\begin{aligned} \mathcal{D}(\phi(\phi(T))) &= \text{ran}\phi(T) \boxplus W' = (\mathcal{D}(T) \cap \overline{\text{ran}T}) \boxplus \ker T \\ &= (\mathcal{D}(T) \cap (V \ominus \ker T)) \boxplus \ker T = \mathcal{D}(T) \end{aligned}$$

and $\phi(\phi(T))w' = 0 = Tw' \quad \forall w' \in W' = \ker T$. It remains to show that $\phi(\phi(T))$ and T agree also on $\mathcal{D}(T) \cap \overline{\text{ran}T}$. In fact, if v is a vector in such a subspace, then $v = \phi(T)Tv$ and in view of $\phi(\phi(T))\phi(T)Tv = Tv$ one has $\phi(\phi(T))v = Tv$. This completes the proof that $\phi(\phi(T))v = Tv$ for any $v \in \mathcal{D}(T)$ and since the two operators have also the same domain, the conclusion is $\phi(\phi(T)) = T$. \square

We are now in the condition of re-stating the main results of the KVB extension theory established in Section 2 in the equivalent form that follows.

Theorem 3.4 (Classification of self-adjoint extensions – operator version). *Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$). There is a one-to-one correspondence between the family of all self-adjoint extensions of S on \mathcal{H} and the family of the self-adjoint operators on Hilbert subspaces of $\ker S^*$. If T is any such operator, in the correspondence $T \leftrightarrow S_T$ each self-adjoint extension S_T of S is given by*

$$\begin{aligned} S_T &= S^* \upharpoonright \mathcal{D}(S_T) \\ \mathcal{D}(S_T) &= \left\{ f + S_F^{-1}(Tv + w) + v \left| \begin{array}{l} f \in \mathcal{D}(\bar{S}), v \in \mathcal{D}(T) \\ w \in \ker S^* \cap \mathcal{D}(T)^{\perp} \end{array} \right. \right\}. \end{aligned} \quad (3.2)$$

Theorem 3.5 (Characterisation of semi-bounded extensions). *Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$). If, with respect to the notation of (3.2), S_T is a self-adjoint extension of S , and if $\alpha < m(S)$, then*

$$\begin{aligned} \langle g, S_T g \rangle &\geq \alpha \|g\|^2 \quad \forall g \in \mathcal{D}(S_T) \\ &\Updownarrow \\ \langle v, Tv \rangle &\geq \alpha \|v\|^2 + \alpha^2 \langle v, (S_F - \alpha \mathbb{1})^{-1} v \rangle \quad \forall v \in \mathcal{D}(T). \end{aligned} \quad (3.3)$$

As an immediate consequence, $m(T) \geq m(S_T)$ for any semi-bounded S_T . In particular, positivity or strict positivity of the bottom of S_T is equivalent to

the same property for T , that is,

$$\begin{aligned} m(S_T) \geq 0 &\Leftrightarrow m(T) \geq 0 \\ m(S_T) > 0 &\Leftrightarrow m(T) > 0. \end{aligned} \quad (3.4)$$

Moreover, if $m(T) > -m(S)$, then

$$m(T) \geq m(S_T) \geq \frac{m(S)m(T)}{m(S) + m(T)}. \quad (3.5)$$

Theorem 3.6 (Characterisation of semi-bounded extensions – form version).

Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$) and, with respect to the notation of (3.2), let S_T be a semi-bounded (not necessarily positive) self-adjoint extension of S . Then

$$\mathcal{D}[T] = \mathcal{D}[S_T] \cap \ker S^* \quad (3.6)$$

and

$$\begin{aligned} \mathcal{D}[S_T] &= \mathcal{D}[S_F] \dot{+} \mathcal{D}[T] \\ S_T[f + v, f' + v'] &= S_F[f, f'] + T[v, v'] \\ \forall f, f' \in \mathcal{D}[S_F], \forall v, v' \in \mathcal{D}[T]. \end{aligned} \quad (3.7)$$

As a consequence,

$$S_{T_1} \geq S_{T_2} \quad \Leftrightarrow \quad T_1 \geq T_2 \quad (3.8)$$

and

$$T \geq S_T. \quad (3.9)$$

Proposition 3.7 (Parametrisation of S_F and S_N). Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$) and let S_T be a positive self-adjoint extension of S , parametrised by T according to Theorems 3.4 and 3.6.

- (i) S_T is the Friedrichs extension when $\mathcal{D}[T] = \{0\}$ (“ $T = \infty$ ”).
- (ii) S_T is the Kreĭn-von Neumann extension when $\mathcal{D}(T) = \mathcal{D}[T] = \ker S^*$ and $Tu = 0 \forall u \in \ker S^*$ ($T = \mathbb{O}$).

Proof of Theorem 3.4. Let S_B be a generic self-adjoint extension of S , parametrised by B according to Theorem 2.12, formula (2.24). Correspondingly, let B_\star^{-1} be the Birman’s operator introduced in (2.26)-(2.27). First of all, we claim that S_B is precisely of the form S_T in (3.2) above where $T = B_\star^{-1}$. To prove that, consider a generic element $g = f + (S_F^{-1} + B)\tilde{u}_1 + u_0$ of $\mathcal{D}(S_B)$, as given by the decomposition (2.24) for some $f \in \mathcal{D}(\overline{S})$, $\tilde{u}_1 \in \tilde{U}_1 = \mathcal{D}(B)$, and $u_0 \in U_0 = \ker S^* \cap \mathcal{D}(B)^\perp = \ker S_B$. We write $\tilde{u}_1 = z + w$ for some $w \in \ker B$ and some $z \in \overline{\mathcal{D}(B)} \cap \overline{\text{ran} B}$ that are uniquely identified by the decomposition $U_1 = \overline{\mathcal{D}(B)} = \overline{\text{ran} B} \oplus \ker B$, $\mathcal{D}(B) = (\mathcal{D}(B) \cap \overline{\text{ran} B}) \boxplus \ker B$. Owing to (2.27), $v := B\tilde{u}_1 + u_0 = Bz + u_0 \in \mathcal{D}(B_\star^{-1})$ and $B_\star^{-1}v = z$. Moreover, from

$$\ker S^* = U_0 \oplus U_1 = \ker S_B \oplus \overline{\text{ran} B} \oplus \ker B = \overline{\mathcal{D}(B_\star^{-1})} \oplus \ker B$$

one deduces that $\ker B = \ker S^* \cap \mathcal{D}(B_\star^{-1})^\perp$. Therefore,

$$\begin{aligned} g &= f + S_F^{-1}\tilde{u}_1 + B\tilde{u}_1 + u_0 = f + S_F^{-1}(z + w) + v \\ &= f + S_F^{-1}(B_\star^{-1}v + w) + v \\ &\quad v \in \mathcal{D}(B_\star^{-1}), w \in \ker S^* \cap \mathcal{D}(B_\star^{-1})^\perp, \end{aligned}$$

that is, g is an element of $\mathcal{D}(S_T)$ defined in (3.2) above with $T = B_\star^{-1}$. It is straightforward to go through the same arguments and decompositions in reverse order to conclude that *any* vector of the form $S_F^{-1}(B_\star^{-1}v + w) + v$, where $v \in \mathcal{D}(B_\star^{-1})$ and $w \in \ker S^* \cap \mathcal{D}(B_\star^{-1})^\perp$, can be re-written as $(S_F^{-1} + B)\tilde{u}_1 + u_0$ for $\tilde{u}_1 \in \tilde{U}_1 = \mathcal{D}(B)$, and $u_0 \in U_0$ determined by

$$\begin{aligned} B_\star^{-1}v + w &= \tilde{u}_1 \\ v &= B\tilde{u}_1 + u_0, \end{aligned}$$

which proves that any $g \in \mathcal{D}(S_T)$ is also an element of $\mathcal{D}(S_B)$. Thus, (2.24) and (3.2) define the same domain: $\mathcal{D}(S_B) = \mathcal{D}(S_T)$ for $T = B_\star^{-1}$. Since S_B and S_T are the restrictions to such a common domain of the same operator S^* , then $S_B = S_T$ for $T = B_\star^{-1}$, and the initial claim is proved. As a consequence of this and of the one-to-one correspondence $S_B \leftrightarrow B$ of Theorem 2.12, the self-adjoint extensions of S are *all* of the form S_T of (3.2) for some self-adjoint operator T on a Hilbert subspace of $\ker S^*$. What remains to be proved is that when T runs in the family $\mathcal{S}(\ker S^*)$ of the self-adjoint operators on Hilbert subspaces of $\ker S^*$, the corresponding S_T 's give the whole family of self-adjoint extensions of S . This follows at once by Proposition 3.1, since by (2.24) $B_\star^{-1} = \phi(B)$ and ϕ is a bijection in $\mathcal{S}(\ker S^*)$. \square

Proof of Theorem 3.5, Theorem 3.6, and Proposition 3.7. All statements follow at once from their original versions, respectively Theorem 2.15, Theorem 2.17, and Proposition 2.19, and from the fact that the extension parameter T is precisely the parameter B_\star^{-1} in Theorem 2.15, Theorem 2.17, and Proposition 2.19. \square

Remark 3.8 (Equivalence of Theorems 2.12 and 3.4). Our arguments in the proof of Theorem 3.4 actually show also that the original Višik-Birman representation Theorem 2.12 can be *deduced* from Theorem 3.4 and that therefore the two Theorems are equivalent. Indeed, assuming the representation (3.2) for a generic self-adjoint extension S_T of S , our argument shows that the ϕ -inverse $B := \phi(T)$ of the parameter T allows to rewrite $\mathcal{D}(S_T)$ in the form $\mathcal{D}(S_B)$ of (2.24) and therefore all self-adjoint extensions of S have the form $S_B = S^* \upharpoonright \mathcal{D}(S_B)$ for some $B \in \mathcal{S}(\ker S^*)$; moreover, since by Proposition 3.1 ϕ is a bijection on $\mathcal{S}(\ker S^*)$, one concludes that when B runs in $\mathcal{S}(\ker S^*)$ the corresponding S_B exhausts the whole family of self-adjoint extensions of S , thus obtaining Theorem 2.12.

Let us discuss in the last part of this Section yet another equivalent formulation of the general representation theorem for self-adjoint extensions.

Theorem 3.9 (Classification of self-adjoint extensions – operator version). *Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$). There is a one-to-one correspondence between the family of all self-adjoint extensions of S on \mathcal{H} and the family of the self-adjoint operators on Hilbert subspaces of $\ker S^*$. If T is any such operator, $P_T : \mathcal{H} \rightarrow \mathcal{H}$ is the orthogonal projection onto $\overline{\mathcal{D}(T)}$, and $P_* : \mathcal{D}(S^*) \rightarrow \mathcal{D}(S^*)$ is the (non-orthogonal, in general) projection onto $\ker S^*$ with respect to Kreĭn's decomposition formula $\mathcal{D}(S^*) = \mathcal{D}(S_F) \dot{+} \ker S^*$ (Lemma 2.1), then in the correspondence $T \leftrightarrow S_T$ each self-adjoint extension S_T of S is given by*

$$S_T = S^* \upharpoonright \mathcal{D}(S_T)$$

$$\mathcal{D}(S_T) = \left\{ g \in \mathcal{D}(S^*) \left| \begin{array}{l} P_*g \in \mathcal{D}(T) \text{ and} \\ P_T S^*g = T P_*g \end{array} \right. \right\}. \quad (3.10)$$

Proposition 3.10. *The parameter T in (3.10) is precisely the same as in (3.2), that is, the representation given in Theorem 3.9 is the same as the one given in Theorem 3.4. In other words, the two theorems are equivalent. In particular, given a self-adjoint extension \tilde{S} of S , its extension parameter T (i.e., the operator T for which $\tilde{S} = S_T$) is the operator acting on the Hilbert space $P_*\mathcal{D}(\tilde{S})$ with domain $\mathcal{D}(T) = P_*\mathcal{D}(\tilde{S})$ and action $T P_*g = P_T S_T g \forall g \in \mathcal{D}(\tilde{S})$.*

Proof of Theorem 3.9 and Proposition 3.10. All one needs to prove is that the domain $\mathcal{D}(S_T)$ given by (3.2) can be re-written in the form (3.10) with the same T . If $g = f + S_F^{-1}(Tv + w) + v$ is a generic element of the space $\mathcal{D}(S_T)$ defined by (3.2), then $P_*g = v$ (by Kreĭn's decomposition formula), $S^*g = \bar{S}f + Tv + w$, and $P_T S^*g = Tv$. Thus, $P_*g \in \mathcal{D}(T)$ and $T P_*g = Tv = P_T S^*g$, which proves that g belongs to the domain defined in (3.10). For the converse, recall that for any $g \in \mathcal{D}(S^*)$ the Višik-Birman decomposition formula (2.5) gives $g = f + S_F^{-1}u + P_*g$ for some $f \in \mathcal{D}(\bar{S})$ and $u \in \ker S^*$. If now g belongs to the domain defined in (3.10), then $v := P_*g \in \mathcal{D}(T) \subset \ker S^*$ for some $T \in \mathcal{S}(\ker S^*)$, and the decomposition $\ker S^* = \overline{\mathcal{D}(T)} \oplus (\ker S^* \cap \mathcal{D}(T)^\perp)$ gives $u = P_T u + w$ for some $w \in \ker S^* \cap \mathcal{D}(T)^\perp$: since $P_T S^*g = P_T(\bar{S}f + u) = P_T u$ and (3.10) prescribes also $P_T S^*g = Tv$, then $P_T u = Tv$ and $u = Tv + w$: this proves that $g = f + S_F^{-1}(Tv + w) + v$, which belongs to the domain $\mathcal{D}(S_T)$ given by (3.2). Thus, (3.2) and (3.10) define (for the same T) the same space $\mathcal{D}(S_T)$. \square

4. Comparisons with the subsequent literature in English

Before proceeding on to the further aspects of the theory (Sections 5 and 6), the discussion developed so far gives the opportunity of a short historical retrospective.

The KVB self-adjoint extension theory was developed (in Russian) in the course of a decade between the mid 1940's and the mid 1950's. This was not the result of a coherent programme.

Kreĭn’s focus in [30] was the complete answer to the problem, risen up by von Neumann [63], of finding and characterising semi-bounded extensions of a given semi-bounded and densely defined symmetric operator S . von Neumann himself had provided one particular solution (the extension S_N , in the present notation) and later Stone [60, Theorem 9.21] had proved, for the finite deficiency indices case, the existence of a self-adjoint extension \tilde{S} with the much more interesting feature that $m(\tilde{S}) = m(S)$, followed by Friedrichs [19] who had constructed his eponymous extension (S_F , in the present notation). The framework for Viřik’s work [62] was instead the study of the boundary conditions needed for certain resolvability properties of boundary value problems associated with an elliptic differential operator L , say, $Lu = h$ with datum h and unknown u in a region $\Omega \subset \mathbb{R}^d$. Two operators on $L^2(\Omega)$ are naturally associated to L , a “minimal” operator L_0 and a “maximal” L_1 (with $L_0 \subset L_1$), and one considers a suitable family of realisations \tilde{S} of L between them ($L_0 \subset \tilde{S} \subset L_1$) that are determined by boundary conditions at $\partial\Omega$; the question is to find such conditions for any considered realisation \tilde{S} , each boundary condition being expressed in terms of boundary operators $\mathcal{D}(\tilde{S}) \rightarrow \mathcal{D}'(\partial\Omega)$ and operators between functional spaces over $\partial\Omega$. Viřik focused, among other cases, on the case where $L_0 = S$ is densely defined and symmetric on $L^2(\Omega)$, $L_1 = S^*$, and \tilde{S} is a self-adjoint extension of S , and he provided the one-to-one representation $\tilde{S} \equiv S_B \leftrightarrow B$ of Theorem 2.12, where B is a suitable boundary operator. Concerning Birman, the motivation in [8] was to characterise further the correspondence $S_B \leftrightarrow B$ along a two-fold direction: to relate the semi-boundedness and other spectral properties of S_B with the analogous properties of the parameter B (both in the operator and in the quadratic form sense), and to include also the case of infinite deficiency indices, which had not been covered by Kreĭn.

