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ONE-DIMENSIONAL GRAPH PERTURBATIONS OF SELFADJOINT RELATIONS

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Abstract. Let A be a selfadjoint operator (or a selfadjoint relation) in a Hilbert space $\mathfrak{H}$, let Z be a one-dimensional subspace of $\mathfrak{H}^2$ such that $A \cap Z = \{0,0\}$ and define $S = A \cap Z^*$. Then S is a closed, symmetric operator (or relation) with defect numbers $(1,1)$ and, conversely, each such S and a selfadjoint extension A are related in this way. This allows us to interpret the selfadjoint extensions of S in $\mathfrak{H}$ as one-dimensional graph perturbations of A. If $Z = \operatorname{span}\{\varphi, \psi\}$, then the function $Q(l) = l[\varphi,\varphi] + [(A-l)^{-1}(l\varphi - \psi), \bar{l}\varphi - \psi]$, generated by A and the pair $\{\varphi,\psi\}$, is a Q-function of $S = A \cap Z^*$ and A. It belongs to the class $\mathbf{N}$ of Nevanlinna functions and essentially determines S and A. Calculation of the corresponding resolvent operators in the perturbation formula leads to Kreĭn's description of (the resolvents of) the selfadjoint extensions of S. The class $\mathbf{N}$ of Nevanlinna functions has subclasses $\mathbf{N}_1 \supset \mathbf{N}_0 \supset \mathbf{N}_{-1} \supset \mathbf{N}_{-2}$, each defined in terms of function-theoretic properties. We characterize the Q-functions belonging to each of these classes in terms of the pair $\{\varphi,\psi\}$. If $Q(l)$ belongs to the subclass $\mathbf{N}_k$, $k = 1, 0, -1, -2$, then all but one of the selfadjoint extensions of S have a Q-function in the same class, while the exceptional extension has a Q-function in $\mathbf{N} \setminus \mathbf{N}_1$. In particular, if S is semi-bounded, the exceptional selfadjoint extension is precisely the Friedrichs extension. We consider our perturbation formula in the case where the Q-function $Q(l)$ belongs to the subclass $\mathbf{N}_k$, $k = 1, 0, -1, -2$, or if it is an exceptional function associated with this subclass. The resulting perturbation formulas are made explicit for the case that A or its orthogonal operator part is the multiplication operator in a Hilbert space $L^2(d\rho)$.

0. Introduction

Let S be a closed symmetric relation in a Hilbert space $\mathfrak{H}$, whose defect numbers are $(1,1)$. Then S has canonical selfadjoint extensions, i.e., selfadjoint extensions within the space $\mathfrak{H}$. In this paper we fix a canonical selfadjoint extension A of S. The other canonical selfadjoint extensions of S are now described as one-dimensional graph perturbations of A. Our description of the graph perturbations is in terms of a one-dimensional subspace Z of $\mathfrak{H}^2$, which connects S and A by $S = A \cap Z^*$ (here Z^* denotes the adjoint of the subspace Z in the graph sense), and which satisfies $A \cap Z = \{0,0\}$. Note that S is obtained from A by a restriction on the graph of A. Special choices of the subspace Z provide restrictions on the domain and restrictions on the range of A, respectively.

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The use of finite-dimensional subspaces to restrict a symmetric relation goes back to [C2], [CD1], [CD2], and was continued in [DSS]. In these papers the underlying idea was to broaden the classes of boundary value problems. In the present context this method seems appropriate as it provides us with coordinates to describe perturbations.

It is the purpose of this paper to give various forms of the perturbation formula depending on the behaviour of the so-called Q-function $Q(l)$ of A and $S = A \cap Z^*$, and to relate them to known results in terms of operator models. The Q-function belongs to the class $\mathbf{N}$ of Nevanlinna functions, i.e., it is holomorphic on $\mathbf{C} \setminus \mathbf{R}$, satisfies $Q(l)^* = Q(\bar{l})$ and $\operatorname{Im} Q(l)/\operatorname{Im} l \geq 0$. Conversely, for each Nevanlinna function $Q(l)$ there exist a symmetric relation (which may be taken to be completely nonselfadjoint and hence is an operator) and a canonical selfadjoint extension, which generate $Q(l)$ as the corresponding Q-function, cf. [HLS], [LT]. The Q-function $Q(l)$ is an ingredient in Kreĭn's formula, which describes the resolvent operators of the canonical selfadjoint extensions of S in terms of one-dimensional range perturbations of the resolvent operator of A. Calculation of the resolvent operators in terms of our perturbation formula gives Kreĭn's formula.

The class of Nevanlinna functions has subclasses $\mathbf{N}_1$ and $\mathbf{N}_0 \subset \mathbf{N}_1$ of functions $Q(l)$ in $\mathbf{N}$ with the property that

$$\int_1^\infty \frac{\operatorname{Im} Q(iy)}{y}\, dy < \infty,$$

and that

$$\sup_{y>0} y \operatorname{Im} Q(iy) < \infty,$$

respectively. The theory of the class $\mathbf{N}_1$ goes back to Kac, cf. [Ka]; see also [HLS] and [KK]. The class $\mathbf{N}_0$ in its turn has subclasses $\mathbf{N}_{-1}$ and $\mathbf{N}_{-2} \subset \mathbf{N}_{-1}$ of functions $Q(l)$ in $\mathbf{N}_0$ with the property that

$$\int_1^\infty \Big(\sup_{y>0} y \operatorname{Im} Q(iy) - y \operatorname{Im} Q(iy) \Big)\, dy < \infty,$$

and

$$\sup_{y>0} y^2 \Big(\sup_{y>0} y \operatorname{Im} Q(iy) - y \operatorname{Im} Q(iy) \Big) < \infty,$$

respectively, cf. [HS1].

If there is a canonical selfadjoint extension with a Q-function belonging to $\mathbf{N}_1$, $\mathbf{N}_0$, $\mathbf{N}_{-1}$, or $\mathbf{N}_{-2}$, then, with the exception of one, all the other canonical selfadjoint extensions have a Q-function belonging to $\mathbf{N}_1$, $\mathbf{N}_0$, $\mathbf{N}_{-1}$, or $\mathbf{N}_{-2}$, respectively. In each case the exceptional canonical selfadjoint extension has a Q-function which belongs to $\mathbf{N} \setminus \mathbf{N}_1$.

We will give some examples of exceptional extensions. The first example occurs when S is a densely defined, semibounded operator: then all but one of its canonical selfadjoint extensions have a Q-function in $\mathbf{N}_1$ and the exceptional selfadjoint extension is the Friedrichs extension, cf. [HLS] and [C1], [CS], [K1], [K2], [KY]. This case has also been considered from the point of view of rank one perturbations: see [GS], [KS], and [S]. Related results concerning nonnegative relations in a Kreĭn space setting were obtained in [JL1] and [JL2]. Another example occurs when S is a nondensely defined operator: then all but one of its selfadjoint extensions are operators and the exceptional selfadjoint extension is a proper relation. It coincides with the Friedrichs extension when S in addition is semibounded, see [CS]. An exposition of these facts can be found in [HLS]. In this paper a model space was constructed for a Nevanlinna function $Q(l)$ belonging to $\mathbf{N}_1$ in which all the canonical selfadjoint extensions, including the exceptional one, were exhibited. The present graph perturbation formula covers this case.

Let A be a selfadjoint relation and let $Z = \operatorname{span}\{\varphi, \psi\}$ satisfy $A \cap Z = \{0, 0\}$. Without loss of generality we assume that $S = A \cap Z^*$ is a closed symmetric operator and that A is a selfadjoint relation whose multivalued part is at most one-dimensional. We characterize when the Q-function $Q(l)$ of A and $S = A \cap Z^*$ belongs to the above subclasses of Nevanlinna functions by means of $\{\varphi, \psi\}$. The Q-function $Q(l)$ of A and $S = A \cap Z^*$ belongs to $\mathbf{N}_1$ or $\mathbf{N}_0$ if and only if A is an operator and $\varphi \in \operatorname{dom} |A|^{1/2}$ or $\varphi \in \operatorname{dom} A$, respectively. In addition, the Q-function $Q(l)$ of A and $S = A \cap Z^*$ belongs to $\mathbf{N}_{-1}$ or $\mathbf{N}_{-2}$, if and only if A is an operator, $\varphi \in \operatorname{dom} A$, and $A\varphi - \psi$ belongs to $\operatorname{dom} |A|^{1/2}$ or to $\operatorname{dom} A$, respectively.