Since the mid 1950’s, as already commented, the self-adjoint extension theory based in the results of Kreĭn, Viřik, and Birman has found a rather limited space within the mathematical literature in English, presumably for a multiplicity of reasons that, language and geo-political barriers apart, are related with the distance between the fields which such results were applied to, boundary value problems for PDE on the one hand, and quantum-mechanical Hamiltonians on the other. This refers both to Kreĭn’s characterisation of the semi-bounded extensions (that is, Theorem A.10), which at least received a partial discussion in 1954’s Riesz and Nagy’s treatise on Functional Analysis [53, §125], and to a much larger extent to the Viřik-Birman representation Theorem 2.12 as well as its application to semi-bounded extensions, Theorems 2.15, and 2.17.

As oversimplified as the following statement may appear, the main *comprehensive discussions* of the KVB theory of self-adjoint extensions that were produced within the “western” mathematical literature are,

1. from the perspective of boundary value problems for elliptic differential operators: Grubb’s 1968 theory on the “universal parametrisation of extensions” [24];

2. from the perspective of general operator theory on Hilbert spaces (with the point of view of quantum-mechanical and Schrödinger operator applications): Faris's 1975 lecture notes on self-adjoint operators [18] and, above all, Alonso's and Simon's 1980 "propaganda" article on the KVB theory [3].

Grubb's work [24] (see also its modern survey in [26, Chapter 13]) lies within the general study of boundary conditions for elliptic partial differential operators and the associated boundary value problem, therefore a field that is closely related with Višik's approach. As a tool, [24] develops an abstract extension theory for closed and densely defined operators on Hilbert space, with a specific treatment of the symmetric case and the corresponding self-adjoint extensions. This is done by means of Hilbert space and operator graph methods that resemble very much those used by Kreĭn, Višik, and Birman some 20 years earlier, so that it is fair to regard [24, Chapter II] as an independent route to the general self-adjoint extension characterisation already provided by the KVB theory, together with a novel generalisation to a wider class of extensions. The form by which the work [24] classifies the self-adjoint extensions of a given densely defined (and closed) symmetric operator S with positive bottom is essentially that of Theorem 3.9 (see [24, Theorem II.2.1]), that here we have derived directly from (and actually proved to be equivalent to) Višik-Birman representation Theorem 2.12.² [24] reproduces also the bound on $m(S_T)$ in terms of $m(T)$, expressed here by (3.5) of Theorem 3.5 (see [26, Theorem 13.17]), as well as Kreĭn's decomposition formula for quadratic forms, here expressed by (A.21) of Theorem A.10(iii) (see [26, Theorem 13.19]). *Grubb's theory, however, does not cover the quadratic form side of the extension scheme*, it only concerns the operator level.

Faris's presentation in [18], on the other hand, is explicitly motivated by general mathematical problems for quantum mechanics (with no reference to Grubb's previous work). It includes a concise derivation of formula (3.7) of Theorem 3.6, limited to the case of *positive* self-adjoint extensions of a given densely defined symmetric operator S with positive bottom (see [18, Theorem 15.3]), which is obtained independently in the same spirit as Birman's work.

Along the same line, in fact independently from Grubb's and Faris's previous discussions, Alonso and Simon in [3] revisit a large part of the KVB theory (again, only for *positive* extensions of S , with $m(S) > 0$) with some originality of viewpoint that gives primary emphasis to the notion of quadratic form. First, they classify the positive extensions in terms of positive forms on $\ker S^*$, thus reproducing both Kreĭn's extension theorem, with a statement that is essentially Theorem A.10(ii), and Birman's characterisation of the forms of positive extensions, essentially stating it as (3.7) and

²The positivity of the bottom, $m(S) > 0$, is in fact only a special case of a more general assumption discussed in [24, Section II §2], that is, the assumption that \bar{S} has a bounded and everywhere defined inverse: in this general case S_F^{-1} is replaced by the inverse of another self-adjoint extension \tilde{S}_0 of S with bounded inverse – the existence of such \tilde{S}_0 is a result originally proved by Calkin [12].

(3.8) in Theorem 3.6 (see [3, Section 2]). Then, by means of operator graph techniques, they derive the operator version of the corresponding classification, with the same statement as in Theorem here 3.4 (see [3, Section 3]).

It is worth remarking that all the above-mentioned works use the parametrisation of the operator domains of the extensions in terms of the operator T used in Section 3, instead of the original parameter B used by Višik and Birman for Theorem 2.12.

One further relevant contribution is the work of Ando and Nishio [5] that appears immediately after Grubb's and is practically ignored by Faris's and by Alonso's and Simon's. By means of an ad hoc analysis that in fact does not use the general tools and formulas of the KVB theory, [5] investigates the structure of the (quadratic form of the) Kreĭn-von Neumann extension S_N of a densely defined and positive symmetric operator S , and characterises it in the form of Theorem A.7 in the Appendix. [5] also provides a necessary and sufficient condition for S to admit positive self-adjoint extensions (even when the $\mathcal{D}(S)$ is not dense or closed), as reviewed in Theorem A.9.

The *positive* self-adjoint extensions of a given positive and densely defined symmetric operator are also the object of a recent study by Arlinskiĭ and Tsekanovskiĭ [6], where several results of the KVB theory are reproduced in a somewhat alternative form.

As mentioned already, in more recent times the extension picture of Kreĭn, Višik, and Birman, as well as that of Grubb's approach (following an idea that can be traced back to Calkin [11]), has found at an abstract analytic and operator-theoretic level a natural generalisation in the form of the modern theory of boundary triplets (introduced by Kočubeĭ [29] and Bruk [10]) and gamma fields and Weyl functions associated with boundary triplets (invented by Derkach and Malamud [16]). This is a vast subject with applications to abstract extension theory, to elliptic boundary value problems, and to the theory of local point interactions, with many fundamental contributions that can be traced in the works of Derkach and Malamud [16], Gorbachuk, Gorbachuk, and Kochubeĭ [22, 21], Albeverio and Kurasov [2], Amrein and Pearson [4], Behrndt and Langer [7], Ryzhov [54, 55], Posilicano [50], Brown, Grubb, and Wood [9], Grubb [26], Kostenko and Malamud [28], Malamud [32, 33], Malamud and Neidhardt [34], Derkach, Hassi, Malamud and de Snoo [15], and in the references therein. For example, in [56, Chapter 14] one may find a detailed derivation of Theorems 3.4 and 3.6 (but only for *positive* extensions of S with $m(S) > 0$) by means of boundary triplet techniques. Remark 5.6 below collects further references to fundamental works of the modern theory of boundary triplets that reproduce results that one can obtain directly within the original KVB theory.

One of the purposes of the present work is not to use these modern instances and to discuss instead the emergence of the KVB theory, both in its original formulation and in what today is the 'boundary-triplet-derived' modern formulation, but using only the 'elementary' operator-theoretic setting. This makes the theory particularly suited to the application we are

concerned most, that is, models of quantum mechanical Hamiltonians of particle systems with zero-range (or very singular) interaction. In this context, for the classification of all possible self-adjoint realisation of the ‘physically driven’ Hamiltonian, the characterisation provided by Theorems 3.4, 3.5, and 3.6, and Proposition 3.7, turns out to be the most applicable and fruitful, as may be found in many past and recent works on the subject [48, 47, 41, 49, 35, 36, 59, 42, 43, 44, 46, 45, 40, 39, 37, 38].

5. Invertibility, semi-boundedness, and negative spectrum

In this Section we complete the discussion of the main results that can be proved within the KVB theory, focusing on the link between relevant features (such as invertibility, semi-boundedness, structure of the negative spectrum) of a self-adjoint extension of a given densely defined symmetric operator S with positive bottom, and the corresponding features of the extension parameter given by the theory. Such a close link allows one to appreciate even more the effectiveness of the KVB extension parameter, as compared to von Neumann’s parametrisation. We adopt here the notation $T \leftrightarrow S_T$ for the parametrisation of the extensions – see Section 3.

A first link between S_T and T , which is straightforward although it is not explicitly present in Birman’s original work, is the following.

Theorem 5.1 (Invertibility). *Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$) and let S_T be a generic self-adjoint extension of S according to the parametrisation (3.2) of Theorem 3.4. Then*

- (i) S_T is injective $\Leftrightarrow T$ is injective,
- (ii) S_T is surjective $\Leftrightarrow T$ is surjective,
- (iii) S_T is invertible on the whole $\mathcal{H} \Leftrightarrow T$ is invertible on the whole $\overline{\mathcal{D}(T)}$.

Proof. Assume that S_T is injective and let $v \in \mathcal{D}(T)$ be such that $Tv = 0$. Then v is an element in $\mathcal{D}(S_T)$, because it is a vector of the form (3.2), $g = f + S_F^{-1}(Tv + w) + v$, with $f = w = 0$. Since $S_T v = 0$, by injectivity of S_T one concludes that $v = 0$. Conversely, if T is injective and for some $g = f + S_F^{-1}(Tv + w) + v \in \mathcal{D}(S_T)$ one has $S_T g = 0$, then $\overline{S}f + Tv + w = 0$. Since $\overline{S}f + Tv + w \in \text{ran}\overline{S} \boxplus \text{ran}T \boxplus (\ker S^* \cap \mathcal{D}(T)^\perp)$, one must have $\overline{S}f = Tv = w = 0$. Owing to the injectivity of \overline{S} and T , $f = v = 0$ and hence $g = 0$. This completes the proof of (i). As for (ii), in the notation of (3.2) one has that $\text{ran}S_T = \text{ran}\overline{S} \boxplus \text{ran}T \boxplus (\ker S^* \cap \mathcal{D}(T)^\perp)$ and in fact $\overline{\text{ran}S} = \overline{\text{ran}\overline{S}}$ (Remark 2.5). Thus, T is surjective $\Leftrightarrow \text{ran}T \boxplus (\ker S^* \cap \mathcal{D}(T)^\perp) = \overline{\text{ran}T} \oplus (\ker S^* \cap \mathcal{D}(T)^\perp) = \ker S^* \Leftrightarrow \text{ran}S_T = \overline{\text{ran}\overline{S}} \oplus \ker S^* = \mathcal{H} \Leftrightarrow S_T$ is surjective. (iii) is an obvious consequence of (i) and (ii). \square

Remark 5.2. Noticeably, Višik-Birman’s original parametrisation $S_B \leftrightarrow B$ for the extensions does not allow to control invertibility, as opposed to the parametrisation $S_T \leftrightarrow T$. Indeed, the identity $\ker S_B = U_0 \equiv \ker S^* \cap \mathcal{D}(B)^\perp$

(that follows immediately from (2.13) and (2.24)) shows that the injectivity of S_B and the injectivity of B are unrelated, and the identity $\text{ran} S_B = \text{ran} \overline{S} \oplus \mathcal{D}(B)$ shows that the surjectivity of S_B and the surjectivity of B are unrelated too.

Semi-boundedness is another relevant feature of the self-adjoint extensions that can be controlled in terms of the KVB extension parameter. The sub-family of the semi-bounded self-adjoint extensions of S is the object of Theorem 2.15 (equivalently, of Theorem 3.5). Here below we supplement the information of that theorem with the answer to the question on whether the semi-boundedness of S_T and of T are *equivalent*. This is another result that is not explicitly present in Birman's discussion, although it follows from it. As a consequence, we derive within the KVB theory the fact that when S has a finite deficiency index all its self-adjoint extensions are bounded below.

Theorem 5.3 (Semi-boundedness). *Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$), $P_K : \mathcal{H} \rightarrow \mathcal{H}$ be the orthogonal projection onto $\ker S^*$, and for each $\alpha < m(S)$ let*

$$M(\alpha) := P_K(\alpha\mathbb{1} + \alpha^2(S_F - \alpha\mathbb{1})^{-1})P_K = P_K(\alpha S_F(S_F - \alpha\mathbb{1})^{-1})P_K. \quad (5.1)$$

Let S_T be a generic self-adjoint extension of S according to the parametrisation (3.2) of Theorem 3.4. Assume that $m(T) \in [-\infty, 0)$, that is, T is either unbounded below or with finite negative bottom (otherwise it is already known by (3.4) in Theorem 3.5 that $m(T) \geq 0 \Leftrightarrow m(S_T) \geq 0$). Then the two conditions

- (i) S_T is bounded below (on \mathcal{H})
- (ii) T is bounded below (on $\overline{\mathcal{D}(T)}$)

are equivalent if and only if $M(\alpha)$ “diverges to $-\infty$ uniformly as $\alpha \rightarrow -\infty$ ”, meaning that $\forall R > 0 \exists \alpha_R < 0$ such that $M(\alpha) \leq -R\mathbb{1}$ for each $\alpha \leq \alpha_R$.

Proof. Since (i) \Rightarrow (ii) is always true (owing to (3.3) in Theorem 3.5), what must be proven is the equivalence between the implication (ii) \Rightarrow (i) and the condition of uniform divergence to $-\infty$ for $M(\alpha)$. Assume (ii) \Rightarrow (i), that is, assume that for arbitrary $R > -m(T)$ the condition $T \geq -R\mathbb{1}$ implies $S_T \geq \alpha_R\mathbb{1}$ for some $\alpha_R < 0$ and hence also $S_T \geq \alpha\mathbb{1} \forall \alpha \leq \alpha_R$ (if the lower bound α_R was non-negative, then $m(T)$ would be non-negative too, against the assumption). In turn, owing to (3.3) and (5.1), $S_T \geq \alpha\mathbb{1} \forall \alpha \leq \alpha_R$ is equivalent to $T \geq M(\alpha) \forall \alpha \leq \alpha_R$. Then, for $T \geq -R\mathbb{1}$ to imply $T \geq M(\alpha) \forall \alpha \leq \alpha_R$, necessarily $M(\alpha) \leq -R\mathbb{1} \forall \alpha \leq \alpha_R$. Conversely, assume now that for arbitrary $R > 0$ there exists α_R such that $M(\alpha) \leq -R\mathbb{1} \forall \alpha \leq \alpha_R$: we want to deduce (ii) \Rightarrow (i). To this aim, assume that T is bounded below and apply the assumption for $R = -m(T)$: for the corresponding α_R one has $M(\alpha_R) \leq -R\mathbb{1} = m(T)\mathbb{1} \leq T$, which by (3.3) implies $S_T \geq \alpha_R\mathbb{1}$. \square

Corollary 5.4 (Finite deficiency index). *If S is a semi-bounded and densely defined symmetric operator on a Hilbert space \mathcal{H} with finite deficiency index, then*

- (i) the semi-boundedness of S_T is equivalent to the semi-boundedness of T ;
- (ii) any self-adjoint extension of S is bounded below.

Proof. It is not restrictive to assume $m(S) > 0$ and hence $\dim \ker S^* < \infty$. Part (ii) follows from (i) because T is now defined on a finite-dimensional Hilbert space and is therefore bounded. Part (i) follows from Theorem 5.3 once one shows that $M(\alpha)$ diverges uniformly to $-\infty$. Irrespectively of whether $\dim \ker S^*$ is finite or not,

$$\lim_{\alpha \rightarrow -\infty} \langle u, M(\alpha)u \rangle = -\infty \quad \forall u \in \ker S^*. \quad (5.2)$$

Indeed, for any $u \in \ker S^*$ one has $u \notin \mathcal{D}[S_F]$ (see (A.14)), whence

$$\int_{[0, +\infty)} \lambda \, d\langle u, E^{(S_F)}(\lambda)u \rangle = +\infty,$$

where $dE^{(S_F)}$ denotes the spectral measure of S_F ; therefore, since $\frac{\lambda\alpha}{\lambda-\alpha} \rightarrow -\lambda$ as $\alpha \rightarrow -\infty$,

$$\langle u, M(\alpha)u \rangle = \int_{[0, +\infty)} \frac{\lambda\alpha}{\lambda-\alpha} \, d\langle u, E^{(S_F)}(\lambda)u \rangle \xrightarrow{\alpha \rightarrow -\infty} -\infty.$$

Under the additional assumption $\dim \ker S^* < \infty$ let us now show that (5.2) implies a *uniform* divergence in the sense of Theorem 5.3. For arbitrarily fixed $R > 0$ decompose $u = f_R + v_R$ with

$$f_R := E^{(S_F)}([0, 2R])u, \quad v_R := E^{(S_F)}((2R, +\infty))u.$$

Observe that $f_R \in \mathcal{D}(S_F)$, because

$$\int_{[0, +\infty)} \lambda^2 \, d\langle f_R, E^{(S_F)}(\lambda)f_R \rangle = \int_{[0, 2R]} \lambda^2 \, d\langle f_R, E^{(S_F)}(\lambda)f_R \rangle \leq 4R^2 \|f_R\|^2,$$

while necessarily $v_R \notin \mathcal{D}(S_F)$ because $u \notin \mathcal{D}(S_F)$. One has

$$\begin{aligned} \langle u, M(\alpha)u \rangle &= \langle u, M(\alpha)u \rangle = \int_{[0, +\infty)} \frac{\lambda\alpha}{\lambda-\alpha} \, d\langle u, E^{(S_F)}(\lambda)u \rangle \\ &= \int_{[0, 2R]} \frac{\lambda\alpha}{\lambda-\alpha} \, d\langle f_R, E^{(S_F)}(\lambda)f_R \rangle + \int_{(2R, +\infty)} \frac{\lambda\alpha}{\lambda-\alpha} \, d\langle v_R, E^{(S_F)}(\lambda)v_R \rangle. \end{aligned} \quad (a)$$

In the second integral in the r.h.s above $\lambda > 2R$, whence $2R > \frac{2R\lambda}{2\lambda-2R}$: therefore, choosing $\alpha < -2R$ implies $-\alpha > \frac{2R\lambda}{2\lambda-2R}$ and the latter condition is equivalent to $\frac{\lambda\alpha}{\lambda-\alpha} < -R$, thus

$$\int_{(2R, +\infty)} \frac{\lambda\alpha}{\lambda-\alpha} \, d\langle v_R, E^{(S_F)}(\lambda)v_R \rangle < -R \|v_R\|^2 \quad (\alpha < -2R). \quad (b)$$

Let us now exploit the assumption $\dim \ker S^* = d$ for some $d \in \mathbb{N}$ in order to estimate the first integral in the r.h.s of (a). Obviously there is $d_R \in \mathbb{N}$, $d_R \leq d$, such that

$$\dim E^{(S_F)}([0, 2R]) \ker S^* = d_R \quad (c)$$

and let $\{\varphi_{R,1}, \dots, \varphi_{R,d_R}\}$ be an orthonormal basis of this d_R -dimensional subspace of $\mathcal{D}(S_F)$. Decompose $f_R = f_{R,1} + \dots + f_{R,d_R}$ with $f_{R,j} := \langle \varphi_{R,j}, f_R \rangle \varphi_{R,j}$, $j = 1, \dots, d_R$. Then

$$\begin{aligned} \int_{[0, 2R]} \frac{\lambda \alpha}{\lambda - \alpha} d\langle f_R, E^{(S_F)}(\lambda) f_R \rangle &= \sum_{j=1}^{d_R} \int_{[0, 2R]} \frac{\lambda \alpha}{\lambda - \alpha} d\langle f_{R,j}, E^{(S_F)}(\lambda) f_{R,j} \rangle \\ &= \sum_{j=1}^{d_R} |\langle \varphi_{R,j}, f_R \rangle|^2 \int_{[0, 2R]} \frac{\lambda \alpha}{\lambda - \alpha} d\langle \varphi_{R,j}, E^{(S_F)}(\lambda) \varphi_{R,j} \rangle \\ &= \sum_{j=1}^{d_R} |\langle \varphi_{R,j}, f_R \rangle|^2 \langle \tilde{\varphi}_{R,j}, M(\alpha) \tilde{\varphi}_{R,j} \rangle. \end{aligned}$$

Where the $\tilde{\varphi}_{R,j} \in \ker S^*$ are preimages under $E^{(S_F)}([0, 2R])$ of the orthonormal basis, so that the last line just uses the fact that $E^{(S_F)}([0, 2R])$ is a orthogonal projection. Owing to (5.2), each $\langle \tilde{\varphi}_{R,j}, M(\alpha) \tilde{\varphi}_{R,j} \rangle$ diverges to $-\infty$ as $\alpha \rightarrow -\infty$: there is only a *finite* number of them (and it does not exceed d), so there is a common threshold $\alpha_R < 0$ such that

$$\sup_{j \in \{1, \dots, d_R\}} \langle \tilde{\varphi}_{R,j}, M(\alpha) \tilde{\varphi}_{R,j} \rangle \leq -R \quad \forall \alpha \leq \alpha_R.$$

Therefore

$$\int_{[0, 2R]} \frac{\lambda \alpha}{\lambda - \alpha} d\langle f_R, E^{(S_F)}(\lambda) f_R \rangle \leq -R \|f_R\|^2 \quad (\alpha \leq \alpha_R) \quad (d)$$

(α_R only depends on R (and on d), *not* on f_R). Plugging the bounds (b) and (d) into (a) yields

$$\langle u, M(\alpha) u \rangle < -R \|f_R\|^2 - R \|v_R\|^2 = -R \|u\|^2$$

for $\alpha < \min\{-2R, \alpha_R\}$. From the arbitrariness of $u \in \ker S^*$ and of $R > 0$ one concludes that $M(\alpha) \rightarrow -\infty$ uniformly as $\alpha \rightarrow -\infty$. \square

Corollary 5.5. *If S is a semi-bounded and densely defined symmetric operator on a Hilbert space \mathcal{H} , whose bottom is positive ($m(S) > 0$) and whose Friedrichs extension has compact inverse S_F^{-1} , then the semi-boundedness of S_T is equivalent to the semi-boundedness of T .*

Proof. Since S_F^{-1} is compact, the spectrum of S_F only consists of a discrete set of eigenvalues, each of finite multiplicity, whence the bound (c) in the proof of Corollary 5.4 and the same conclusion as in Corollary 5.4(i). \square

Remark 5.6. The question of Theorem 5.3 and its corollaries deal with is sometimes referred to as the “*semi-boundedness problem*”, that is, the problem of finding conditions under which the semi-boundedness of S_T and of T are equivalent (in general or under special circumstances). The fact that the compactness of S_F^{-1} is a sufficient condition (that is, Corollary 5.5) was noted originally by Grubb [25] and by Gorbačuk and Mihailec [23] in the mid 1970’s. More than a decade later the same property, and more generally the necessary

and sufficient condition provided by Theorem 5.3, was proved *with a boundary triplets language* by Derkach and Malamud [16]. In fact, it is easy to recognise that the operator-valued function $\alpha \mapsto M(\alpha)$ defined in (5.1) is the Weyl function of a standard boundary triplet [56, Example 14.12]. In [16, Section 3] one can also find examples in which such a condition is violated. The conclusion of Corollary 5.4(ii) is easy to establish also with general Hilbert space and spectral arguments, with no reference to the KVB theory – see, e.g., [17, Lemma XIII.7.22] or [52, Theorem X.1, first corollary].

Theorem 5.3 and (the proof of) Corollary 5.4 have a further noticeable consequence.

Corollary 5.7 (“Finite-dimensional” extensions are always semi-bounded).

Given a semi-bounded and densely defined symmetric operator S on a Hilbert space \mathcal{H} , whose bottom is positive ($m(S) > 0$), all the self-adjoint extensions of S_T of S for which the parameter T , in the parametrisation (3.2) of Theorem 3.4, is a self-adjoint operator acting on a finite-dimensional subspace of $\ker S^$ are semi-bounded. For the occurrence of unbounded below self-adjoint extensions it is necessary (not sufficient) that $\dim \overline{\mathcal{D}(T)} = \infty$.*

Proof. T is bounded (and hence also semi-bounded) because the Hilbert space $\overline{\mathcal{D}(T)}$ it acts on has finite dimension. Let $P_T : \mathcal{H} \rightarrow \mathcal{H}$ be the orthogonal projection onto $\overline{\mathcal{D}(T)}$ and set

$$\widetilde{M}(\alpha) := P_T(\alpha \mathbb{1} + \alpha^2(S_F - \alpha \mathbb{1})^{-1})P_T = P_T M(\alpha) P_T, \quad \alpha < m(S).$$

One can repeat for $\widetilde{M}(\alpha)$ the same arguments used in the proof of Corollary 5.4 to establish the uniform divergence of $M(\alpha)$ to $-\infty$, thus obtaining the same property for $\widetilde{M}(\alpha)$ on the finite-dimensional space $\overline{\mathcal{D}(T)}$ (the assumption $\dim \overline{\mathcal{D}(T)} = d < +\infty$ implies $\dim E^{(S_F)}([0, 2R])\overline{\mathcal{D}(T)} = d_R \leq d$, which is the analogue of formula (c) in the proof of Corollary 5.4, whence the same conclusion). Therefore $\exists \alpha < 0$, with $|\alpha|$ sufficiently large, such that

$$\alpha \|v\|^2 + \alpha^2 \langle v, (S_F - \alpha \mathbb{1})^{-1} v \rangle < m(T) \|v\|^2 \leq \langle v, T v \rangle \quad \forall v \in \mathcal{D}(T),$$

which implies $m(S_T) > \alpha$ owing to (3.3). \square

Remark 5.8. It is also worth remarking that unless S is essentially self-adjoint, in all other cases (i.e., whenever $\dim \ker S^* \geq 1$) there is no *uniform* lower bound to the bottoms of the semi-bounded self-adjoint extensions of S . This is an immediate consequence of the bound $m(T) \geq m(S_T)$ given by (3.3) in Theorem 3.5, since it is enough to consider extension parameters $T = -\gamma \mathbb{1}$ for arbitrary $\gamma > 0$.

In the remaining part of this Section we turn to the negative spectrum of an extension S_T . It turns out that relevant properties of the negative discrete spectrum of S_T are controlled by the analogous properties for T . We cast in Theorem 5.9 and Corollary 5.10 below results that are found in Birman’s original work [8] (formulated therein with the original parametrisation

$S_B \leftrightarrow B$), apart from a number of ambiguities and redundancies that we have cleaned up.

For convenience let us define

$$\begin{aligned}\sigma_-(S_T) &:= \sigma(S_T) \cap (-\infty, 0) \\ \sigma_-(T) &:= \sigma(T) \cap (-\infty, 0).\end{aligned}\tag{5.3}$$

Theorem 5.9 (Negative spectrum). *Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$) and let S_T be a generic self-adjoint extension of S according to the parametrisation (3.2) of Theorem 3.4. Then $\sigma_-(S_T)$ consists of a bounded below set of finite-rank eigenvalues of S_T whose only possible accumulation point is 0 if and only if $\sigma_-(T)$ has the same property. When this is the case, and $\lambda_1 \leq \lambda_2 \leq \dots < 0$ and $t_1 \leq t_2 \leq \dots < 0$ are the ordered sequences of negative eigenvalues (counted with multiplicity) of S_T and of T respectively, then*

- ground state of $S_T = \lambda_1 \leq t_1 =$ ground state of T ,
- $\lambda_k \leq t_k$ for $k = 1, 2, \dots$

Corollary 5.10. *For some $N \in \mathbb{N}$, $\sigma_-(S_T)$ consists of N eigenvalues if and only if $\sigma_-(T)$ consists of N eigenvalues. (Here the eigenvalues are counted with multiplicity.)*

Remark 5.11. We observe that no restriction is assumed on the dimension of $\ker S^*$, that is, the deficiency index of S can be infinite as well. In fact, as long as $\dim \ker S^* < +\infty$, Corollary 5.10 could be deduced directly by combining Theorems 19 and 20 of Kreĭn’s original work [30] with the subsequent results of Viřik and Birman that are stated here in Theorems 3.4 and 3.6.

A further consequence is the following.

Corollary 5.12.

- (i) *If S has finite deficiency index ($\dim \ker S^* < +\infty$), then all self-adjoint extensions of S have finite negative spectrum, with finite-dimensional eigenvalues.*
- (ii) *If, in the sense of the parametrisation (3.2) of Theorem 3.4, S_T is a self-adjoint extension of S where the parameter T acts on a finite-dimensional subspace of $\ker S^*$, then the negative spectrum $\sigma_-(S_T)$ of S_T is finite, with finite-dimensional eigenvalues.*

In preparation for the proof of Theorem 5.9 and its corollaries, let us denote by $dE^{(S_T)}$ and by $dE^{(T)}$, respectively, the spectral measure of S_T and of T on \mathbb{R} . For generic $v \in \mathcal{D}(T)$ one also has $v \in \mathcal{D}[S_T]$ with $\langle v, Tv \rangle = S_T[v]$, owing to (3.7) (see also (2.30)), whence

$$\int_{[m(T), +\infty)} t \langle v, dE^{(T)}(t)v \rangle = \int_{[m(S_T), +\infty)} \lambda \langle v, dE^{(S_T)}(\lambda)v \rangle \geq \int_{[m(S_T), 0)} \lambda \langle v, dE^{(S_T)}(\lambda)v \rangle.\tag{5.4}$$

Let us also single out two useful facts (the first is straightforward).