We will present the perturbation formula according to the behaviour of the Q-function of A and $S = A \cap Z^*$, including a description of the exceptional extension.

The first case is where A is an operator. If $Q(l)$ belongs to $\mathbf{N}_1$ some refinements of our perturbation formula can be given. In particular, if $Q(l)$ belongs to $\mathbf{N}_0$ the general graph perturbation can be reduced to a one-dimensional perturbation of the range of A: $A + \tau R$, $\tau \in \mathbf{R}$, where R is the orthogonal projection onto a one-dimensional subspace. The exceptional selfadjoint extension corresponds to the parameter $\tau = \infty$; it is the only canonical selfadjoint extension which is not an operator and its domain is equal to the domain of S. See [D, Chapter 6] for the case of a selfadjoint operator in a finite-dimensional Hilbert space. The Q-function $Q(l)$ belongs to $\mathbf{N}_{-1}$ or $\mathbf{N}_{-2}$ if and only if the range of R belongs to $\operatorname{dom} |A|^{1/2}$ or $\operatorname{dom} A$, respectively. The case when $Q(l)$ belongs to $\mathbf{N}_1 \setminus \mathbf{N}_0$ is similar to the case $Q(l) \in \mathbf{N}_0$, but not so explicit. In this case a description in terms of space triplets (see the last section of this paper) is more suitable. Further details are given in [HKS], [HS2].

The second case is when A is a selfadjoint relation whose multivalued part is one-dimensional. Then the Q-function $Q(l)$ is an exceptional function corresponding to the class $\mathbf{N}_0$. We can obtain an appropriate version of the perturbation result. Refinements in this case can be given depending on whether $Q(l)$ is an exceptional function corresponding to $\mathbf{N}_{-1}$ or $\mathbf{N}_{-2}$, see also [HS1].

The results described above are specialized for the selfadjoint operator of multiplication by the independent variable in a Hilbert space $L^2(d\rho)$ with ρ a nondecreasing function on $\mathbf{R}$, to which is possibly orthogonally added a one-dimensional multivalued part. We will give a description of all canonical selfadjoint extensions; in the case where the Q-function belongs to $\mathbf{N}_1$ or to $\mathbf{N}_0$ the description reduces by means of an explicit isometric isomorphism to the results in [HLS].

In Section 1 of this paper we will present some preliminary results concerning Q-functions associated with symmetric and selfadjoint relations. In Section 2 we then give the general perturbation formula and in Section 3 show the connection with Kreĭn's formula. We will reformulate some facts concerning Q-functions of A and $S = A \cap Z^*$ in terms of Z in Section 4. In Sections 5 and 6 we study the perturbation formula in the cases, where A is an operator or that A has a one-dimensional multivalued part and S is an operator, respectively. Finally, Section 7 contains further refinements of the perturbation formula when A or its operator part is a multiplication operator in some $L^2(d\rho)$-space, where ρ is a nondecreasing function on $\mathbf{R}$.

1. Preliminaries

In this section we will give a short introduction and present some notation and terminology, concerning relations in Hilbert spaces and Q-functions.

Consider a Hilbert space $\mathfrak{H}$ with inner product $[\cdot,\cdot]$. A linear relation S in $\mathfrak{H}$ is just a linear subspace of the orthogonal sum $\mathfrak{H} \oplus \mathfrak{H}$ of $\mathfrak{H}$ with itself. For instance, a linear operator is a linear relation when we identify the operator and its graph. The relation is said to be closed if it is closed as a subspace of $\mathfrak{H} \oplus \mathfrak{H}$. The null space $\ker S$ is given by $\ker S = \{f \in \mathfrak{H} : \{f,0\} \in S\}$ and the multivalued part $\operatorname{mul} S$ is given by $\operatorname{mul} S = \{g \in \mathfrak{H} : \{0,g\} \in S\}$. A linear relation S is (the graph of) an operator if and only if $\operatorname{mul} S = \{0\}$. Its domain and range are given by $\operatorname{dom} S = \{f : \{f,g\} \in S\}$ and $\operatorname{ran} S = \{g : \{f,g\} \in S\}$, respectively. By S^{-1} we mean the linear relation $S^{-1} = \{\{g,f\} : \{f,g\} \in S\}$. Note that $\operatorname{dom} S^{-1} = \operatorname{ran} S$. Clearly, $\ker S^{-1} = \operatorname{mul} S$. We define the linear relation S_∞ by $S_\infty = \{0\} \oplus \operatorname{mul} S$. When S is closed, the operator part S_s of S is defined by

$$S_s = \{\{f,g\} \in S : g \perp \operatorname{mul} S\}.$$

In this sense a relation $S = S_s \oplus S_\infty$ is a multivalued linear operator.

For each $l \in \mathbf{C}$ we define the linear relation $S - l = \{\{f, g - lf\} : \{f,g\} \in S\}$. Clearly, $\ker (S-l)^{-1} = \operatorname{mul} S$. When S is closed, the resolvent set $\rho(S)$ is the set of all $l \in \mathbf{C}$ for which $(S-l)^{-1} = \{\{g - lf, f\} : \{f,g\} \in S\}$ is (the graph of) a bounded linear operator defined on all of $\mathfrak{H}$. The resolvent set $\rho(S)$ is open and the resolvent operator $(S-l)^{-1}$, $l \in \rho(S)$, satisfies

$$(S-l)^{-1}-(S-\lambda)^{-1}=(l-\lambda)(S-l)^{-1}(S-\lambda)^{-1}, \qquad l,\lambda \in \rho(S),$$

which is the usual resolvent identity.

For any subset S in $\mathfrak{H}^2$ we define the adjoint S^* by

$$S^*=\big\{\{h,k\}\in \mathfrak{H}^2 : \langle\{h,k\},\{f,g\}\rangle=0, \text{ for all } \{f,g\}\in S\big\},$$

where the form $\langle\{f,g\},\{h,k\}\rangle$ is defined by $[g,h]-[f,k]$. Then S^* is automatically a closed linear relation and $(S^*)^*$ is the closure of the linear subspace spanned by S. A linear relation S is called symmetric if $S\subset S^*$ and selfadjoint if $S=S^*$. For a closed symmetric relation S we have von Neumann's formula, which expresses S^* as a direct sum:

$$S^*=S\dot{+}M_{\bar\mu}(S^*)\dot{+}M_\mu(S^*), \qquad \mu\in\mathbf{C}\setminus\mathbf{R}, \tag{1.1}$$

where $M_\lambda(S^*)=\big\{\{f,g\}\in S^* : g=\lambda f\big\}$, $\lambda\in\mathbf{C}$; note that $\ker(S^*-\lambda)=\operatorname{dom} M_\lambda(S^*)$. The symbol $\dot{+}$ denotes the componentwise sum in $\mathfrak{H}\oplus\mathfrak{H}$. The defect numbers (m,n) of S are the dimensions of the defect subspaces $\ker(S^*-\bar\mu)$ and of $\ker(S^*-\mu)$, respectively, if $\mu\in\mathbf{C}^+$. In general, the symmetric relation S has selfadjoint extensions if we extend the original Hilbert space. The operator S has canonical selfadjoint extensions, i.e., selfadjoint extensions in the original Hilbert space if and only if the defect numbers of S are equal. Finally we observe that

$$\ker(S^*-l)\cap\operatorname{dom} S=\{0\}, \qquad l\in\mathbf{C}\setminus\mathbf{R}. \tag{1.2}$$

To see this, let $\{\chi(l),l\chi(l)\}\in S^*$ be nontrivial and assume that $\chi(l)\in\operatorname{dom} S$. Then there exists an element k such that $\{\chi(l),k\}\in S$, so that

$$[k,\chi(l)]-\bar l[\chi(l),\chi(l)]=\langle\{\chi(l),k\},\{\chi(l),l\chi(l)\}\rangle=0,$$

which contradicts the fact that $[k,\chi(l)]$ is real.

For any closed symmetric linear relation S the relation S_∞ is selfadjoint in $\operatorname{mul} S$ and S_s is a closed symmetric operator in $\mathfrak{H}\ominus\operatorname{mul} S$ with the same defect numbers as S. A symmetric relation is called completely nonselfadjoint if it is not the nontrivial orthogonal sum of a symmetric and a selfadjoint relation. By the above reasoning a completely nonselfadjoint symmetric relation is automatically an operator. A closed symmetric relation S is completely nonselfadjoint if and only if

$$\mathfrak{H}=\overline{\operatorname{span}}\,\{\ker(S^*-l) : l\in\mathbf{C}\setminus\mathbf{R}\}.$$

This characterization goes back to M.G. Kreĭn, cf. [LT, Proposition 1.1].