Lemma 5.13. *If V and W are closed subspaces of \mathcal{H} with $\dim V < +\infty$ and $\dim W > \dim V$, then $W \cap V^\perp \neq \{0\}$.*

Lemma 5.14. *If $\varepsilon > 0$ and, for some $N \in \mathbb{N}$, g_1, \dots, g_N are linearly independent elements in $\mathcal{D}(S_T) \cap E^{(S_T)}((-\infty, -\varepsilon])\mathcal{H}$, then the corresponding v_1, \dots, v_N given by the decomposition (3.2) $g_k = f_k + S_F^{-1}(Tv_k + w_k) + v_k$, $k = 1, \dots, N$, are linearly independent in $\mathcal{D}(T)$.*

Proof. If $\sum_{k=1}^N c_k v_k = 0$ for some $c_1, \dots, c_N \in \mathbb{C}$, then $g := \sum_{k=1}^N c_k g_k = \sum_{k=1}^N c_k (f_k + S_F^{-1}(Tv_k + w_k)) \in \mathcal{D}(S_F)$, whence $\langle g, S_T g \rangle = \langle g, S_F g \rangle \geq m(S) \|g\|^2 \geq 0$. On the other hand,

$$\begin{aligned} \langle g, S_T g \rangle &= \int_{[m(S_T), +\infty)} \lambda \langle g, dE^{(S_T)}(\lambda)g \rangle = \int_{[m(S_T), -\varepsilon]} \lambda \langle g, dE^{(S_T)}(\lambda)g \rangle \\ &\leq -\varepsilon \int_{[m(S_T), -\varepsilon]} \langle g, dE^{(S_T)}(\lambda)g \rangle \leq 0 \end{aligned}$$

(where in the second identity we used that $g \in \mathcal{D}(S_T) \cap E^{(S_T)}((-\infty, -\varepsilon])\mathcal{H}$), therefore $g = 0$ and hence, by assumption, $c_1 = \dots = c_N = 0$. \square

Proof of Theorem 5.9. Assume that $\sigma_-(S_T)$ consists of a bounded below set of finite-rank eigenvalues of S_T whose only possible accumulation point is 0. In particular, $-\infty < m(S_T) < 0$ which, by (3.3)-(3.4), implies also $m(S_T) \leq m(T) < 0$. If, for contradiction, $\sigma_-(T)$ does not satisfy the same property of $\sigma_-(S_T)$, then there exists $\varepsilon > 0$ such that $\dim E^{(T)}([m(T), -\varepsilon])\overline{\mathcal{D}(T)} = +\infty$, whereas by assumption $\dim E^{(S_T)}([m(S_T), -\frac{1}{2}\varepsilon])\mathcal{H} < +\infty$. By Lemma 5.13 $\exists v \in E^{(T)}([m(T), -\varepsilon])\overline{\mathcal{D}(T)}$, $v \neq 0$, $v \perp E^{(S_T)}([m(S_T), -\frac{1}{2}\varepsilon])\mathcal{H}$. As a consequence of this and of (5.4),

$$\begin{aligned} -\varepsilon \|v\|^2 &\geq \int_{[m(T), -\varepsilon]} t \langle v, dE^{(T)}(t)v \rangle = \int_{[m(T), +\infty)} t \langle v, dE^{(T)}(t)v \rangle \\ &\geq \int_{[m(S_T), 0]} \lambda \langle v, dE^{(S_T)}(\lambda)v \rangle = \int_{(-\frac{1}{2}\varepsilon, 0)} \lambda \langle v, dE^{(S_T)}(\lambda)v \rangle \geq -\frac{\varepsilon}{2} \|v\|^2, \end{aligned}$$

which is a contradiction because $v \neq 0$. For the converse, assume that $\sigma_-(T)$ consists of a bounded below set of finite-rank eigenvalues of T whose only possible accumulation point is 0. In particular, $-\infty < m(T) < 0$. If, for contradiction, $\sigma_-(S_T)$ does not satisfy the same property of $\sigma_-(T)$, then $\dim E^{(S_T)}((-\infty, -\varepsilon])\mathcal{H} = +\infty$ for some $\varepsilon > 0$. Therefore also

$$\dim E^{(S_T)}((-\infty, -\varepsilon])\mathcal{H} \cap \mathcal{D}(S_T) = +\infty \quad (*)$$

because $E^{(S_T)}((-\infty, -\varepsilon])\mathcal{H} \cap \mathcal{D}(S_T)$ is dense in $E^{(S_T)}((-\infty, -\varepsilon])\mathcal{H}$. Based on the decomposition (3.2) for generic $g \in \mathcal{D}(S_T)$ (namely, $g = f + S_F^{-1}(Tv + w) + v$), set

$$V_\varepsilon := \left\{ v \in \mathcal{D}(T) \left| \begin{array}{l} g - v \in \mathcal{D}(S_F) \text{ for some} \\ g \in E^{(S_T)}(-\infty, -\varepsilon])\mathcal{H} \cap \mathcal{D}(S_T) \end{array} \right. \right\}.$$

In fact, owing to Lemma 5.14, any $v \in V_\varepsilon$ identifies uniquely the corresponding $g \in E^{(S_T)}(-\infty, -\varepsilon])\mathcal{H} \cap \mathcal{D}(S_T)$. Furthermore, Lemma 5.14 and

(*) yield $\dim V_\varepsilon = +\infty$. On the other hand, let $h \in \mathbb{R}$ with $0 < h < \min\{-m(T), \frac{\varepsilon m(S)}{2m(S)+\varepsilon}\}$: by assumption

$$\dim E^{(T)}([m(T), -h])\overline{\mathcal{D}(T)} < +\infty. \quad (**)$$

Lemma 5.13 and (*)-(**) then imply the existence of a non-zero $v \in V_\varepsilon$ with $v \perp E^{(T)}([m(T), -h])\overline{\mathcal{D}(T)}$. For such v one has

$$\begin{aligned} \langle v, Tv \rangle &= \int_{[m(T), +\infty)} t \langle v, dE^{(T)}(t)v \rangle = \int_{(-h, +\infty)} t \langle v, dE^{(T)}(t)v \rangle \geq -h\|v\|^2 \\ &\geq -\frac{\varepsilon m(S)}{2m(S) + \varepsilon} \|v\|^2 \end{aligned}$$

which can be re-written equivalently as

$$\langle v, Tv \rangle + \frac{\varepsilon}{2} \|v\|^2 \geq \frac{\varepsilon^2}{4} \frac{1}{m(S) + \frac{1}{2}\varepsilon} \|v\|^2.$$

The last inequality implies

$$\langle v, Tv \rangle + \frac{\varepsilon}{2} \|v\|^2 \geq \frac{\varepsilon^2}{4} \langle v, (S_F + \frac{1}{2}\varepsilon)^{-1}v \rangle.$$

If g is the vector in $E^{(S_T)}(-\infty, -\varepsilon])\mathcal{H} \cap \mathcal{D}(S_T)$ that corresponds to such $v \in V_\varepsilon$, by repeating the very same reasoning as in the proof of Theorem 2.15 one sees that the latter condition is *equivalent* to $\langle g, S_T g \rangle \geq -\frac{\varepsilon}{2}\|g\|^2$. However, this last finding is not compatible with the fact that

$$\langle g, S_T g \rangle = \int_{[m(S_T), +\infty)} \lambda \langle g, dE^{(S_T)}(\lambda)g \rangle = \int_{[m(S_T), -\varepsilon)} \lambda \langle g, dE^{(S_T)}(\lambda)g \rangle \leq -\varepsilon\|g\|^2,$$

whence the contradiction. This completes the proof of the equivalence of the considered condition for $\sigma_-(S_T)$ and $\sigma_-(T)$. When such a condition holds and the eigenvalues are labelled as in the statement of the theorem, obviously $\lambda_1 = m(S_T) \leq m(T) = t_1$ (by (3.3)), while the fact that $\lambda_k \leq t_k$ for $k = 1, 2, \dots$ is a consequence of the min-max principle for the self-adjoint operators S_T and T , owing to the fact (Theorem 3.6) that $S_T \leq T$. \square

Proof of Corollary 5.10. Owing to Theorem 5.9,

$$\sigma_-(S_T) = \{\text{eigenvalues } \lambda_1 \leq \dots \leq \lambda_N < 0\} \quad \text{for some } N \in \mathbb{N}$$

is equivalent to

$$\sigma_-(T) = \{\text{eigenvalues } t_1 \leq \dots \leq t_M < 0\} \quad \text{for some } M \in \mathbb{N}$$

and when this is the case $\lambda_1 = m(S_T) \leq m(T) = t_1$. If $M > N$, then $\exists v \in (E^{(T)}([m(T), -\varepsilon])\overline{\mathcal{D}(T)}) \cap (E^{(S_T)}([m(S_T), 0])\mathcal{H})^\perp$, $v \neq 0$, for some $\varepsilon > 0$ (in fact, $\forall \varepsilon \in (0, |t_M|)$), as a consequence of Lemma 5.13. Moreover, $v \in \mathcal{D}(T)$ because

$$\int_{[m(T), +\infty)} t^2 \langle v, dE^{(T)}(t)v \rangle = \int_{[m(T), -\varepsilon]} t^2 \langle v, dE^{(T)}(t)v \rangle < +\infty,$$

whence also $v \in \mathcal{D}[S_T]$ with $S_T[v] = \langle v, Tv \rangle$, owing to (3.7). As a consequence of this and of (5.4),

$$0 > \int_{[m(T), -\varepsilon]} t \langle v, dE^{(T)}(t)v \rangle = \int_{[m(T), +\infty)} t \langle v, dE^{(T)}(t)v \rangle \geq \int_{[m(S_T), 0)} \lambda \langle v, dE^{(S_T)}(\lambda)v \rangle = 0,$$

a contradiction. If instead $M < N$, let us use the fact that for some $\varepsilon > 0$ (in fact $\forall \varepsilon \in (0, |\lambda_N|)$) Lemma 5.14 applied to the space V_ε introduced in the proof of Theorem 5.9 yields $\dim V_\varepsilon \geq N$: then, owing to Lemma 5.13, $\exists v \in V_\varepsilon \cap (E^{(T)}([m(T), 0))\overline{\mathcal{D}(T)})^\perp$, $v \neq 0$. In turn, as already observed in the proof of Theorem 5.9, this v identifies uniquely a non-zero element $g \in E^{(S_T)}([m(S_T), -\varepsilon])\mathcal{H} \subset \mathcal{D}(S_T)$ for which $g - v \in \mathcal{D}(S_F)$. For such g and v , (3.7) yields $\langle g, S_T g \rangle \geq \langle v, Tv \rangle$. With these findings,

$$\begin{aligned} 0 > \int_{[m(S_T), -\varepsilon]} \lambda \langle g, dE^{(S_T)}(\lambda)g \rangle &= \int_{[m(S_T), +\infty)} \lambda \langle g, dE^{(S_T)}(\lambda)g \rangle = \langle g, S_T g \rangle \\ &\geq \langle v, Tv \rangle = \int_{[m(T), +\infty)} t \langle v, dE^{(T)}(t)v \rangle \geq \int_{[m(T), 0)} t \langle v, dE^{(T)}(t)v \rangle = 0, \end{aligned}$$

another contradiction. Thus, the conclusion is necessarily $M = N$. \square

Proof of Corollary 5.12. In either case (i) and (ii) the extension parameter T is self-adjoint on a finite-dimensional space, therefore its spectrum only consists of a finite number of (finite-dimensional) eigenvalues. This is true in particular for the negative spectrum of T . Then the conclusion follows from Corollary 5.10. \square

6. Resolvents of self-adjoint extensions

We turn now to the discussion of the structure of the resolvent of self-adjoint extensions.

In fact, this is a context in which the theory of boundary triplets (the modern theory that has “incorporated” the original KVB results, see Section 4) has deepest results, including the appropriate abstract language to reproduce in full generality the celebrated Kreĭn-Naimark resolvent formula – see, e.g., the comprehensive overview in [56, Chapter 14]. Here we content ourselves to discuss some direct applications of the KVB theory. We thus derive the formula of the inverse of an invertible extension *in terms of its KVB extension parameter* and of the “canonical” Friedrichs extension (Theorem 6.1), and from it we derive resolvent formulas (Corollary 6.4 and Theorem 6.6) originally established, in implicit form, by Kreĭn [30, Theorem 20].

Theorem 6.1 (Resolvent formula for invertible extensions). *Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$). Let, in terms of the decomposition and parametrisation (3.2) of Theorem 3.4, S_T be a generic self-adjoint extension of S and $P_T : \mathcal{H} \rightarrow \mathcal{H}$ be the*

orthogonal projection onto $\overline{\mathcal{D}(T)}$. If S_T is invertible on the whole \mathcal{H} , then T is invertible on the whole $\overline{\mathcal{D}(T)}$ and

$$S_T^{-1} = S_F^{-1} + P_T T^{-1} P_T. \quad (6.1)$$

Proof. The invertibility (with everywhere defined inverse) of T is guaranteed by Theorem 5.1(iii). Thus, (6.1) is an identity between bounded self-adjoint operators (their boundedness following by the inverse mapping theorem). For a generic $h \in \mathcal{H} = \text{ran } S_T$ one has $h = S_T g$ for some $g = f + S_F^{-1}(Tv+w) + v = F + v$, where $f \in \mathcal{D}(\overline{S})$, $v \in \mathcal{D}(T)$, $w = \ker S^* \cap \mathcal{D}(T)$ (Theorem 3.4), and hence $F \in \mathcal{D}(S_F)$ (Remark 2.3). Then

$$\langle h, S_T^{-1} h \rangle = \langle g, S_T g \rangle = \langle F, S_F F \rangle + \langle v, Tv \rangle.$$

On the other hand

$$\langle F, S_F F \rangle = \langle S_F F, S_F^{-1} S_F F \rangle = \langle S_T g, S_F^{-1} S_T g \rangle = \langle h, S_F^{-1} h \rangle$$

and

$$\langle v, Tv \rangle = \langle Tv, T^{-1} Tv \rangle = \langle P_T S_T g, T^{-1} P_T S_T g \rangle = \langle h, P_T T^{-1} P_T h \rangle,$$

whence the conclusion $\langle h, S_T^{-1} h \rangle = \langle h, S_F^{-1} h \rangle + \langle h, P_T T^{-1} P_T h \rangle$. \square

Remark 6.2. In terms of the equivalent parametrisation $S_B \leftrightarrow B$ of the self-adjoint extensions of S (Theorem 2.12), and denoting with $P_B : \mathcal{H} \rightarrow \mathcal{H}$ the orthogonal projection onto $\overline{\mathcal{D}(B)}$, Theorem 6.1 takes the following form: if S_B is invertible on the whole \mathcal{H} , then

$$S_B^{-1} = S_F^{-1} + P_B B P_B \quad (6.2)$$

(and B is not the zero operator on the whole $\ker S^*$, unless $S_B = S_F$). Indeed, re-doing the proof above, for generic $g \in \mathcal{D}(S_B)$ the parametrisation (2.24) yields $g = f + (S_F^{-1} + B)\tilde{u}_1 + u_0$ for some $f \in \mathcal{D}(\overline{S})$, $\tilde{u}_1 \in \mathcal{D}(B)$, and $u_0 \in \ker S^* \cap \mathcal{D}(B)^\perp$, whence $F := f + S_F^{-1}\tilde{u}_1 \in \mathcal{D}(S_F)$, $h := S_B g = S_F F = \overline{S}f + \tilde{u}_1$, and $\tilde{u}_1 = P_B S_B g$. Therefore,

$$\begin{aligned} \langle h, S_B^{-1} h \rangle &= \langle g, S_B g \rangle = \langle F, S_F F \rangle + \langle \tilde{u}_1, B\tilde{u}_1 \rangle \\ &= \langle h, S_F^{-1} h \rangle + \langle h, P_B B P_B h \rangle. \end{aligned}$$

Remark 6.3. With reference to the historical perspective of Section 4, Theorem 6.1 appears, in a formulation that is virtually the same as the present one, both in Grubb [24, Theorem 1.4] and, limited to S_T 's with positive bottom, in Faris [18, Theorem 15.1].

Corollary 6.4. *Let \tilde{S} be a self-adjoint extension of S and let $z < m(S)$ be such that $\tilde{S} - z\mathbb{1}$ is invertible on the whole \mathcal{H} (for example a semi-bounded extension \tilde{S} and a real number $z < m(\tilde{S})$). Let $T(z)$ be the extension parameter, in the sense of the KVB parametrisation (3.2) of Theorem 3.4, of the operator $\tilde{S} - z\mathbb{1}$ considered as a self-adjoint extension of the densely defined and bottom-positive symmetric operator $S(z) := S - z\mathbb{1}$. Correspondingly, let $P(z)$ be the orthogonal projection onto $\overline{\mathcal{D}(T(z))}$. Then*

$$(\tilde{S} - z\mathbb{1})^{-1} = (S_F - z\mathbb{1})^{-1} + P(z) T(z)^{-1} P(z). \quad (6.3)$$

Proof. Since $m(S(z)) = m(S) - z > 0$, the assumptions of Theorem 6.1 are matched and (6.1) takes the form (6.3) owing to the fact that the Friedrichs extension of $S(z)$ is precisely $S_F - z\mathbb{1}$ (Theorem A.2(vii)). \square

Remark 6.5. Formula (6.3), in particular, shows that the resolvent difference $(\tilde{S} - z\mathbb{1})^{-1} - (S_F - z\mathbb{1})^{-1}$ has non-zero matrix elements only on a suitable subspace of $\ker(S^* - z\mathbb{1})$. (The dependence on z of the term $P(z)T(z)^{-1}P(z)$ remains here somewhat implicit, although of course $T(z)$ and $P(z)$ are unambiguously and constructively well defined in terms of the given $\tilde{S} - z\mathbb{1}$, as described in Proposition 3.10.)

Let us now make (6.3) more explicit by reproducing a Kreĭn-like resolvent formula (see, e.g., [1, Theorems A.2-A.3]).

Theorem 6.6 (Kreĭn's resolvent formula for deficiency index = 1). *Let S be a densely defined symmetric operator on a Hilbert space \mathcal{H} with positive bottom ($m(S) > 0$) and with deficiency index $\dim \ker S^* = 1$. Let \tilde{S} be a self-adjoint extension of S other than the Friedrichs extension S_F . Let $v \in \ker S^* \setminus \{0\}$ and for each $z \in (-\infty, m(S)) \cap \rho(\tilde{S})$ set*

$$v(z) := v + z(S_F - z\mathbb{1})^{-1}v. \quad (6.4)$$

Then there exists an analytic function $\beta : (-\infty, m(S)) \cap \rho(\tilde{S}) \rightarrow \mathbb{R}$, with $\beta(z) \neq 0$, such that

$$(\tilde{S} - z\mathbb{1})^{-1} = (S_F - z\mathbb{1})^{-1} + \beta(z)|v(z)\rangle\langle v(z)|. \quad (6.5)$$

$\beta(z)$, $v(z)$, and (6.5) admit an analytic continuation to $\rho(S_F) \cap \rho(\tilde{S})$.

Proof. Because of the constance of the deficiency index, $\dim \ker(S^* - z\mathbb{1}) = \dim \ker S^* = 1$. \tilde{S} is semi-bounded (Corollary 5.4). Since $z < m(\tilde{S})$, $\tilde{S} - z\mathbb{1}$ is a bottom-positive self-adjoint extension of the densely defined and bottom-positive symmetric operator $S(z) := S - z\mathbb{1}$. Its extension parameter $T(z)$, in the sense of the KVB parametrisation, is the bottom-positive self-adjoint operator $T(z)$ on the space $\ker(S^* - z\mathbb{1})$ which acts as the multiplication by a positive number $t(z)$. (The positivity of the bottom of $T(z)$ follows from $m(T(z)) \geq m(\tilde{S} - z\mathbb{1}) > 0$, Theorem 5.3.) Clearly, $v(z) \in \ker(S^* - z\mathbb{1})$. Moreover, $v(z) \neq 0$ for each admissible z : this is obviously true if $z = 0$, and if it was not true for $z \neq 0$, then $z(S_F - z\mathbb{1})^{-1}v = -v \neq 0$, which would contradict $\mathcal{D}(S_F - z\mathbb{1}) \cap \ker(S^* - z\mathbb{1}) = \{0\}$ (Remark 2.3, formula (2.7)). Thus, $v(z)$ spans $\ker(S^* - z\mathbb{1})$ and $P_T := \|v(z)\|^{-2}|v(z)\rangle\langle v(z)| : \mathcal{H} \rightarrow \mathcal{H}$ is the orthogonal projection onto $\ker(S^* - z\mathbb{1})$. In this case, the resolvent formula (6.3) takes precisely the form (6.5) where $\beta(z) := \|v(z)\|^{-2}t(z)^{-1}$. Being a product of positive quantities, $\beta(z) > 0$. Moreover, $z \mapsto (\tilde{S} - z\mathbb{1})^{-1}$ and $z \mapsto (S_F - z\mathbb{1})^{-1}$ are analytic operator-valued functions on the whole $\rho(S_F) \cap \rho(\tilde{S})$ (because of the analyticity of resolvents) and so is the vector-valued function $z \mapsto v(z)$ (because of the construction (6.4)). Therefore, taking the expectation of both sides of (6.5) on $v(z)$ shows at once that $z \mapsto \beta(z)$ is analytic on $\rho(S_F) \cap \rho(\tilde{S})$, and real analytic on $(-\infty, m(S)) \cap \rho(\tilde{S})$. \square

7. Examples

7.1. “Free quantum particle” on half-line

On the Hilbert space $\mathcal{H} = L^2[0, +\infty)$ one considers the densely defined symmetric operator

$$S = -\frac{d^2}{dx^2} + \mathbb{1}, \quad \mathcal{D}(S) = C_0^\infty(0, +\infty). \quad (7.1)$$

S has bottom $m(S) = 1$. One has

$$S^* = -\frac{d^2}{dx^2} + \mathbb{1} \\ \mathcal{D}(S^*) = H^2(0, +\infty) = \left\{ f \in L^2[0, +\infty) \mid \begin{array}{l} f, f' \in AC[0, +\infty) \\ f'' \in L^2[0, +\infty) \end{array} \right\}, \quad (7.2)$$

thus all the extensions of S act as $-\frac{d^2}{dx^2} + \mathbb{1}$ on suitable restrictions of $H^2(0, +\infty)$. In particular,

$$\mathcal{D}(\bar{S}) = H_0^2(0, +\infty) = \{f \in H^2(0, +\infty) \mid f(0) = 0, f'(0) = 0\} \quad (7.3)$$

and the Friedrichs extension of S has domain

$$\mathcal{D}(S_F) = H^2(0, +\infty) \cap H_0^1(0, +\infty) = \{f \in H^2(0, +\infty) \mid f(0) = 0\}, \quad (7.4)$$

that is, $\mathcal{D}(S^*)$ with Dirichlet boundary condition at the origin.

Applying von Neumann’s theory one finds (see, e.g., [20, Chapter 6.2]) that the self-adjoint extensions of S constitute the family $\{S_\nu \mid \nu \in (-\frac{\pi}{2}, \frac{\pi}{2})\}$, where each S_ν acts as $-\frac{d^2}{dx^2} + \mathbb{1}$ on the domain

$$\mathcal{D}(S_\nu) = \{g \in H^2(0, +\infty) \mid g(0) \sin \nu = g'(0) \cos \nu\}. \quad (7.5)$$

By inspection one sees that the Friedrichs extension of S is $S_{\pi/2}$.

In order to apply the KVB theory, one needs to identify $\ker S^*$ and S_F^{-1} . One easily finds

$$\ker S^* = \text{Span}\{e^{-x}\}. \quad (7.6)$$

All self-adjoint extensions of S are therefore semi-bounded (Corollary 5.4). One also finds that the integral kernel of S_F^{-1} is

$$S_F^{-1}(x, y) = \frac{1}{2}(e^{-|x-y|} - e^{-(x+y)}) \quad (7.7)$$

(see, e.g., [20, Chapter 6.2]). In fact, since S_F^{-1} only enters the formulas as acting on $\ker S^*$, instead of (7.7) one can rather limit oneself to the problem

$$\begin{cases} -\eta''(x) + \eta(x) = e^{-x}, & x \in [0, +\infty) \\ \eta(0) = 0, \end{cases}$$

whose only solution in $L^2[0, +\infty)$ is $\eta(x) = \frac{1}{2} x e^{-x}$. Thus, for fixed $a \in \mathbb{C}$,

$$S_F^{-1}(a e^{-x}) = \frac{a}{2} x e^{-x}. \quad (7.8)$$

According to Theorem 3.4, the self-adjoint extensions of S are operators of the form S_T where T is a self-adjoint operator on subspaces of

$\ker S^* = \text{Span}\{e^{-x}\}$, precisely the zero-dimensional subspace $\{0\}$ or the whole $\text{Span}\{e^{-x}\}$. In the former case $S_T = S_F$ (Proposition 3.7). In the latter, each such T acts as the multiplication $T_\beta : e^{-x} \mapsto \beta e^{-x}$ by a fixed $\beta \in \mathbb{R}$, $\mathcal{D}(T_\beta) = \text{Span}\{e^{-x}\} = \ker S^*$, and $\ker S^* \cap \mathcal{D}(T_\beta)^\perp = \{0\}$: by (3.2) and (7.8), the corresponding self-adjoint extension $S_\beta \equiv S_{T_\beta}$ of S acts as $-\frac{d^2}{dx^2} + \mathbb{1}$ on the domain

$$\begin{aligned}
 \mathcal{D}(S_\beta) &= \left\{ g = f + S_F^{-1}(\beta a e^{-x}) + a e^{-x} \mid \begin{array}{l} f \in H_0^2(0, +\infty) \\ a \in \mathbb{C} \end{array} \right\} \\
 &= \left\{ g \mid \begin{array}{l} g(x) = f(x) + a(\frac{1}{2}\beta x + 1)e^{-x} \\ x \in [0, 1], f \in H_0^2(0, +\infty), a \in \mathbb{C} \end{array} \right\}.
 \end{aligned} \tag{7.9}$$

Observing that $g(0) = a$ and $g'(0) = a(\frac{1}{2}\beta - 1)$ for any $g \in \mathcal{D}(S_\beta)$, (7.9) can be re-written as

$$\mathcal{D}(S_\beta) = \left\{ g \in H^2(0, +\infty) \mid g'(0) = \left(\frac{\beta}{2} - 1\right)g(0) \right\}. \tag{7.10}$$

Comparing (7.10) with (7.5) above, we see that S_β is the extension S_ν of von Neumann's parametrisation with

$$\beta/2 - 1 = \tan \nu \tag{7.11}$$

which includes the Friedrichs extension ($\nu = \frac{\pi}{2}$) if one let $\beta = +\infty$.

The same analysis can be equivalently performed in terms of the quadratic forms of the self-adjoint extensions of S , following Theorem 3.6 (which applies to this example since *all* extensions are semi-bounded). The reference form is the Friedrichs one, that is,

$$\begin{aligned}
 \mathcal{D}[S_F] &= H_0^1(0, +\infty) = \{f \in H^1[0, +\infty) \mid f(0) = 0\} \\
 S_F[F_1, F_2] &= \int_0^{+\infty} \overline{F_1'(x)} F_2'(x) dx + \int_0^{+\infty} \overline{F_1(x)} F_2(x) dx,
 \end{aligned} \tag{7.12}$$

as one deduces from (7.4). Owing to (3.7), the form domain of any other extension is obtained by taking the direct sum of $\mathcal{D}[S_T] = \mathcal{D}[S_F] \dot{+} \mathcal{D}[T]$ where $T \equiv T_\beta =$ the multiplication by a real β on $\mathcal{D}(T) = \text{Span}\{e^{-x}\} = \mathcal{D}[T]$. Then (3.7) and (7.12) yield

$$\begin{aligned}
 \mathcal{D}[S_\beta] &= H_0^1(0, +\infty) \dot{+} \text{Span}\{e^{-x}\} = H^1(0, +\infty) \\
 S_\beta[g_1, g_2] &= S_\beta[F_1 + a_1 e^{-x}, F_2 + a_2 e^{-x}] \\
 &= \int_0^{+\infty} \overline{F_1'(x)} F_2'(x) dx + \int_0^{+\infty} \overline{F_1(x)} F_2(x) dx + \frac{\beta}{2} \overline{a_1} a_2 \\
 &= \int_0^{+\infty} \overline{g_1'(x)} g_2'(x) dx + \int_0^{+\infty} \overline{g_1(x)} g_2(x) dx + \left(\frac{\beta}{2} - 1\right) \overline{g_1(0)} g_2(0).
 \end{aligned} \tag{7.13}$$

Going backwards from this (closed and semi-bounded) form to the uniquely associated self-adjoint operator, a straightforward exercise would yield the domain $\mathcal{D}(S_\beta)$ already determined by (7.10).

Concerning the bottom and the negative spectrum of a generic extension S_β , one has $m(T_\beta) = \beta$ and $\sigma(T_\beta) = \{\beta\}$, therefore Theorem 3.5 gives

$$\begin{aligned}
 m(S_\beta) &\leq \min\{1, \beta\} && \forall \beta \in \mathbb{R} \\
 \frac{\beta}{1 + \beta} &\leq m(S_\beta) \leq \min\{1, \beta\} && \text{if } \beta > -1
 \end{aligned}
 \tag{7.14}$$

and Corollary 5.10 implies that $\sigma_-(S_\beta)$ consists of one single eigenvalue whenever $\beta < 0$. The explicit spectral analysis of S_β gives $\sigma_-(S_\beta) = \emptyset$ if $\beta \geq 2$ and $\sigma_-(S_\beta) = \{1 - (\beta/2 - 1)^2\}$ if $\beta < 2$ with normalised eigenfunction $g_\beta(x) = \sqrt{2 - \beta} e^{-(1 - \beta/2)x}$, whence

$$m(S_\beta) = \begin{cases} 1 & \beta \geq 2 \\ 1 - (\beta/2 - 1)^2 & \beta < 2. \end{cases}
 \tag{7.15}$$

We thus see that the bounds (7.14) are consistent with the ‘‘exact result’’ (7.15) (and that there are extensions other than the Friedrichs one whose bottom coincide with that of S).

As for the resolvents, for $z > 0$ one sees that $e^{-zx} \in \ker(S^* + (z^2 - 1)\mathbb{1})$ and by means of the formula ([20, Chapter 6.2])

$$(S_F + (z^2 - 1)\mathbb{1})^{-1}(x, y) = \frac{1}{2z} (e^{-z|x-y|} - e^{-z(x+y)}) \quad (z > 0)
 \tag{7.16}$$

one finds

$$\begin{aligned}
 (S_\beta + (z^2 - 1)\mathbb{1})^{-1} &= \\
 &= (S_F + (z^2 - 1)\mathbb{1})^{-1} + \frac{1}{(\beta/2 - 1) + z} |e^{-zx}\rangle \langle e^{-zx}|, \quad z > 0,
 \end{aligned}
 \tag{7.17}$$

for $z > 0$ and $z \neq -(\beta/2 - 1)$ if $\beta < 2$. This is precisely a Kreĭn resolvent formula of the type (6.5). The corresponding integral kernel is

$$(S_\beta + (z^2 - 1)\mathbb{1})^{-1}(x, y) = \frac{1}{2z} \left(e^{-z|x-y|} - \frac{\beta/2 - 1 - z}{\beta/2 - 1 + z} e^{-z(x+y)} \right).
 \tag{7.18}$$

This expression can be continued analytically to complex z ’s as stated in general in Theorem 6.6, see (7.23) below.