Let S be a closed symmetric relation in a Hilbert space $\mathfrak{H}$ with defect numbers $(1,1)$, and let A be a canonical selfadjoint extension of S. For some $\mu \in \mathbf{C}\setminus\mathbf{R}$ we choose a nontrivial element $\chi(\mu) \in \ker(S^*-\mu)$ and we define the vector function $\chi(l)$, $l \in \mathbf{C}\setminus\mathbf{R}$, by

$$\chi(l) = \big(I + (l-\mu)(A-l)^{-1}\big)\chi(\mu). \tag{1.3}$$

Then $\ker(S^*-l)$ is spanned by $\chi(l)$ and furthermore

$$S = \big\{\{f,g\} \in A : [g - lf, \chi(\bar{l})] = 0\big\}, \tag{1.4}$$

as it is easily verified that the righthand side of (1.4) defines a closed symmetric extension of S with defect numbers $(1,1)$. A function $Q(l)$ is a Q-function of A and S if it is a solution of:

$$\frac{Q(l)-Q(\lambda)^*}{l-\bar{\lambda}} = [\chi(l),\chi(\lambda)], \qquad l,\lambda \in \mathbf{C}\setminus\mathbf{R}. \tag{1.5}$$

Up to a real constant the function $Q(l)$ is uniquely defined and

$$Q(l) = Q(\mu)^* + (l-\bar{\mu})\big[\big(I+(l-\mu)(A-l)^{-1}\big)\chi(\mu),\chi(\mu)\big]. \tag{1.6}$$

It is clear from the definition of the Q-function of S and A that we may always take out selfadjoint parts of S. In particular, we may assume that S is completely nonselfadjoint, see also [LT]. Conversely, a Q-function essentially determines a pair (S,A) in a model space, where S is completely nonselfadjoint. These model spaces can be constructed in various ways, see [LT] and, for instance, [HLS].

We denote the orthogonal projection onto $\mathfrak{H} \ominus \operatorname{mul} A$ by P and the spectral family of the operator part A_s of A (in $\mathfrak{H} \ominus \operatorname{mul} A$) by $E(t)$. We recall [HLS, Proposition 2.1]:

Proposition 1.1. *Let S be a closed symmetric relation with defect numbers $(1,1)$ and let A be a selfadjoint extension of S. Let $Q(l)$ be the Q-function of S and A with the representation* (1.6)*. Then $Q(l)$ admits an integral representation*

$$Q(l) = \alpha + \beta l + \int_{\mathbf{R}} \Big(\frac{1}{t-l} - \frac{t}{t^2+1}\Big)\, d\sigma(t), \tag{1.7}$$

where

(i) $\alpha = Q(i)^* + i[\chi(i),\chi(i)] = \operatorname{Re} Q(i)$,
(ii) $\beta = [(I-P)\chi(i),(I-P)\chi(i)]$ $(= \lim_{y\to\infty} \operatorname{Im} Q(iy)/y)$,
(iii) $d\sigma(t)/(t^2+1) = d\big([E(t)P\chi(i),P\chi(i)]\big)$,

and where the function $\sigma(t)$ is nondecreasing on $\mathbf{R}$ and satisfies

$$\int_{\mathbf{R}} \frac{d\sigma(t)}{t^2+1} < \infty. \tag{1.8}$$

The singular part S_∞ is selfadjoint and we may reduce S to the Hilbert space $\mathfrak{H} \ominus \operatorname{mul} S$. In that case the multivalued part of any selfadjoint extension of S is at most one-dimensional as stated in the following proposition.

Proposition 1.2. *Let S be a closed symmetric relation with defect numbers $(1,1)$ and let A be a selfadjoint extension of S. Then the multivalued part* mul S *of S is given by*

$$\text{mul } S = \{g \in \text{mul } A : [g, (I-P)\chi(\bar{\mu})] = 0\}. \tag{1.9}$$

Hence

$$\dim(\text{mul } A \ominus \text{mul } S) \leq 1. \tag{1.10}$$

In particular, if S is an operator then

$$\text{mul } A = \text{span}\,\{(I-P)\chi(\bar{\mu})\},$$

and mul A *is at most one-dimensional.*

Proof. The inclusion mul $S \subset$ mul A and the identity

$$\text{mul } S = \{g \in \text{mul } A : [g, \chi(\bar{\mu})] = 0\}$$

follow immediately from (1.4). For $g \in$ mul A we may write

$$[g, \chi(\bar{\mu})] = [(I-P)g, \chi(\bar{\mu})] = [g, (I-P)\chi(\bar{\mu})],$$

so that (1.9) follows. Clearly, $(I-P)\chi(\bar{\mu}) \in$ mul A and (1.10) follows. Now assume that S is an operator. If A is an operator then the identity mul $A =$ span $\{(I-P)\chi(\bar{\mu})\}$ is trivially true. Next suppose that A is not an operator. As S is an operator it follows from (1.9) that $(I-P)\chi(\bar{\mu}) \neq 0$ and that mul A is one-dimensional. This completes the proof.

The following result is a slight extension of [HLS, Proposition 2.2] where it was assumed that S is completely nonselfadjoint. Moreover, we include some information about the classes $\mathbf{N}_{-1}$ and $\mathbf{N}_{-2}$.

Proposition 1.3. *Let $Q(l)$ be a Q-function belonging to S and A. Then*

(i) $\lim_{y\to\infty} \text{Im}\, Q(iy)/y = 0$ *if and only if* $\chi(l) \in \overline{\text{dom}\, A}$ *for some (and, hence, for all) $l \in \mathbf{C} \setminus \mathbf{R}$.*

Assume that S is a closed operator. Then

(ii) $\lim_{y\to\infty} \text{Im}\, Q(iy)/y = 0$ *if and only if A is an operator.*

(iii) $Q(l) \in \mathbf{N}_1$ *if and only if A is an operator and* $\chi(l) \in \text{dom}\, |A|^{1/2}$ *for some (and, hence, for all) $l \in \mathbf{C} \setminus \mathbf{R}$.*

(iv) $Q(l) \in \mathbf{N}_0$ *if and only if A is an operator and* $\chi(l) \in \text{dom}\, A$ *for some (and, hence, for all) $l \in \mathbf{C} \setminus \mathbf{R}$.*

(v) $Q(l) \in \mathbf{N}_{-1}$ *if and only if A is an operator and* $\chi(l) \in \text{dom}\, |A|^{3/2}$ *for some (and, hence, for all) $l \in \mathbf{C} \setminus \mathbf{R}$.*

(vi) $Q(l) \in \mathbf{N}_{-2}$ *if and only if A is an operator and* $\chi(l) \in \text{dom}\, A^2$ *for some (and, hence, for all) $l \in \mathbf{C} \setminus \mathbf{R}$.*

As for the statements (i)–(iv), it suffices to discuss (ii). First assume that A is an operator. Then $P = I$ and hence $\beta = 0$ in (1.7). Conversely, assume that $\beta = 0$. According to (i) $\chi(l) \in \overline{\text{dom}\, A}$. From (1.1) it then follows that dom $S^* \subset (\text{mul } A)^\perp$. However, by assumption, $(\text{dom } S^*)^\perp = \text{mul } S^{**} = \text{mul } S = \{0\}$, which implies that S^* is densely defined. Therefore, it follows that mul $A = \{0\}$, and A is an operator. The items (v) and (vi) follow from Proposition 1.1, in the same way as (iii) and (iv), cf. [HLS, Proposition 2.1] and [HS1, Proposition 1.2].

The next result is similar to (iv) and (vi) of Proposition 1.3, but stated in terms of the symmetric operator S. For this purpose, suppose that $Q(l)$ belongs to $\mathbf{N}_0$. Let A be the corresponding selfadjoint operator extension of S. Then $\chi(l) \in \text{dom } A$ and it follows from von Neumann's formula (1.1) that dom $S^* \subset$ dom A, so that

$$\text{dom } S^* = \text{dom } A.$$

Proposition 1.4. *Assume that S is a closed operator.*

(i) *There is a Q-function $Q(l) \in \mathbf{N}_0$ of S if and only if S is not densely defined.*

(ii) *There is a Q-function $Q(l) \in \mathbf{N}_{-2}$ of S if and only if S is not densely defined and* mul $S^* \subset$ dom S^*, *or equivalently, if and only if* dom $S^* =$ dom $S +$ mul S^*.