The shift by a unit constant introduced in the definition (7.1) of S guarantees that S has positive bottom. After having determined with (7.12)-(7.13) the quadratic forms of a generic self-adjoint extension of S , one can remove the shift and deduce that the self-adjoint extensions of the operator $S' = -\frac{d^2}{dx^2}$, $\mathcal{D}(S') = C_0^\infty(0, +\infty)$, constitute the family $\{S'_\beta \mid \beta \in (-\infty, +\infty]\}$ where for each $\beta \in \mathbb{R}$ the element S'_β is the extension with quadratic form

$$\begin{aligned}
 \mathcal{D}[S'_\beta] &= H^1(0, +\infty) \\
 S'_\beta[g_1, g_2] &= \int_0^{+\infty} \overline{g'_1(x)} g'_2(x) dx + \left(\frac{\beta}{2} - 1\right) \overline{g_1(0)} g_2(0),
 \end{aligned}
 \tag{7.19}$$

and hence with

$$\begin{aligned} \mathcal{D}(S'_\beta) &= \left\{ g \in H^2(0, +\infty) \mid g'(0) = \left(\frac{\beta}{2} - 1\right)g(0) \right\} \\ S'_\beta g &= -g'', \end{aligned} \quad (7.20)$$

whereas for $\beta = \infty$ one has the Friedrichs extensions

$$\begin{aligned} \mathcal{D}[S'_F] &= H_0^1(0, +\infty), \quad S'_\beta[g_1, g_2] = \int_0^{+\infty} \overline{g'_1(x)} g'_2(x) dx, \\ \mathcal{D}(S'_F) &= H^2(0, +\infty) \cap H_0^1(0, +\infty), \quad S'_F f = -f''. \end{aligned} \quad (7.21)$$

Similarly, one deduces from (7.18)

$$(S'_\beta + z^2 \mathbb{1})^{-1}(x, y) = \frac{1}{2z} \left(e^{-z|x-y|} - \frac{\beta/2 - 1 - z}{\beta/2 - 1 + z} e^{-z(x+y)} \right) \quad (7.22)$$

for $z > 0$ and $z \neq -(\beta/2 - 1)$ if $\beta < 2$. This expression admits the analytic continuation

$$(S'_\beta - k^2 \mathbb{1})^{-1}(x, y) = \frac{i}{2k} \left(e^{ik|x-y|} - \frac{(\beta/2 - 1) + ik}{(\beta/2 - 1) - ik} e^{ik(x+y)} \right) \quad (7.23)$$

for $k \in \mathbb{C}$ with $\Im k > 0$ and $k \neq -i(\beta/2 - 1)$ if $\beta < 2$, that is, the operator-valued map $\mathbb{C} \ni k^2 \mapsto (S'_\beta - k^2 \mathbb{1})^{-1}$ is holomorphic.

7.2. “Free quantum particle” on an interval

On the Hilbert space $\mathcal{H} = L^2[0, 1]$ one considers the densely defined symmetric operator

$$S = -\frac{d^2}{dx^2}, \quad \mathcal{D}(S) = C_0^\infty(0, 1). \quad (7.24)$$

The positivity of the bottom of S can be seen by applying twice (to f, f' and to f', f'') Poincaré’s inequality

$$\int_0^1 |f'(x)|^2 dx \geq \pi^2 \int_0^1 |f(x)|^2 dx \quad \forall f \in C_0^\infty(0, 1),$$

thus obtaining

$$m(S) = \pi^2. \quad (7.25)$$

One has

$$\begin{aligned} S^* &= -\frac{d^2}{dx^2} \\ \mathcal{D}(S^*) &= H^2(0, 1) = \left\{ f \in L^2[0, 1] \mid \begin{array}{l} f, f' \in AC[0, 1] \\ f'' \in L^2[0, 1] \end{array} \right\}, \end{aligned} \quad (7.26)$$

thus all the extensions of S act as $-\frac{d^2}{dx^2}$ on suitable restrictions of $H^2(0, 1)$. In particular,

$$\mathcal{D}(\bar{S}) = H_0^2(0, 1) = \left\{ f \in H^2(0, 1) \mid \begin{array}{l} f(0) = 0 = f(1) \\ f'(0) = 0 = f'(1) \end{array} \right\} \quad (7.27)$$

and the Friedrichs extension of S has domain

$$\mathcal{D}(S_F) = H^2(0, 1) \cap H_0^1(0, 1) = \{f \in H^2(0, 1) \mid f(0) = 0 = f(1)\}, \quad (7.28)$$

that is, S_F is the negative Laplacian with Dirichlet boundary conditions. Considering its spectrum, $\sigma(S_F) = \{n^2\pi^2 \mid n \in \mathbb{N}\}$, one re-obtains (7.25) without using Poincaré’s inequality.

Applying von Neumann’s theory one finds (see, e.g., [20, Chapter 6.2]) that the self-adjoint extensions of S constitute the family $\{S_U \mid U \in U(2)\}$ where each S_U acts as $-\frac{d^2}{dx^2}$ on the domain

$$\mathcal{D}(S_U) = \left\{ g \in H^2(0, 1) \mid \begin{pmatrix} g(1) - ig'(1) \\ g(0) + ig'(0) \end{pmatrix} = U \begin{pmatrix} g(1) + ig'(1) \\ g(0) - ig'(0) \end{pmatrix} \right\}. \quad (7.29)$$

By inspection one sees that in this case the Friedrichs extension of S is the extension S_U indexed by $U = -\mathbb{1}$.

Let us apply now the KVB theory, identifying first of all $\ker S^*$ and S_F^{-1} . One has

$$\ker S^* = \text{Span}\{\mathbf{1}, x\}. \quad (7.30)$$

All self-adjoint extensions of S are therefore semi-bounded (Corollary 5.4). As for S_F^{-1} , all what we need here is its action on $\ker S^*$ (the general inversion formula for the problem $S_F\eta = h$ with datum h can be found, for instance, in [20, Chapter 6.2]), therefore we consider the problem

$$\begin{cases} -\eta''(x) = a + bx, & x \in [0, 1] \\ \eta(0) = 0 = \eta(1) \end{cases}$$

for given $a, b \in \mathbb{C}$, whose only solution is $\eta(x) = (\frac{a}{2} + \frac{b}{6})x - \frac{a}{2}x^2 - \frac{b}{6}x^3$. Thus,

$$S_F^{-1}(a + bx) = \left(\frac{a}{2} + \frac{b}{6}\right)x - \frac{a}{2}x^2 - \frac{b}{6}x^3, \quad x \in [0, 1]. \quad (7.31)$$

Owing to (7.27), (7.30), and (7.31) above, the decomposition (2.6) reads

$$H^2(0, 1) \cap H_0^1(0, 1) = H_0^2(0, 1) \dot{+} S_F^{-1}\text{Span}\{\mathbf{1}, x\}$$

i.e., any $F \in H^2(0, 1) \cap H_0^1(0, 1)$ determines uniquely $f \in H_0^2(0, 1)$ and $a, b \in \mathbb{C}$ such that $F(x) = f(x) + (\frac{a}{2} + \frac{b}{6})x - \frac{a}{2}x^2 - \frac{b}{6}x^3$. Explicitly,

$$F(x) = f(x) + F'(0)x - (2F'(0) + F'(1))x^2 + (F'(0) + F'(1))x^3.$$

Analogously, the decomposition (2.4) reads

$$H^2(0, 1) = H^2(0, 1) \cap H_0^1(0, 1) + \text{Span}\{\mathbf{1}, x\},$$

that is, any $g \in H^2(0, 1)$ can be written as

$$g(x) = F(x) + g(0) + (g(1) - g(0))x$$

for a unique $F \in H^2(0, 1) \cap H_0^1(0, 1)$.

According to Theorem 3.4, the self-adjoint extensions of S are operators of the form S_T where T is a self-adjoint operator on subspaces of $\ker S^* = \text{Span}\{\mathbf{1}, x\}$, precisely

- the zero-dimensional subspace $\{0\}$, in which case $S_T = S_F$ (Proposition 3.7)
- or the one-dimensional subspaces $\text{Span}\{\mathbf{1}\}$ or $\text{Span}\{a\mathbf{1} + x\}$, $a \in \mathbb{C}$, in which case T acts as the multiplication by a real number,

- or the whole two-dimensional space $\text{Span}\{\mathbf{1}, x\} \cong \mathbb{C}^2$, in which case T acts as the multiplication by a hermitian matrix.

For concreteness, let us work out in detail the case of the one-dimensional space $\text{Span}\{\mathbf{1}\}$ and of the self-adjoint operator T_β on it, defined by $T_\beta \mathbf{1} := \beta \mathbf{1}$ for fixed $\beta \in \mathbb{R}$. In this case $\mathcal{D}(T_\beta) = \text{Span}\{\mathbf{1}\}$ and $\ker S^* \cap \mathcal{D}(T_\beta)^\perp = \text{Span}\{2x - \mathbf{1}\}$: therefore, according to (3.2), the corresponding self-adjoint extension $S_\beta \equiv S_{T_\beta}$ of S acts as $-\frac{d^2}{dx^2}$ on the domain

$$\mathcal{D}(S_\beta) = \left\{ g = f + S_F^{-1}(\beta\gamma\mathbf{1} + \delta(2x - \mathbf{1})) + \gamma\mathbf{1} \mid \begin{array}{l} f \in H_0^2(0, 1) \\ \gamma, \delta \in \mathbb{C} \end{array} \right\}.$$

By means of (7.31) (upon renaming the coefficients γ, δ), this is re-written as

$$\mathcal{D}(S_\beta) = \left\{ g \mid \begin{array}{l} g(x) = f(x) + 2\gamma + (\beta\gamma - \delta)x - (\beta\gamma - 3\delta)x^2 - 2\delta x^3 \\ x \in [0, 1], \quad f \in H_0^2(0, 1), \quad \gamma, \delta \in \mathbb{C} \end{array} \right\} \quad (7.32)$$

which in turn, observing that $g(0) = 2\gamma = g(1)$ and $g'(0) - g'(1) = 2\beta\gamma$ for any $g \in \mathcal{D}(S_\beta)$, can be further re-written as

$$\mathcal{D}(S_\beta) = \left\{ g \in H^2(0, 1) \mid \begin{array}{l} g(0) = g(1) \\ g'(0) - g'(1) = \beta g(0) \end{array} \right\}. \quad (7.33)$$

The special case $\beta = 0$ corresponds to the self-adjoint extension with periodic boundary conditions: in the parametrisation (7.29) of von Neumann's theory, this is the extension S_U with $U = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Concerning the bottom of the extensions of the form S_β , clearly $m(T_\beta) = \beta$, thus Theorem 3.5 gives

$$\begin{aligned} m(S_\beta) &\leq \min\{\pi^2, \beta\} && \forall \beta \in \mathbb{R} \\ \frac{\beta\pi^2}{\beta + \pi^2} &\leq m(S_\beta) \leq \min\{\pi^2, \beta\} && \text{if } \beta > -\pi^2. \end{aligned} \quad (7.34)$$

This is consistent with the explicit knowledge of $\sigma(S_\beta)$: for example $\sigma(S_{\beta=0}) = \{4\pi^2 n^2 \mid n \in \mathbb{Z}\}$, whence indeed $m(S_{\beta=0}) = 0$. Moreover, since $\sigma(T_\beta) = \{\beta\}$ (simple eigenvalue), Corollary 5.10 implies that $\sigma_-(S_\beta)$ consists of one single eigenvalue whenever $\beta < 0$.

All other cases of the above list can be discussed analogously: along the same line, (3.2) and (7.31) produce each time an expression like (7.32) for $\mathcal{D}(S_T)$ that can be then cast in the form (7.33). For completeness, we give here the summary of all possible conditions of self-adjointness. The family of all self-adjoint extension of S is described by the following four families of boundary conditions:

$$g'(0) = b_1 g(0) + c g(1), \quad g'(1) = -\bar{c} g(0) - b_2 g(1), \quad (7.35)$$

$$g'(0) = b_1 g(0) + \bar{c} g'(1), \quad g(1) = c g(0), \quad (7.36)$$

$$g'(1) = -b_1 g(1), \quad g(0) = 0, \quad (7.37)$$

$$g(0) = 0 = g(1), \quad (7.38)$$

where $c \in \mathbb{C}$ and $b_1, b_2 \in \mathbb{R}$ are arbitrary parameters. For each boundary condition, the corresponding extension is the operator $-\frac{d^2}{dx^2}$ acting on the

$H^2(0, 1)$ -functions that satisfy that one boundary condition. For instance, the extension S_β determined by (7.33) correspond to the boundary condition of type (7.36) with $c = 1$ and $b_1 = \beta$. In term of the Višik-Birman extension parameter T , conditions of type (7.35) occur when $\dim \mathcal{D}(T) = 2$, conditions of type (7.36) or (7.37) occur when $\dim \mathcal{D}(T) = 1$, and condition (7.38) is precisely that occurring when $\dim \mathcal{D}(T) = 0$ (Dirichlet boundary conditions, Friedrichs extension). The well-known conditions (7.35)-(7.38) can be also found by means of boundary triplet techniques: see, e.g., [56, Example 4.10].

The same analysis can be equivalently performed in terms of the quadratic forms of the self-adjoint extensions of S , according to Theorem 3.6 (in the present case *all* extensions are semi-bounded). The reference form is the Friedrichs one, that is,

$$\begin{aligned} \mathcal{D}[S_F] &= H_0^1(0, 1) = \left\{ f \in L^2[0, 1] \mid \begin{array}{l} f \in AC[0, 1], f' \in L^2[0, 1], \\ f(0) = 0 = f(1) \end{array} \right\} \\ S_F[F_1, F_2] &= \int_0^1 \overline{F_1'(x)} F_2'(x) \, dx \quad \forall F_1, F_2 \in \mathcal{D}[S_F], \end{aligned} \tag{7.39}$$

as one deduces from (7.28). The property $m(S_F) = \pi^2$ reads

$$\int_0^1 |f'(x)|^2 dx \geq \pi^2 \int_0^1 |f(x)|^2 dx \quad \forall f \in H_0^1(0, 1), \tag{7.40}$$

that is, Poincaré’s inequality. Owing to (3.7), the form domain of each extension is obtained by taking the direct sum of $\mathcal{D}[S_T] = \mathcal{D}[S_F] \dot{+} \mathcal{D}[T]$: in the present case $\mathcal{D}[T] = \mathcal{D}(T)$, because of the finiteness of the deficiency index of S . For example, in the concrete case worked out above, that is, $T \equiv T_\beta =$ multiplication by a real β on $\mathcal{D}(T) = \text{Span}\{\mathbf{1}\}$, (3.7) and (7.39) yield

$$\begin{aligned} \mathcal{D}[S_\beta] &= H_0^1(0, 1) \dot{+} \text{Span}\{\mathbf{1}\} = \{g \in H^1(0, 1) \mid g(0) = g(1)\} \\ S_\beta[g_1, g_2] &= S_\beta[F_1 + \gamma_1 \mathbf{1}, F_2 + \gamma_2 \mathbf{1}] = \int_0^1 \overline{F_1'(x)} F_2'(x) dx + \beta \overline{\gamma_1} \gamma_2 \\ &= \int_0^1 \overline{g_1'(x)} g_2'(x) dx + \beta \overline{g_1(0)} g_2(0). \end{aligned} \tag{7.41}$$

Then, going from this (closed and semi-bounded) form to the uniquely associated self-adjoint operator, a straightforward exercise would yield the domain $\mathcal{D}(S_\beta)$ already determined by (7.33).

As for the Kreĭn-von Neumann extension S_N of S , this is the extension S_T with $T : \ker S^* \rightarrow \ker S^*$, $Tv = 0 \, \forall v \in \ker S^*$ (Proposition 3.7), in which case (3.7) and (7.39) yield the quadratic form

$$\begin{aligned} \mathcal{D}[S_N] &= H_0^1(0, 1) \dot{+} \text{Span}\{\mathbf{1}, x\} = H^1(0, 1) \\ S_N[g_1, g_2] &= S_N[F_1 + a_1 \mathbf{1} + b_1 x, F_2 + a_2 \mathbf{1} + b_2 x] \\ &= \int_0^1 \overline{F_1'(x)} F_2'(x) \, dx \\ &= \int_0^1 \overline{g_1'(x)} g_2'(x) \, dx - (\overline{g_1(1)} - \overline{g_1(0)})(g_2(1) - g_2(0)). \end{aligned} \tag{7.42}$$

The corresponding S_N is either found by determining the self-adjoint operator associated to $S_N[\cdot]$ or by applying directly (3.2) to the operator T under consideration:

$$\begin{aligned} \mathcal{D}(S_N) &= H_0^2(0, 1) \dot{+} \text{Span}\{\mathbf{1}, x\} \\ &= \{g \in H^2(0, 1) \mid g'(0) = g'(1) = g(1) - g(0)\}. \end{aligned} \tag{7.43}$$

(The latter boundary condition is of the form (7.35) with $b_1 = b_2 = -c = 1$.) S_N has not to be confused with the self-adjoint extension with Neumann boundary conditions $S_{N.bc}$, that is, the operator $S_{N.bc} = \frac{d^2}{dx^2}$ with domain

$$\mathcal{D}(S_{N.bc}) = \{g \in H^2(0, 1) \mid g'(0) = 0 = g'(1)\} \tag{7.44}$$

and quadratic form

$$\mathcal{D}[S_{N.bc}] = H^1(0, 1), \quad S_{N.bc}[g_1, g_2] = \int_0^1 \overline{g_1'(x)} g_2'(x) \, dx. \tag{7.45}$$

Although S_N and $S_{N.bc}$ have the same form domain and the same (zero) bottom, S_N is the smallest among all positive self-adjoint extensions of S (Theorem A.6(i)) – the inequality $S_N[g] \leq S_{N.bc}[g]$ (which is strict whenever $g(0) \neq g(1)$) can be also checked explicitly by comparing (7.42) with (7.45). In fact it is easy to compute explicitly (see, e.g., [3, Example 5.1])

$$\begin{aligned} \sigma(S_N) &= \{\lambda_n \mid n \in \mathbb{N}\} \quad \text{with} \quad \lambda_n = \begin{cases} (n-1)^2 \pi^2 & n \text{ odd} \\ k_{n/2}^2 & n \text{ even} \end{cases} \\ \sigma(S_{N.bc}) &= \{(n-1)^2 \pi^2 \mid n \in \mathbb{N}\}, \end{aligned}$$

where k_j is the unique solution to $\frac{1}{2}k = \tan(\frac{1}{2}k)$ in $(2\pi(j-1), 2\pi(j-\frac{1}{2}))$ (moreover, $k_j \rightarrow 2\pi(j-\frac{1}{2})$ as $j \rightarrow +\infty$), thus any even eigenvalue of S_N is strictly smaller than the corresponding eigenvalue of $S_{N.bc}$.

Appendix A. Summary of von Neumann’s vs Kreĭn’s extension theory

The material of this Appendix is completely classical and stems from the original works of von Neumann [63], Stone [60], Friedrichs [19], and Kreĭn [30]. We give here a concise summary from a more modern perspective (see, e.g., [52, 56]) that includes also the Ando-Nishio characterisation of the Kreĭn-von Neumann extension (first obtained in the work of Ando and Nishio [5] and later generalised by Coddington and de Snoo [13], and by Prokaj, Sebestyén, and Stochel [57, 51, 58]) as well as Kadison’s characterisation of the Friedrichs extension [27].

Roughly speaking, von Neumann’s theory can be regarded as the “complex version” and Kreĭn’s theory as the “real version” of the same idea, that consists of checking whether a complex number w is *real* by seeing whether $\frac{w-i}{w+i}$ is a phase (complex version), or alternatively checking whether w is *real positive* by seeing whether $\frac{w-1}{w+1}$ lies in $[-1, 1)$ (real version), based on the

fact that $w \mapsto \frac{w-i}{w+i}$ is a bijection of the real axis onto the complex unit circle without the point 1, and that $w \mapsto \frac{w-1}{w+1}$ is a bijection of the non-negative half-line onto the interval $[-1, 1)$.

A.1. von Neumann's theory

Fixed $z \in \mathbb{C} \setminus \mathbb{R}$ and a Hilbert space \mathcal{H} , the Cayley transform

$$S \mapsto V_S := (S - z\mathbb{1})(S - \bar{z}\mathbb{1})^{-1}, \quad \mathcal{D}(V_S) = \text{ran}(S - \bar{z}\mathbb{1}), \quad (\text{A.1})$$

is a bijective map of the set of densely defined symmetric operators on \mathcal{H} onto the set of all isometric (i.e., norm-preserving) operators V on \mathcal{H} for which $\text{ran}(\mathbb{1} - V)$ is dense in \mathcal{H} . One has

$$\text{ran}(\mathbb{1} - V_S) = \mathcal{D}(S). \quad (\text{A.2})$$

S is closed if and only if V_S is, and if S' is another symmetric operator on \mathcal{H} , then $S \subset S'$ if and only if $V_S \subset V_{S'}$. The inverse map is the inverse Cayley transform

$$V \mapsto S_V := (z\mathbb{1} - \bar{z}V)(\mathbb{1} - V)^{-1}. \quad (\text{A.3})$$

As a consequence, a densely defined symmetric operator S is self-adjoint if and only if its Cayley transform V_S is unitary: indeed, $S = S^*$ if and only if $\mathcal{H} = \text{ran}(S - z\mathbb{1}) = \text{ran}(S - \bar{z}\mathbb{1})$, which is equivalent to $\mathcal{H} = \text{ran}(V_S) = \mathcal{D}(V_S)$.

Thus, finding a self-adjoint extension of S , call it \tilde{S} , is equivalent to finding a unitary extension of V_S , which turns out to be $V_{\tilde{S}}$, and this is in turn equivalent to (taking the operator closure and) finding a unitary operator from $\mathcal{D}(V_S)^\perp$ to $(\text{ran}V_S)^\perp$, i.e., from $\ker(S^* - z\mathbb{1})$ to $\ker(S^* - \bar{z}\mathbb{1})$. This way the isometric V_S is extended to the unitary $V_{\tilde{S}}$ on the whole \mathcal{H} so that

$$\begin{aligned} V_S : \overline{\text{ran}(S - \bar{z}\mathbb{1})} &\xrightarrow{\cong} \overline{\text{ran}(S - z\mathbb{1})} \\ V_{\tilde{S}} \upharpoonright \ker(S^* - z\mathbb{1}) : \ker(S^* - z\mathbb{1}) &\xrightarrow{\cong} \ker(S^* - \bar{z}\mathbb{1}). \end{aligned} \quad (\text{A.4})$$

Obviously, this is possible if and only if $\dim \ker(S^* - z\mathbb{1}) = \dim \ker(S^* - \bar{z}\mathbb{1})$.

For a generic densely defined symmetric operator S each of the two dimensions above is actually constant in z throughout each of the two complex half-planes.³ This justifies the unambiguous (z -independent) terminology of “deficiency indices” of S .

When the condition of equal deficiency indices is matched, then from (A.2) and from $(\mathbb{1} - V_{\tilde{S}}) = (\mathbb{1} - V_{\tilde{S}}) \upharpoonright \mathcal{D}(V_S) + (\mathbb{1} - V_{\tilde{S}}) \upharpoonright \mathcal{D}(V_S)^\perp$ one has

$$\mathcal{D}(\tilde{S}) = \text{ran}(\mathbb{1} - V_{\tilde{S}}) = \mathcal{D}(\bar{S}) + (\mathbb{1} - V_{\tilde{S}}) \ker(S^* - z\mathbb{1}), \quad (\text{A.5})$$

and on a generic $f + u - V_{\tilde{S}}u$ in $\mathcal{D}(\tilde{S})$ ($f \in \mathcal{D}(\bar{S})$, $u \in \ker(S^* - z\mathbb{1})$) the action of \tilde{S} , in view of (A.3), gives

$$\begin{aligned} \tilde{S}(f + u - V_{\tilde{S}}u) &= \bar{S}f + (z\mathbb{1} - \bar{z}V_{\tilde{S}})(\mathbb{1} - V_{\tilde{S}})^{-1}(\mathbb{1} - V_{\tilde{S}})u \\ &= \bar{S}f + zu - \bar{z}V_{\tilde{S}}u. \end{aligned} \quad (\text{A.6})$$

³In fact, this is a result of Krasnosel'skii and Kreĭn [31].

Because of (A.4), $V_{\bar{S}}$ in the r.h.s. of (A.5) and of (A.6) has to be thought of as a unitary map $\ker(S^* - z\mathbb{1}) \xrightarrow{\cong} \ker(S^* - \bar{z}\mathbb{1})$. Thus, summarising:

Theorem A.1 (von Neumann's theorem on self-adjoint extensions). *A densely defined symmetric operator S on a Hilbert space \mathcal{H} admits self-adjoint extensions if and only if S has equal deficiency indices. In this case there is a one-to-one correspondence between the self-adjoint extensions of S and the isomorphisms between $\ker(S^* - z\mathbb{1})$ and $\ker(S^* - \bar{z}\mathbb{1})$, where $z \in \mathbb{C} \setminus \mathbb{R}$ is fixed and arbitrary. Each self-adjoint extension is of the form S_U for some $U : \ker(S^* - z\mathbb{1}) \xrightarrow{\cong} \ker(S^* - \bar{z}\mathbb{1})$, where*

$$\begin{aligned} \mathcal{D}(S_U) &= \mathcal{D}(\bar{S}) \dot{+} (\mathbb{1} - U) \ker(S^* - z\mathbb{1}) \\ S_U(f + u - Uu) &= \bar{S}u + zu - \bar{z}Uu = S^*(f + u - Uu). \end{aligned} \quad (\text{A.7})$$

For each S_U , the unitary U is the restriction to $\ker(S^* - z\mathbb{1})$ of the Cayley transform of S_U .

A.2. Friedrichs extension and Kreĭn-von Neumann extension

If a given densely defined symmetric operator S on a Hilbert space \mathcal{H} is bounded below, then it surely admits self-adjoint extensions (see, e.g., [52], Corollary to Theorem X.1). In fact, in this case S has two distinguished extensions (possibly coinciding), the Friedrichs extension and Kreĭn-von Neumann extension.

Theorem A.2 (Friedrichs extension). *Let S be a semi-bounded and densely defined symmetric operator on a Hilbert space \mathcal{H} .*

- (i) *The form $(f, g) \mapsto \langle f, Sg \rangle$ with domain $\mathcal{D}(S)$ is closable. Its closure is the form whose domain, denoted by $\mathcal{D}[S]$, is given by the completion of $\mathcal{D}(S)$ with respect to the norm $f \mapsto \langle f, Sf \rangle + (1 - m(S))\|f\|^2$, where $m(S)$ is the bottom of S , and whose value $S[f, g]$ on any two $f, g \in \mathcal{D}[S]$ is given by $S[f, g] = \lim_{n \rightarrow \infty} \langle f_n, Sg_n \rangle$, where $(f_n)_n$ and $(g_n)_n$ are two sequences in $\mathcal{D}(S)$ that converge, respectively, to f and g in the above norm.*
- (ii) *The form $(S[\cdot], \mathcal{D}[S])$ is bounded below and closed. Therefore, the operator associated with $(S[\cdot], \mathcal{D}[S])$ is self-adjoint. It is called the Friedrichs extension of S and denoted by S_F . By definition*

$$\begin{aligned} \mathcal{D}(S_F) &= \left\{ f \in \mathcal{D}[S] \left| \begin{array}{l} \exists u_f \in \mathcal{H} \text{ such that} \\ S[f, g] = \langle u_f, g \rangle \quad \forall g \in \mathcal{D}[S] \end{array} \right. \right\} \\ S_F f &:= u_f. \end{aligned} \quad (\text{A.8})$$

- (iii) *S_F is a bounded below self-adjoint extension of S with the same greatest lower bound as S , i.e.,*

$$m(S_F) = m(S), \quad (\text{A.9})$$

and whose associated quadratic form coincides with the closure if the form $(f, g) \mapsto \langle f, Sg \rangle$ considered in (i)-(ii), i.e.,

$$\mathcal{D}[S_F] = \mathcal{D}[S], \quad S_F[f, g] = S[f, g]. \quad (\text{A.10})$$

- (iv) $\mathcal{D}(S_F) = \mathcal{D}(S^*) \cap \mathcal{D}[S]$ and $S_F = S^* \upharpoonright \mathcal{D}[S]$.
- (v) S_F is the only self-adjoint extension of S whose operator domain is contained in $\mathcal{D}[S]$.
- (vi) If \tilde{S} is another bounded below self-adjoint extension of S , then $S_F \geq \tilde{S}$.
- (vii) $(S + \lambda \mathbb{1})_F = S_F + \lambda \mathbb{1}$ for $\lambda \in \mathbb{R}$.

Theorem A.3 (Friedrichs extension – Kadison’s construction [27]). *Let S be a semi-bounded, closed, and densely defined symmetric operator on a Hilbert space \mathcal{H} .*

- (i) *The inner product $(f, g) \mapsto \langle f, Sg \rangle + (1 - m(S))\langle f, g \rangle$ on $\mathcal{D}(S)$ is positive definite. The corresponding completion \mathcal{D}' is a subspace of \mathcal{H} (in fact, $\mathcal{D}' = \mathcal{D}[S]$) with $\|g\| \leq \|g\|_{\mathcal{D}'}$.*
- (ii) *For each $g \in \mathcal{H}$, the functional $f \mapsto \langle g, f \rangle$ on $\mathcal{D}(S)$ extends to a bounded linear functional on $(\mathcal{D}', \|\cdot\|_{\mathcal{D}'})$ with norm not exceeding $\|g\|$, and consequently $\exists ! g' \in \mathcal{D}(S^*) \cap \mathcal{D}'$ such that*

$$\langle g, f \rangle = \langle g', (S + \mathbb{1} - m(S)\mathbb{1})f \rangle = \langle g', f \rangle_{\mathcal{D}'} \quad \forall f \in \mathcal{D}(S).$$

The map $g \mapsto g'$ is realised by a linear operator K (i.e., $g' = Kg$) such that $K \in \mathcal{B}(\mathcal{H})$, $\|K\| \leq 1$, $K \geq \mathbb{0}$, and K is injective.

- (iii) *The operator $S_K := K^{-1} - \mathbb{1} + m(S)\mathbb{1}$ is a self-adjoint extension of S with $m(S_K) = m(S)$ and $\mathcal{D}(S_K) \subset \mathcal{D}'$. It is the unique extension of S satisfying the last two properties.*

By comparison with Theorem A.2(v) one has that S_K is precisely the Friedrichs extension of S : $S_K = S_F$.

Corollary A.4. *Under the assumptions of Theorem A.3, the Friedrichs extension S_F ($= S_K$) of S is characterised by*

$$\mathcal{D}(S_F) = \left\{ g' \in \mathcal{H} \left| \begin{array}{l} \langle g', (S + \mathbb{1} - m(S)\mathbb{1})f \rangle = \langle g', f \rangle \quad \forall f \in \mathcal{D}(S) \\ \text{for some } g \in \mathcal{H} \end{array} \right. \right\} \quad (\text{A.11})$$

$$\langle S_F g', f \rangle = \langle g', S f \rangle \quad \forall f \in \mathcal{D}(S), \quad \forall g' \in \mathcal{D}(S_F).$$

The uniqueness of the Friedrichs extension (in the sense of Theorem A.2(v) or Theorem A.3(iii)) implies the additional noticeable property that follows. It is through this property that the Friedrichs extension plays a crucial, albeit somewhat hidden, role in the Tomita-Takesaki duality theory for von Neumann algebras and positive cones [61, §15].

Proposition A.5 (The Friedrichs extension preserves the affiliation with a von Neumann algebra).