Proof. We first prove (i). Assume that there is a Q-function $Q(l) \in \mathbf{N}_0$. Then the previous proposition shows that the corresponding selfadjoint extension A is an operator and that $\chi(l) \in \text{dom } A$. Hence it follows from (1.4) that

$$\text{dom } S = \{ f \in \text{dom } A : [f, (A-\mu)\chi(\mu)] = 0 \}, \qquad \mu \in \mathbf{C} \setminus \mathbf{R}, \tag{1.11}$$

which implies that S is not densely defined. Conversely, assume that S is not densely defined, in which case there is a nontrivial $\gamma \in \text{mul } S^*$. We choose a selfadjoint operator extension A of S. Then it follows from the definition that $(A-l)^{-1}\gamma \in \ker(S^*-l)$, so that the defect subspaces of S are contained in dom A. Hence the Q-function $Q(l)$ of A belongs to $\mathbf{N}_0$, by the previous proposition.

Next we prove (ii). Assume that there is a Q-function $Q(l) \in \mathbf{N}_{-2}$. In particular $Q(l)$ belongs to $\mathbf{N}_0$, so that the corresponding selfadjoint extension A is an operator and (1.11) holds, which implies that $(A-\mu)\chi(\mu) \in \text{mul } S^*$. Moreover, the previous proposition shows that $\chi(l) \in \text{dom } A^2$. Therefore $(A-\mu)\chi(\mu) \in \text{dom } A$ and, by dimension arguments, we conclude that mul $S^* = \text{span}\{(A-\mu)\chi(\mu)\} \subset$ dom A and that dom $A =$ dom $S +$ mul S^*, which is the same as dom $S^* =$ dom $S +$ mul S^*. Conversely, assume that dom $S^* =$ dom $S +$ mul S^*. Then S is nondensely defined, since otherwise dom $S^* =$ dom S, which is impossible, see (1.1) and (1.2). By (i) there is a selfadjoint operator extension A of S whose Q-function $Q(l)$ belongs to $\mathbf{N}_0$, and hence $\chi(\mu) \in \text{dom } A$. Again, it follows from (1.11) that mul $S^* = \text{span}\{(A-\mu)\chi(\mu)\}$, and consequently

$$(A-\mu)\chi(\mu) \in \text{dom } S^* = \text{dom } A,$$

which implies $\chi(\mu) \in \operatorname{dom} A^2$. Therefore $Q(l) \in \mathbf{N}_{-2}$.

The equivalence of the last two statements in (ii) is obvious by the above reasoning. This completes the proof.

A corresponding statement about the classes $\mathbf{N}_1$ or $\mathbf{N}_{-1}$ would involve the theory of triplets of Hilbert spaces, see [HKS] and Section 7 of the present paper.

2. One-dimensional perturbations

In this section we consider a closed symmetric relation with defect numbers $(1,1)$. Its canonical selfadjoint extensions are interpreted as perturbations of the graph of one fixed canonical selfadjoint extension.

We associate with a selfadjoint relation A and a one-dimensional subspace Z of $\mathfrak{H}^2$ the relation $S = A \cap Z^*$. Clearly, S is a closed symmetric relation and if $Z = \operatorname{span}\{\varphi, \psi\}$, then

$$S = \big\{\{f,g\} \in A : \langle \{f,g\}, \{\varphi,\psi\} \rangle = 0\big\}. \tag{2.1}$$

Moreover, the adjoint S^* is given by the componentwise sum in $\mathfrak{H}^2$:

$$S^* = A \dot{+} Z. \tag{2.2}$$

To prove this identity we note that

$$S^* = (A \cap Z^*)^* = \overline{\operatorname{span}}\,(A \dot{+} \overline{\operatorname{span}}\, Z) = \overline{\operatorname{span}}\,(A \dot{+} Z) = A \dot{+} Z,$$

where the second equality holds since A is selfadjoint, and hence closed, and the last two equalities hold since Z is one-dimensional and hence closed.

Lemma 2.1. *The closed symmetric relation $S = A \cap Z^*$ is selfadjoint and equal to A if and only if $Z \subset A$.*

Proof. Suppose that S is selfadjoint, then $S = A = S^*$ and it follows from (2.2) that $Z \subset A$. Conversely, let $Z \subset A$. Then (2.2) shows that $S^* = A$, and hence $S = A$. This completes the proof.

Since Z is one-dimensional, it is clear that Z is not contained in A if and only if the componentwise sum $A \dot{+} Z$ is direct, i.e.,

$$A \cap Z = \{0, 0\}. \tag{2.3}$$

Unless otherwise stated, this condition will be assumed in the rest of this paper. A more general version of the first part of the following lemma can be found in [DSS, Lemma 5.1].

Lemma 2.2. *Let the selfadjoint relation A and the one-dimensional subspace Z satisfy* (2.3)*. Then $S = A \cap Z^*$ is a closed symmetric relation with defect numbers* $(1,1)$*. Conversely, if S is a closed symmetric relation with defect numbers* $(1,1)$ *and A is a canonical selfadjoint extension of S, then there exists a one-dimensional subspace Z, which satisfies* (2.3)*, such that $S = A \cap Z^*$.*

Proof. Let $Z = \operatorname{span}\{\varphi, \psi\}$. Choose $l \in \mathbf{C} \setminus \mathbf{R}$, then since A is selfadjoint, there is an element $\{\tilde{\varphi}, \tilde{\psi}\} \in A$ for which $\tilde{\psi} - l\tilde{\varphi} = \psi - l\varphi$. Define $\tilde{\chi} = \tilde{\varphi} - \varphi$. Then $\{\tilde{\chi}, l\tilde{\chi}\} = \{\tilde{\varphi}, \tilde{\psi}\} - \{\varphi, \psi\} \in S^*$ by (2.2). Moreover, $\tilde{\chi} \neq 0$ by (2.3). This shows that $\ker(S^* - l) \geq 1$. Now let $\{\chi, l\chi\} \in S^*$. Then $\{\chi, l\chi\} = \{f, g\} - c\{\varphi, \psi\}$ for some $\{f, g\} \in A$ and $c \in \mathbf{C}$ by (2.2). Hence, $\{\chi, l\chi\} - c\{\tilde{\chi}, l\tilde{\chi}\} = \{f, g\} - c\{\tilde{\varphi}, \tilde{\psi}\} \in A$, and since A has no eigenvalue at $l \in \mathbf{C} \setminus \mathbf{R}$, this shows that $\chi = c\tilde{\chi}$. We conclude that $\dim\ker(S^* - l) = 1$, $l \in \mathbf{C} \setminus \mathbf{R}$, i.e., the symmetric relation has defect numbers $(1,1)$.

Next we prove the converse. We have that $S \subset A \subset S^*$ and $\dim S^*/S = 2$. Therefore, since A is selfadjoint, we have that $\dim S^*/A = 1$. Hence, we can choose a one-dimensional subspace $Z \subset S^*$ such that $S^* = A \dot{+} Z$ and $A \cap Z = \{0, 0\}$. Then clearly $S = A \cap Z^*$. This completes the proof.

Let A be a selfadjoint relation in a Hilbert space $\mathfrak{H}$. We call two pairs $\{\varphi, \psi\}$ and $\{\tilde{\varphi}, \tilde{\psi}\}$ equivalent (with respect to A) if $\{\varphi - \tilde{\varphi}, \psi - \tilde{\psi}\} \in A$. Two subspaces Z and $\tilde{Z}$ are called equivalent if they are spanned by equivalent pairs. If Z and $\tilde{Z}$ are equivalent and if Z satisfies (2.3), then also $\tilde{Z}$ satisfies (2.3). In particular, if $Z = \operatorname{span}\{\varphi, \psi\}$ and $\tilde{Z} = \operatorname{span}\{\varphi, P\psi\}$, where P is the orthogonal projection onto $\mathfrak{H} \ominus \operatorname{mul} A$, then the subspaces Z and $\tilde{Z}$ are equivalent, as $\{\varphi, \psi\} - \{\varphi, P\psi\} = \{0, (I - P)\psi\} \in A$. Observe that in the definition of $S = A \cap Z^*$ we can always replace Z by an equivalent subspace $\tilde{Z}$.