- (i) *Let S be a closed, densely defined, and positive symmetric operator on a Hilbert space \mathcal{H} and let S_F its Friedrichs extension. If U is a unitary operator on \mathcal{H} that commutes with S , in the sense that $U\mathcal{D}(S) \subset \mathcal{D}(S)$ and $USU^* = S$ on $\mathcal{D}(S)$, then U commutes with all the spectral projections of S_F .*

- (ii) *More generally, if S is a closed, densely defined, and positive symmetric operator on a Hilbert space \mathcal{H} affiliated ⁴ with a von Neumann algebra \mathfrak{M} on \mathcal{H} , then its Friedrichs extension S_F too is affiliated with \mathfrak{M} .*

The Friedrichs extension of S is a form construction, obtained canonically given the datum S . In contrast, the Kreĭn-von Neumann extension of S is relative to a chosen reference lower bound to the bottom of S . Up to a trivial shift $S \mapsto S + \lambda \mathbb{1}$ for $\lambda \geq 0$ sufficiently large, one can always assume S to be a positive and densely defined symmetric operator and the reference lower bound to be zero.

Theorem A.6 (Kreĭn-von Neumann extension). *Let S be a positive and densely defined symmetric operator on a Hilbert space \mathcal{H} .*

- (i) *Among all positive self-adjoint extensions of S there exists a unique smallest extension S_N in the sense of the operator ordering, that is, a unique extension with the property that $\tilde{S} \geq S_N$ for any positive self-adjoint extension \tilde{S} of S . It is called the Kreĭn-von Neumann extension.*
- (ii) *One has*

$$\begin{aligned} \mathcal{D}(S_N) &= \mathcal{D}(\overline{S}) + \ker S^* \\ S_N(f + u) &= \overline{S}f \quad \forall f \in \mathcal{D}(\overline{S}), \forall u \in \ker S^* \end{aligned} \quad (\text{A.12})$$

and (recall that $\mathcal{D}[S] = \mathcal{D}[S_F]$)

$$\begin{aligned} \mathcal{D}[S_N] &= \mathcal{D}[S_F] + \ker S^* \\ S_N[f + u, f' + u'] &= S_F[f, f'] \quad \forall f, f' \in \mathcal{D}[S_F], \forall u, u' \in \ker S^*. \end{aligned} \quad (\text{A.13})$$

In particular, $S_N u = 0 \quad \forall u \in \ker S^*$.

- (iii) *If, in addition, S has positive bottom ($m(S) > 0$), then the sums in (A.12) and (A.13) are direct, that is,*

$$\begin{aligned} \mathcal{D}(S_N) &= \mathcal{D}(\overline{S}) \dot{+} \ker S^* \\ \mathcal{D}[S_N] &= \mathcal{D}[S_F] \dot{+} \ker S^*, \end{aligned} \quad (\text{A.14})$$

and S_N is the only positive self-adjoint extension of S satisfying the two properties $\ker S^* \subset \mathcal{D}(S_N)$ and $S_N u = 0 \quad \forall u \in \ker S^*$.

Theorem A.7 (Kreĭn-von Neumann extension: Ando-Nishio version). *Let S be a positive and densely defined symmetric operator on a Hilbert space \mathcal{H} .*

- (i) *The linear space*

$$\mathcal{E}(S) := \left\{ g \in \mathcal{H} \left| \begin{array}{l} \exists c_g \geq 0 \text{ such that} \\ |\langle g, S f \rangle|^2 \leq c_g \langle f, S f \rangle \quad \forall f \in \mathcal{D}(S) \end{array} \right. \right\} \quad (\text{A.15})$$

contains $\mathcal{D}(S)$ as well as the domain of any positive symmetric extension of S , in particular the domain of the Friedrichs extension S_F . $\mathcal{E}(S)$ is therefore dense in \mathcal{H} .

⁴By definition a closed and densely defined operator S on a Hilbert space \mathcal{H} is affiliated with a von Neumann algebra \mathfrak{M} on \mathcal{H} when for any unitary $U \in \mathfrak{M}'$ (the commutant of \mathfrak{M}) one has $U\mathcal{D}(S) \subset \mathcal{D}(S)$ and $USU^* = S$ on $\mathcal{D}(S)$.

(ii) *The Kreĭn-von Neumann extension S_N of S satisfies*

$$\begin{aligned} \mathcal{D}[S_N] &= \mathcal{D}(S_N^{1/2}) = \mathcal{E}(S) \\ S_N[g] &= \|S_N^{1/2}g\|^2 = \nu(g) \end{aligned} \tag{A.16}$$

where $\nu(g) :=$ the smallest number c_g satisfying, for $g \in \mathcal{E}(S)$, the property $|\langle g, Sf \rangle|^2 \leq c_g \langle f, Sf \rangle \forall f \in \mathcal{D}(S)$.

Remark A.8. One has $\nu(g) = \langle g, Sg \rangle \forall g \in \mathcal{D}(S)$ and $\nu(g) = 0 \forall g \in \ker S^*$, consistently with (A.13) above.

Theorem A.7 above has a counterpart when S is positive and symmetric with no a priori assumption on the density of $\mathcal{D}(S)$ in \mathcal{H} . In this case elementary counter-examples (see, e.g., [56, Example 13.2]) show that symmetry plus semi-boundedness of S is not enough to claim the existence of the Friedrichs extension or any other positive self-adjoint extension. On the other hand, there is a class of positive symmetric operators on \mathcal{H} , with possibly neither dense nor closed domain, for which it is crucial for general theoretical purposes to have conditions that ensure the existence of positive self-adjoint extensions: this is the class of shifted Kreĭn transforms of positive and densely defined symmetric operators on \mathcal{H} , see Section A.3. Whence the relevance of the following result.

Theorem A.9 (Ando-Nishio bound and existence theorem). *Let S be a positive symmetric operator on a Hilbert space \mathcal{H} whose domain is not necessarily a dense or a closed subspace of \mathcal{H} .*

- (i) *S admits a positive self-adjoint extension on \mathcal{H} if and only if the set $\mathcal{E}(S)$ defined in (A.15) is dense in \mathcal{H} .*
- (ii) *For given $\gamma > 0$, S has a bounded positive self-adjoint extension \tilde{S} on \mathcal{H} such that $\|\tilde{S}\| \leq \gamma$ if and only if $\|Sf\|^2 \leq \gamma \langle f, Sf \rangle$ for all $f \in \mathcal{D}(S)$.*

A.3. Kreĭn’s theory

Unlike von Neumann’s theory, Kreĭn’s extension theory only deals with densely defined symmetric operators that are *semi-bounded*. In this case the *existence* of self-adjoint extension(s) is not an issue, as proved by Stone [60, Theorem 9.21] and Friedrichs [19]. In fact, in terms of the tools of von Neumann’s theory, semi-boundedness implies the coincidence of the two deficiency indices.⁵

The Kreĭn transform

$$S \mapsto K_S := (S - \mathbb{1})(S + \mathbb{1})^{-1}, \quad \mathcal{D}(K_S) := \text{ran}(S + \mathbb{1}), \tag{A.17}$$

⁵The coincidence of the two deficiency indices of a semi-bounded and densely defined symmetric operator is a classical result (see, e.g., the first corollary to Theorem X.1 in [52]) which is a direct consequence of the above-mentioned Krasnosel’skii-Kreĭn result [31] on the constance of the deficiency indices throughout each of the two complex half-planes. In fact, such an argument is more general and proves as well the coincidence of the deficiency indices of a symmetric and densely defined operator S such that \bar{S} has a real point in its resolvent set (see, e.g., the second corollary to Theorem X.1 in [52]). It is worth highlighting that the existence of a self-adjoint extension of a symmetric and densely defined S with a real point in the resolvent set of \bar{S} is an independent result, proved first by Calkin [12] and later re-proved by Kreĭn [30].

is a bijective map of the set of all positive symmetric operators on a Hilbert space \mathcal{H} onto the set of all bounded symmetric operators K on \mathcal{H} for which $\|K\| \leq 1$ and $\ker(\mathbb{1} - K) = \{0\}$, where for the operators of both sets the domain is possibly neither densely defined nor closed. In particular, if S is unbounded, then $\|K_S\| = 1$. The inverse map is the inverse Kreĭn transform

$$K \mapsto S_K := (\mathbb{1} + K)(\mathbb{1} - K)^{-1}, \quad \mathcal{D}(S_K) = \text{ran}(\mathbb{1} - K). \quad (\text{A.18})$$

In terms of the Kreĭn transform, S is self-adjoint if and only if K_S is self-adjoint. The Kreĭn transform preserves the operator inclusion:

$$S_1 \subset S_2 \Rightarrow K_{S_1} \subset K_{S_2}, \quad (\text{A.19})$$

and on self-adjoint operators it preserves the operator ordering:

$$S_1 = S_1^*, S_2 = S_2^*, \text{ and } S_1 \geq S_2 \Rightarrow K_{S_1} \geq K_{S_2}. \quad (\text{A.20})$$

Theorem A.10 (Kreĭn's theorem on self-adjoint extensions). *Let S be a densely defined and positive symmetric operator on a Hilbert space \mathcal{H} . Assume further that S is unbounded (otherwise the only self-adjoint extension of S is its operator closure \bar{S}).*

- (i) *There is a one-to-one correspondence between the positive self-adjoint extensions of S and the self-adjoint extensions \tilde{K} of the Kreĭn transform K_S that are bounded with $\|\tilde{K}\| = 1$. For each such \tilde{K} one necessarily has $\ker(\mathbb{1} - \tilde{K}) = \{0\}$, which makes the inverse Kreĭn transform of \tilde{K} well defined. Any such \tilde{K} identifies, via its inverse Kreĭn transform, a positive self-adjoint extension \tilde{S} of S (that is, $\tilde{K} = K_{\tilde{S}}$), and any positive self-adjoint extension of S is of this form.*
- (ii) *The family of the self-adjoint extensions \tilde{K} of K_S with $\|\tilde{K}\| = 1$ admits two elements, $K_{S,F}$ and $K_{S,N}$, such that a self-adjoint operator \tilde{K} belongs to this family if and only if $K_{S,N} \leq \tilde{K} \leq K_{S,F}$. The corresponding inverse Kreĭn transforms of $K_{S,F}$ and $K_{S,N}$ are two positive self-adjoint extensions of S , respectively S_F and S_N , such that a self-adjoint operator \tilde{S} is a positive self-adjoint extension of S if and only if $S_N \leq \tilde{S} \leq S_F$. S_F and S_N are nothing but the Friedrichs and the Kreĭn-von Neumann extensions of S (where the latter is defined with respect to the value zero as a reference lower bound), as given by Theorems A.2 and A.6.*
- (iii) *In the special case when S has positive bottom ($m(S) > 0$), for any semi-bounded self-adjoint extension \tilde{S} of S one has*

$$\begin{aligned} \mathcal{D}[\tilde{S}] &= \mathcal{D}[S_F] + \mathcal{D}[\tilde{S}] \cap \ker S^* \\ \tilde{S}[f + u, f' + u'] &= S_F[f, f'] + \tilde{S}[u, u'] \\ \forall f, f' \in \mathcal{D}[S_F], \forall u, u' \in \mathcal{D}[\tilde{S}] \cap \ker S^*. \end{aligned} \quad (\text{A.21})$$

In particular,

$$\tilde{S}[f, u] = 0 \quad \forall f \in \mathcal{D}[S_F], \quad \forall u \in \mathcal{D}[\tilde{S}] \cap \ker S^* \quad (\text{A.22})$$

and

$$\tilde{S} \geq 0 \quad \Leftrightarrow \quad \tilde{S}[u, u] \geq 0 \quad \forall u \in \mathcal{D}[\tilde{S}] \cap \ker S^*. \quad (\text{A.23})$$

The sum in (A.21) is direct for any positive self-adjoint extension of S :

$$\mathcal{D}[\tilde{S}] = \mathcal{D}[S_F] \dot{+} \mathcal{D}[\tilde{S}] \cap \ker S^* \quad (m(S) > 0, m(\tilde{S}) \geq 0). \quad (\text{A.24})$$

Remark A.11. In part (iii) of Theorem A.10 above one actually first establishes (A.22), which is an independent result, valid for any semi-bounded extension of a bottom-positive and densely defined symmetric operator S (see, e.g., [30, Lemma 8]). This automatically implies $\tilde{S}[f+u, f'+u'] = S_F[f, f'] + \tilde{S}[u, u']$ in (A.21). The decomposition $\mathcal{D}[\tilde{S}] = \mathcal{D}[S_F] + \mathcal{D}[\tilde{S}] \cap \ker S^*$ in (A.21) requires an additional analysis, but in the special case of *positive* self-adjoint extensions it is a straightforward consequence of $S_N \leq \tilde{S} \leq S_F$ given by part (ii) and of the property (A.13) for the domain of S_N . In the general case of *semi-bounded* extensions, the route to $\mathcal{D}[\tilde{S}] = \mathcal{D}[S_F] + \mathcal{D}[\tilde{S}] \cap \ker S^*$ (see, e.g., [30, Lemma 7 and Theorem 15]), goes through (A.13) again and the structural property

$$\mathcal{D}(S^*) = \mathcal{D}(S_F) \dot{+} \ker S^* \quad (m(S) > 0) \quad (\text{A.25})$$

for the domain of S^* . For the relevance of the technique used to establish (A.25) we have included it, together with its proof, in the main part of this article (Section 2.2, Lemma 2.1).

Remark A.12. Without the assumption $m(S) > 0$, the decomposition (A.21) for $\mathcal{D}[\tilde{S}]$ fails to be true for arbitrary semi-bounded extensions of S : the inclusion $\mathcal{D}[\tilde{S}] \supset \mathcal{D}[S_F] + \mathcal{D}[\tilde{S}] \cap \ker S^*$ remains trivially valid, but can be proper.

Remark A.13. The Kreĭn transform reduces the (difficult) problem of describing all positive self-adjoint extensions of S to the (possibly easier) problem of finding all the self-adjoint extensions of K_S with unit norm. The price, though, is that K_S is not necessarily densely defined in \mathcal{H} , which makes the search for the “minimal” extension $K_{S,N}$ and the “maximal” extension $K_{S,F}$ of K_S on \mathcal{H} different from the “ordinary” extension theory of densely defined symmetric operators. A more explicit identification of $K_{S,N}$ and $K_{S,F}$ is due to Ando and Nishio [5] (and further developments) and proceeds as follows.

- One considers the positive symmetric operators $K^\pm := \mathbb{1} \pm K_S$ with common domain $\mathcal{D}(K_S)$.
- Although $\mathcal{D}(K_S)$ is not necessarily dense (which prevents one from introducing the Friedrichs extension), from the elementary inequality $\|K^\pm x\|^2 \leq 2\langle x, K^\pm x \rangle \quad \forall x \in \mathcal{D}(K^\pm)$ one sees that they satisfy a Ando-Nishio bound as in Theorem A.9(ii).
- Therefore, both K^+ and K^- admit a bounded positive self-adjoint extension on \mathcal{H} with norm below 2, whence also (Theorem A.6(ii)) the smallest positive self-adjoint extension K_N^\pm , for which $\|K_N^\pm\| \leq 2$ too.

- One then checks that among all the self-adjoint extensions \tilde{K} of K_S on \mathcal{H} which are bounded with $\|\tilde{K}\| = 1$, the extension $K_{S,N} := -(\mathbb{1} - K_N^+)$ is the smallest and $K_{S,F} := \mathbb{1} - K_N^-$ is the largest.
- The corresponding inverse Kreĭn transforms

$$\begin{aligned} S_N &= (\mathbb{1} + K_{S,N})(\mathbb{1} - K_{S,N})^{-1} \\ S_F &= (\mathbb{1} + K_{S,F})(\mathbb{1} - K_{S,F})^{-1} \end{aligned} \tag{A.26}$$

are self-adjoint extensions of S (Theorem A.10(i)) that, because of (A.20), are, respectively, the Kreĭn-von Neumann and the Friedrichs extension of S .

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