Lemma 2.3. *Let the selfadjoint relation A and the one-dimensional subspace Z satisfy* (2.3)*. Then there is a one-dimensional symmetric subspace $\tilde{Z}$ which is equivalent to Z.*

Proof. Let $Z = \operatorname{span}\{\varphi, \psi\}$. Since $A \cap Z = \{0, 0\}$, there is an element $\{h, k\} \in A$ for which $\langle\{h, k\}, \{\varphi, \psi\}\rangle = 1$. Then

$$\{\tilde{\varphi}, \tilde{\psi}\} = \{\varphi, \psi\} - \tfrac{1}{2}\langle\{\varphi, \psi\}, \{\varphi, \psi\}\rangle\{h, k\},$$

spans a one-dimensional symmetric subspace which is equivalent to Z. This completes the proof.

The following theorem gives a description of all canonical selfadjoint extensions of $S = A \cap Z^*$ as perturbations (of the graph) of A, a fixed canonical selfadjoint extension of S. Clearly, Z is symmetric if and only if $S \dot{+} Z$ is a selfadjoint extension of S. Note that only in the case that the subspace Z is symmetric, there is a value $\tau \in \mathbf{R} \cup \{\infty\}$ for which $1/\tau + [\psi, \varphi] = 0$.

Theorem 2.4. *Let A be a selfadjoint relation and let Z be a one-dimensional subspace for which* (2.3) *holds. The canonical selfadjoint extensions of $S = A \cap Z^*$ are in one-to-one correspondence with $\tau \in \mathbf{R} \cup \{\infty\}$. These canonical selfadjoint extensions $A(\tau)$ are given by $A(0) = A$ and for $\tau \neq 0$ and $1/\tau + [\psi, \varphi] \neq 0$ by*

$$A(\tau) = \left\{ \{f, g\} - \frac{\langle \{f, g\}, \{\varphi, \psi\} \rangle}{1/\tau + [\psi, \varphi]} \{\varphi, \psi\} : \{f, g\} \in A \right\}, \tag{2.4}$$

while for $1/\tau + [\psi, \varphi] = 0$ the canonical selfadjoint extension $A(\tau)$ is given by

$$A(\tau) = S \dot{+} Z. \tag{2.5}$$

Proof. By definition the relation A is selfadjoint. The relation $A(\tau)$ in (2.4) when $\tau \neq 0$, $1/\tau + [\psi, \varphi] \neq 0$, and the relation $A(\tau)$ in (2.5) when $1/\tau + [\psi, \varphi] = 0$, are clearly true symmetric extensions of S and therefore they are selfadjoint. Observe that in this last case Z is symmetric.

Now we will show that each selfadjoint extension of S has the indicated form. Let H be a canonical selfadjoint extension of S. The case $H = A$ corresponds to $\tau = 0$.

Next assume that $H \neq A$. Assume that $\{h, k\}$ is a fixed element in H, and write $\{h, k\} = \{f, g\} + c\{\varphi, \psi\}$, according to the decomposition (2.2) with $\{f, g\} \in A$ and $c \in \mathbf{C}$. Assume that $\{h, k\}$ does not belong to S. This implies that $c \neq 0$, as otherwise $\{h, k\}$ would belong to H and A at the same time, which is impossible in the present case $H \neq A$. Since H is selfadjoint, it follows that $\langle \{h, k\}, \{h, k\} \rangle = 0$, which leads to

$$\begin{aligned} 0 &= \langle \{f, g\} + \{\varphi, \psi\}c, \{f, g\} + \{\varphi, \psi\}c \rangle \\ &= \langle \{f, g\}, \{f, g\} \rangle + \langle \{f, g\}, \{\varphi, \psi\} \rangle \bar{c} \\ &\quad + \langle \{\varphi, \psi\}, \{f, g\} \rangle c + \langle \{\varphi, \psi\}, \{\varphi, \psi\} \rangle |c|^2. \end{aligned} \tag{2.6}$$

Clearly, $\langle \{f, g\}, \{f, g\} \rangle = 0$ since $\{f, g\} \in A$. Since $c \neq 0$, we rewrite (2.6) as

$$\frac{1}{c} \langle \{f, g\}, \{\varphi, \psi\} \rangle + \frac{1}{\bar{c}} \langle \{\varphi, \psi\}, \{f, g\} \rangle + \langle \{\varphi, \psi\}, \{\varphi, \psi\} \rangle = 0, \tag{2.7}$$

or equivalently

$$\frac{1}{c} \langle \{f, g\}, \{\varphi, \psi\} \rangle + [\psi, \varphi] = -\frac{1}{\bar{c}} \langle \{\varphi, \psi\}, \{f, g\} \rangle + [\varphi, \psi]. \tag{2.8}$$

As the righthand side of (2.8) is the complex conjugate of the lefthand side, we conclude that the lefthand side must be real, say $-1/\tau$ for some $\tau \in \mathbf{R} \cup \{\infty\}$, $\tau \neq 0$:

$$\frac{1}{c} \langle \{f, g\}, \{\varphi, \psi\} \rangle = -(1/\tau + [\psi, \varphi]). \tag{2.9}$$

First assume that $\langle \{f,g\},\{\varphi,\psi\}\rangle = 0$. According to (2.9) this assumption is equivalent to $1/\tau + [\psi,\varphi] = 0$. It follows from (2.7) that Z is symmetric. Our assumption means that $\{f,g\} \in S$ and thus, $\{h,k\} \in S\dot{+}Z$. Hence, as the element $\{h,k\}$ belongs at the same time to the canonical selfadjoint extensions H and $S\dot{+}Z$ and as it does not belong to S, we conclude that $H = S\dot{+}Z$. Therefore the selfadjoint extension H is equal to $A(\tau)$ for $1/\tau + [\psi,\varphi] = 0$, where $A(\tau)$ is of the form (2.5).

Now assume that $\langle \{f,g\},\{\varphi,\psi\}\rangle \neq 0$. Solve the equation (2.9) for c:

$$c = -\frac{\langle \{f,g\},\{\varphi,\psi\}\rangle}{1/\tau + [\psi,\varphi]}.$$

We observe that

$$\{h,k\} = \{f,g\} + c\{\varphi,\psi\} = \{f,g\} - \frac{\langle \{f,g\},\{\varphi,\psi\}\rangle}{1/\tau + [\psi,\varphi]}\{\varphi,\psi\}.$$

Hence, as the element $\{h,k\}$ belongs at the same time to the canonical selfadjoint extensions H and $A(\tau)$ and does not belong to S, we conclude that $H = A(\tau)$, where $A(\tau)$ is of the form (2.4).

Thus we have shown that any canonical selfadjoint extension of S, different from A, is of the form (2.4) or (2.5) for some $\tau \in \mathbf{R}\cup\{\infty\}$, $\tau \neq 0$. This completes the proof.

3. Q-functions and Kreĭn's formula

In this section we express the Q-function of $S = A\cap Z^*$ and A, Z being a one-dimensional subspace satisfying (2.3), in terms of $Z = \operatorname{span}\{\varphi,\psi\}$. We calculate the resolvent operators in Theorem 2.4 in terms of the resolvent operator for A. In this way we obtain a new proof of Kreĭn's description of all canonical selfadjoint extensions of a closed symmetric relation with defect numbers $(1,1)$, cf. [HLS].

In terms of $\{\varphi,\psi\}$ we introduce the vector function $\chi(l)$, $l \in \mathbf{C}\setminus\mathbf{R}$, by

$$\chi(l) = (A-l)^{-1}(l\varphi - \psi) + \varphi. \tag{3.1}$$

Using the resolvent identity, it can easily be checked that $\chi(l)$ satisfies (1.3). Moreover, $S = A \cap Z^*$ can also be written in the form (1.4), since

$$\langle \{f,g\},\{\varphi,\psi\}\rangle = [g - lf, \chi(\bar{l})] = \langle \{f,g\},\{\chi(\bar{l}), \bar{l}\chi(\bar{l})\}\rangle. \tag{3.2}$$

In particular, $\ker(S^* - l)$ is spanned by $\chi(l)$. We define the function $Q(l)$ by

$$Q(l) = [\chi(l), \bar{l}\varphi - \psi] + [\varphi,\psi], \tag{3.3}$$

or equivalently

$$Q(l) = l[\varphi, \varphi] + [(A-l)^{-1}(l\varphi - \psi), \bar{l}\varphi - \psi]. \tag{3.4}$$

Note that if the condition (2.3) is not satisfied, so that $\{\varphi, \psi\} \in A$, then (3.1) shows that $\chi(l) = 0$. Moreover (3.3) shows that $Q(l) = [\varphi, \psi]$, a real constant, since $\{\varphi, \psi\} \in A$.

Suppose we replace $\{\varphi, \psi\}$ in (3.1) by the equivalent pair of the form $\{\tilde{\varphi}, \tilde{\psi}\} = \{\varphi, \psi\} + \{h, k\}$, with $\{h, k\} \in A$. Since $(A-l)^{-1}(k - lh) = h$, the function $\chi(l)$ remains the same. Note also the converse: if for $\{\varphi, \psi\}, \{\tilde{\varphi}, \tilde{\psi}\} \in \mathfrak{H}^2$

$$(A-l)^{-1}(l\tilde{\varphi} - \tilde{\psi}) + \tilde{\varphi} = (A-l)^{-1}(l\varphi - \psi) + \varphi,$$

then $(A-l)^{-1}\big(l(\tilde{\varphi} - \varphi) - (\tilde{\psi} - \psi)\big) = \varphi - \tilde{\varphi}$, so that $\{\tilde{\varphi} - \varphi, \tilde{\psi} - \psi\} \in A$.

However, the definition of the function $Q(l)$ in (3.3) depends on the choice of the pair $\{\varphi, \psi\}$. When $\{\varphi, \psi\}$ is replaced by $\{\varphi, \psi\} + \{h, k\}$, $\{h, k\} \in A$, then the function in (3.3) is now given by

$$Q(l) + 2\,\mathrm{Re}[h, \psi] + [h, k], \tag{3.5}$$

which differs from the original function $Q(l)$ in (3.3) by a real constant. Of course, when $\{\varphi, \psi\}$ is replaced by $\{\varphi, P\psi\}$, it follows from (3.5) that we obtain precisely the same function.

The element $\chi(l)$ spans $\ker(S^* - l)$. Clearly,

$$\{\chi(l), l\chi(l)\} = \big\{(A-l)^{-1}(l\varphi - \psi), \big(I + l(A-l)^{-1}\big)(l\varphi - \psi)\big\} + \{\varphi, \psi\}. \tag{3.6}$$

This decomposition corresponds to the direct sum (2.2). In particular, for each $l \in \mathbf{C} \setminus \mathbf{R}$ the subspace $\mathrm{span}\{\chi(l), l\chi(l)\}$ is equivalent to $Z = \mathrm{span}\{\varphi, \psi\}$. Note that for each $l \in \mathbf{C} \setminus \mathbf{R}$ the subspace $\mathrm{span}\{\chi(l), l\chi(l)\}$ is nonsymmetric:

$$\mathrm{Im}[l\chi(l), \chi(l)] = (\mathrm{Im}\, l)[\chi(l), \chi(l)].$$

This remark provides a nonsymmetric version of Lemma 2.3. Moreover, with the pair $\{\chi(\bar{l}), \bar{l}\chi(\bar{l})\}$ the definition (2.1) takes the form (1.4).

In case A is a selfadjoint operator and $\varphi \in \mathrm{dom}\, A$, the formulas (3.1) and (3.4) for $\chi(l)$ and $Q(l)$ reduce to

$$\chi(l) = (A-l)^{-1}(A\varphi - \psi), \tag{3.7}$$

and

$$Q(l) = [\psi, \varphi] + [\varphi, \psi] - [A\varphi, \varphi] + [(A-l)^{-1}(A\varphi - \psi), (A\varphi - \psi)]. \tag{3.8}$$

In fact, then the pair $\{\varphi, \psi\}$ is equivalent to the pair $\{0, \psi - A\varphi\}$, as

$$\{\varphi, \psi\} = \{0, \psi - A\varphi\} + \{\varphi, A\varphi\}.$$

Moreover, the symmetric relation $S = A \cap Z^*$ is an operator, and the identity (2.1) reduces to

$$S = \big\{\{f, g\} \in A : [f, A\varphi - \psi] = 0\big\}. \tag{3.9}$$

Proposition 3.1. *The function* $Q(l)$ *satisfies the equation* (1.5). *Hence* $Q(l)$ *is a* Q*-function of* A *and* $S = A \cap Z^*$.

Proof. Write out the inner product

$$[\chi(l), \chi(\lambda)] = [(A-l)^{-1}(l\varphi - \psi) + \varphi, (A-\lambda)^{-1}(\lambda\varphi - \psi) + \varphi].$$

This gives the following terms

$$[(A-l)^{-1}(l\varphi - \psi), (A-\lambda)^{-1}(\lambda\varphi - \psi)] + [(A-l)^{-1}(l\varphi - \psi), \varphi] \\ + [\varphi, (A-\lambda)^{-1}(\lambda\varphi - \psi)] + [\varphi, \varphi].$$

Application of the resolvent identity to the first term leads to the following decomposition:

$$(l-\bar{\lambda})[\chi(l), \chi(\lambda)] = [(A-l)^{-1}(l\varphi - \psi), \lambda\varphi - \psi] \\ - [(l\varphi - \psi), (A-\lambda)^{-1}(\lambda\varphi - \psi)] + (l-\bar{\lambda})[(A-l)^{-1}(l\varphi - \psi), \varphi] \\ + (l-\bar{\lambda})[\varphi, (A-\lambda)^{-1}(\lambda\varphi - \psi)] + (l-\bar{\lambda})[\varphi, \varphi].$$

Combining the first and third term, and the second and the fourth term on the righthand side, it is easily seen, by means of (3.4), that the righthand side is equal to $Q(l) - Q(\lambda)^*$. This completes the proof.

We will now calculate the resolvent operators of the selfadjoint extensions in (2.4) and (2.5). It turns out that we obtain a formula due to Kreĭn describing abstractly all selfadjoint extensions of a symmetric operator. The connection between Kreĭn's formula and von Neumann's formula was made explicit in [HLS].

Theorem 3.2. *The resolvents of the canonical selfadjoint extensions* $A(\tau)$ *of* $S = A \cap Z^*$ *in* (2.4) *and* (2.5) *are given by* $\big(A(0) - l\big)^{-1} = (A-l)^{-1}$ *and for* $\tau \in \mathbf{R} \cup \{\infty\}$, $\tau \neq 0$, *by*

$$\big(A(\tau) - l\big)^{-1} = (A-l)^{-1} - \chi(l)\frac{1}{Q(l) + 1/\tau}[\,\cdot\,, \chi(\bar{l})]. \tag{3.10}$$

Proof. Assume that $\tau \neq 0$ and let $h \in \mathfrak{H}$. Define $k = \big(A(\tau) - l\big)^{-1}h$, so that $\{k, h + lk\} \in A(\tau)$. According to Theorem 2.4 the element $\{k, h + lk\}$ has the decomposition

$$\{k, h + lk\} = \{f, g\} - c\{\varphi, \psi\}. \tag{3.11}$$

If $1/\tau + [\psi, \varphi] \neq 0$ the element $\{f, g\}$ in (3.11) belongs to A, and $c \in \mathbf{C}$ satisfies

$$c(1/\tau + [\psi, \varphi]) = \langle \{f, g\}, \{\varphi, \psi\} \rangle. \tag{3.12}$$

If $1/\tau + [\psi, \varphi] = 0$ the element $\{f, g\}$ in (3.11) belongs to $S \subset A$, and $c \in \mathbf{C}$ is uniquely determined by $\{k, h + lk\}$ because of (2.3). Note that in this case (3.12) is automatically satisfied as the righthand side of (3.12) is now 0. It follows from (3.11) that

$$\{f,g\} = \{k, h+lk\} + c\{\varphi,\psi\} \in A,$$

so that

$$\{g-lf, f\} = \{h,k\} + c\{\psi - l\varphi, \varphi\} \in (A-l)^{-1},$$

or equivalently

$$(A-l)^{-1}h = k + c\big(\varphi + (A-l)^{-1}(l\varphi - \psi)\big).$$

Due to the definition (3.1) and the definition $k = (A(\tau)-l)^{-1}h$, this gives

$$\big(A(\tau)-l\big)^{-1}h = (A-l)^{-1}h - c\chi(l). \tag{3.13}$$

It also follows from (3.11) that $h = g - lf + c(l\varphi - \psi)$, which yields

$$[h, \chi(\bar{l})] = [g-lf, \chi(\bar{l})] + c[l\varphi - \psi, \chi(\bar{l})]. \tag{3.14}$$

Due to the definition (3.3), the inner product in the second term on the righthand side of (3.14) is equal to

$$[l\varphi - \psi, \chi(\bar{l})] = Q(l) - [\psi,\varphi],$$

recall that (1.5) implies that $Q(l)^* = Q(\bar{l})$. Therefore it follows from (3.2) that

$$[h, \chi(\bar{l})] = \langle \{f,g\}, \{\varphi,\psi\}\rangle + c(Q(l) - [\psi,\varphi]). \tag{3.15}$$

First consider the case $1/\tau + [\psi,\varphi] \neq 0$. Substitution of $\langle \{f,g\}, \{\varphi,\psi\}\rangle$ from (3.12) into (3.15) gives

$$[h, \chi(\bar{l})] = c(Q(l) + 1/\tau). \tag{3.16}$$

Next consider the case $1/\tau + [\psi,\varphi] = 0$. The first term on the righthand side of (3.15) is zero as $\{f,g\} \in S$. Hence (3.15) reduces to (3.16). Thus, in both cases $1/\tau + [\psi,\varphi] \neq 0$ and $1/\tau + [\psi,\varphi] = 0$, we can solve the equation (3.16) for c and substitute the result in (3.13). This gives the desired result. Hence, in each case the resolvent of $A(\tau)$ is given by (3.10). This completes the proof.

We recall the following proposition concerning Q-functions, which are normalized as indicated, cf. [HLS, Proposition 3.2].

Proposition 3.3. *Let $Q(l)$ be the Q-function of S and A, normalized by* $\operatorname{Re} Q(\mu) = 0$. *For each $\tau \in \mathbf{R} \cup \{\infty\}$ the Q-function $Q_\tau(l)$ of the canonical selfadjoint extension $A(\tau)$ and S, normalized by* $\operatorname{Re} Q_\tau(\mu) = 0$, *is given by*

$$Q_\tau(l) = \frac{Q(l) - \tau\big(\operatorname{Im} Q(\mu)\big)^2}{\tau Q(l) + 1}, \qquad \tau \in \mathbf{R} \cup \{\infty\}. \tag{3.17}$$

We emphasize that a Q-function of S and A is determined up to a real constant; the only condition on a Q-function is that it satisfies (1.5).

With any Nevanlinna function $Q(l)$ and a parameter $\tau \in \mathbf{R} \cup \{\infty\}$ we may associate the function $Q_\tau(l)$, defined by the linear fractional transform (3.17), see [HLS]. In [HLS] and [HS1] the following facts were proved using a function-theoretic method. If $Q(l)$ belongs to $\mathbf{N}_1$, $\mathbf{N}_0$, $\mathbf{N}_{-1}$ or $\mathbf{N}_{-2}$, then for all but one $\tau \in \mathbf{R} \cup \{\infty\}$, the function $Q_\tau(l)$ belongs to $\mathbf{N}_1$, $\mathbf{N}_0$, $\mathbf{N}_{-1}$ or $\mathbf{N}_{-2}$, respectively, whereas for the exceptional value of τ, given by $1/\tau + \gamma = 0$, the exceptional function $Q_\tau(l)$ does not belong to $\mathbf{N}_1$. Moreover, the exceptional function was characterized in a function-theoretic manner.

4. Characterization of subclasses of Q-functions

Let A be a selfadjoint relation and let $Z = \operatorname{span}\{\varphi, \psi\}$ be a one-dimensional subspace which satisfies (2.3). Associated with S and its selfadjoint extension A is a Q-function $Q(l)$ given by (3.3), see Proposition 3.1. In this section we will give necessary and sufficient conditions in terms of Z for $Q(l)$ to belong to the subclasses $\mathbf{N}_1$, $\mathbf{N}_0$, $\mathbf{N}_{-1}$, or $\mathbf{N}_{-2}$. If $Q(l)$ belongs to $\mathbf{N}_1$ we can evaluate $\lim_{y\to\infty} Q(iy)$ and if $Q(l)$ belongs to $\mathbf{N}_0$, $\mathbf{N}_{-1}$, or $\mathbf{N}_{-2}$ we can evaluate the corresponding moments in terms of A and Z.

In the following we assume that $S = A \cap Z^*$ and A are restricted to the Hilbert space $\mathfrak{H} \ominus \operatorname{mul} S$. According to Proposition 1.2 we may restrict ourselves, without loss of generality, to the situation that $S = A \cap Z^*$ is a closed symmetric operator with defect numbers $(1,1)$ and where A is an operator or A is a multivalued operator whose multivalued part $\operatorname{mul} A$ is one-dimensional. In this case $\operatorname{mul} A = \operatorname{span}\{(I-P)\varphi\}$, cf. Proposition 1.2. Here P denotes the orthogonal projection onto $\mathfrak{H} \ominus \operatorname{mul} A$.

Proposition 4.1. *Let A be a selfadjoint relation in a Hilbert space $\mathfrak{H}$ and let $Z = \operatorname{span}\{\varphi, \psi\}$ be a one-dimensional subspace which satisfies* (2.3). *Assume that $S = A \cap Z^*$ is an operator, so that* $\operatorname{mul} A$ *is at most one-dimensional.*

(i) *If* $\operatorname{mul} A = \{0\}$, *then S is not densely defined if and only if* $\varphi \in \operatorname{dom} A$. *In this case* $\operatorname{mul} S^* = \operatorname{span}\{A\varphi - \psi\}$.

(ii) *If* $\operatorname{mul} A$ *is one-dimensional, then S is not densely defined and* $\operatorname{dom} S = \operatorname{dom} A$ *and* $\operatorname{mul} S^* = \operatorname{span}\{(I-P)\varphi\}$.

Proof. Suppose that $\operatorname{mul} A = \{0\}$, i.e., that A is an operator. We first assume that S is not densely defined. Then there exists a nontrivial element $\{0, g\} \in \operatorname{mul} S^*$ and it follows that $\{0, g\} = \{h, Ah\} + c\{\varphi, \psi\}$ for some $h \in \operatorname{dom} A$ and $c \in \mathbf{C}$. Clearly, $c \neq 0$ and thus $\varphi \in \operatorname{dom} A$ follows. Suppose conversely that $\varphi \in \operatorname{dom} A$. Then the definition (2.1) of S can be written as

$$S = \big\{\{f, g\} \in A : [f, A\varphi - \psi] = 0\big\}.$$

Note that $A\varphi - \psi \neq 0$, due to (2.3). This shows that S is not densely defined and that $\operatorname{mul} S^*$ has the indicated form.

To prove the second statement note that, if $\operatorname{mul} A$ is one-dimensional then A is not an operator, so that A and thus S are not densely defined. Moreover, $(I - P)\varphi \neq 0$. Now let $\{f, g\} \in A$ and denote $c = \langle\{f, g\}, \{\varphi, \psi\}\rangle / [(I - P)\varphi, \varphi]$. Then with $\tilde{g} = g - c(I - P)\varphi$ we have $\{f, \tilde{g}\} \in A$ and it is easy to check that $\langle\{f, \tilde{g}\}, \{\varphi, \psi\}\rangle = 0$, i.e., $\{f, \tilde{g}\} \in S$. This shows that $\operatorname{dom} A \subset \operatorname{dom} S$ and completes the proof.

Proposition 4.2. *Assume that the conditions of Proposition* 4.1 *hold.*

(i) *If* $\varphi \in \operatorname{dom} S$, *then* $S \dot{+} Z$ *is a selfadjoint extension of* S *which is not an operator.*

(ii) *Conversely, if* $S \dot{+} Z$ *is not an operator, then* $\varphi \in \operatorname{dom} S$.

Proof. If $\varphi \in \operatorname{dom} S$, then $\{\varphi, \psi'\} \in S$ for some $\psi' \in \mathfrak{H}$. Since $\langle\{\varphi, \psi'\}, \{\varphi, \psi\}\rangle = 0$, it follows that $[\varphi, \psi] = [\psi', \varphi] \in \mathbf{R}$. Hence, Z is symmetric and $S \dot{+} Z$ is selfadjoint. Moreover $\{0, \psi' - \psi\} \in S \dot{+} Z$ and $\psi' \neq \psi$ on account of (2.3). The converse statement is obvious.

Let $Q(l)$ be the Q-function of $S = A \cap Z^*$ and A as defined by (3.3). From the general theory of Nevanlinna functions we know that

$$\lim_{y\to\infty} \frac{\operatorname{Re} Q(iy)}{y} = 0, \qquad \lim_{y\to\infty} \frac{\operatorname{Im} Q(iy)}{y} \geq 0.$$

It follows from (3.1) that $(I - P)\chi(l) = (I - P)\varphi$. Hence, the last limit can be expressed in terms of Z: if we apply (ii) of Proposition 1.1, we obtain

$$\lim_{y\to\infty} \frac{\operatorname{Im} Q(iy)}{y} = [(I - P)\varphi, (I - P)\varphi]. \tag{4.1}$$

We state Proposition 1.3 in terms of the subspace Z.

Proposition 4.3. *Let* $Q(l)$ *be the* Q*-function of* $S = A \cap Z^*$ *and* A. *Then*

(i) $\lim_{y\to\infty} \operatorname{Im} Q(iy)/y = 0$ *if and only if* $\varphi \in \overline{\operatorname{dom} A}$.

Assume that S *is an operator. Then*

(ii) $\lim_{y\to\infty} \operatorname{Im} Q(iy)/y = 0$ *if and only if* A *is an operator.*

(iii) $Q(l) \in \mathbf{N}_1$ *if and only if* A *is an operator and* $\varphi \in \operatorname{dom} |A|^{1/2}$.
(iv) $Q(l) \in \mathbf{N}_0$ *if and only if* A *is an operator and* $\varphi \in \operatorname{dom} A$.
(v) $Q(l) \in \mathbf{N}_{-1}$ *if and only if* A *is an operator,* $\varphi \in \operatorname{dom} A$, *and* $A\varphi - \psi \in \operatorname{dom} |A|^{1/2}$.
(vi) $Q(l) \in \mathbf{N}_{-2}$ *if and only if* A *is an operator,* $\varphi \in \operatorname{dom} A$, *and* $A\varphi - \psi \in \operatorname{dom} A$.

Proof. The first statement follows immediately from (4.1). Note that the first element on the righthand side of (3.1) belongs to dom A and that $\operatorname{dom} A = \operatorname{dom} |A| \subset \operatorname{dom} |A|^{1/2}$. Therefore, φ belongs to $\operatorname{dom} |A|^{1/2}$ or to dom A if and only if $\chi(l)$ belongs to $\operatorname{dom} |A|^{1/2}$ or to dom A, respectively. If A is an operator and $\varphi \in \operatorname{dom} A$, it follows from (3.7) that $\chi(l)$ belongs to $\operatorname{dom} |A|^{3/2}$ or $\operatorname{dom} |A|^2$, if and only if $A\varphi - \psi$ belongs to $\operatorname{dom} |A|^{1/2}$ or $\operatorname{dom} |A| = \operatorname{dom} A$, respectively. Now apply Proposition 1.3. The proof is completed.

Note that if $\{\tilde{\varphi}, \tilde{\psi}\}$ is equivalent to $\{\varphi, \psi\}$, then $\tilde{\varphi} \in \operatorname{dom} |A|^{1/2}$ if and only if $\varphi \in \operatorname{dom} |A|^{1/2}$, and $\tilde{\varphi} \in \operatorname{dom} A$ if and only if $\varphi \in \operatorname{dom} A$, in which case $A\varphi - \psi = A\tilde{\varphi} - \tilde{\psi}$ spans mul S^*, see Proposition 4.1.

A function $Q(l)$ in $\mathbf{N}$ belongs to $\mathbf{N}_1$ if and only if the integral representation (1.7) of $Q(l)$ reduces to

$$Q(l) = \gamma + \int_{\mathbf{R}} \frac{1}{t-l}\, d\sigma(t), \tag{4.2}$$

where $\gamma \in \mathbf{R}$ and $\int_{\mathbf{R}} d\sigma(t)/(|t|+1) < \infty$, cf. [Ka] and [KK]. It follows from this representation that

$$\gamma = \lim_{y\to\infty} Q(iy). \tag{4.3}$$

In particular, the function $Q(l)$ belongs to $\mathbf{N}_0$ if and only if the function $\sigma(t)$ satisfies $\int_{\mathbf{R}} d\sigma(t) < \infty$. Moreover, the function $Q(l)$ belongs to $\mathbf{N}_{-1}$ or $\mathbf{N}_{-2}$ if and only $\int_{\mathbf{R}}(|t|+1)\, d\sigma(t) < \infty$ or $\int_{\mathbf{R}}(|t|^2+1)\, d\sigma(t) < \infty$, respectively, see [HS1]. Hence, in these cases the moments

$$m_k(\sigma) = \int_{\mathbf{R}} t^k\, d\sigma(t), \tag{4.4}$$

associated with the spectral measure of the function $Q(l)$, are well-defined for $k = 0$, $k = 0, 1$, or $k = 0, 1, 2$, respectively. If $Q(l)$ is the Q-function of $S = A \cap Z^*$ and A, we will express the limit γ and the moments $m_0(\sigma)$, $m_1(\sigma)$, and $m_2(\sigma)$, respectively, in terms of the operator A and the subspace Z, cf. [A], [K3], [KL]. For this we need the polar decomposition of $A = U|A|$. Here the operators U $(= U^* = U^{-1})$ and $|A|$ are given in terms of the spectral decomposition $A = \int_{\mathbf{R}} t\, dE(t)$ of A as follows

$$|A| = \int_{\mathbf{R}} |t|\, dE(t), \qquad U = \int_{\mathbf{R}} \frac{t}{|t|}\, dE(t). \tag{4.5}$$

The functions $\sigma(t)$ in (1.7) and $E(t)$ are related by (iii) of Proposition 1.1. Hence if $Q(l)$ belongs to $\mathbf{N}_0$, it follows from (3.7) that

$$d\sigma(t) = d\big([E(t)(A\varphi - \psi), A\varphi - \psi]\big). \tag{4.6}$$

Proposition 4.4. *Let $Q(l)$ be the Q-function of $S = A \cap Z^*$ and A. If $Q(l) \in \mathbf{N}_1$, then*

$$\gamma = \lim_{y\to\infty} Q(iy) = [\psi, \varphi] + [\varphi, \psi] - [U|A|^{1/2}\varphi, |A|^{1/2}\varphi]. \tag{4.7}$$

Moreover, if $Q(l)$ belongs to $\mathbf{N}_0$, then $\gamma = [\psi, \varphi] + [\varphi, \psi] - [A\varphi, \varphi]$ and $Q(l)$ has the operator representation

$$Q(l) = \gamma + [(A - l)^{-1}\tilde{\psi}, \tilde{\psi}], \tag{4.8}$$

where $\tilde{\psi} = A\varphi - \psi$.

(i) *If $Q(l) \in \mathbf{N}_0$, then*

$$m_0(\sigma) = \lim_{y\to\infty} -iy(Q(iy) - \gamma) = [\tilde{\psi}, \tilde{\psi}].$$

(ii) *If $Q(l) \in \mathbf{N}_{-1}$, then*

$$m_1(\sigma) = \lim_{y\to\infty} -(iy)^2\Big(Q(iy) - \gamma + \frac{m_0(\sigma)}{iy}\Big) = [U|A|^{1/2}\tilde{\psi}, |A|^{1/2}\tilde{\psi}].$$

(iii) *If $Q(l) \in \mathbf{N}_{-2}$, then $m_1(\sigma) = [A\tilde{\psi}, \tilde{\psi}]$ and*

$$m_2(\sigma) = \lim_{y\to\infty} -(iy)^3\Big(Q(iy) - \gamma + \frac{m_0(\sigma)}{iy} + \frac{m_1(\sigma)}{(iy)^2}\Big) = [A\tilde{\psi}, A\tilde{\psi}].$$

Proof. Observe that $Q(l)$ in (3.4) can be written as

$$\begin{aligned} Q(l) &= l[\varphi, \varphi] + [(A - l)^{-1}\psi, \psi] \\ &\qquad - l[(A - l)^{-1}\psi, \varphi] - l[(A - l)^{-1}\varphi, \psi] + l^2[(A - l)^{-1}\varphi, \varphi]. \end{aligned} \tag{4.9}$$

Consider the behaviour of this function for $l = iy$, $y \to \infty$. The second term $[(A - l)^{-1}\psi, \psi]$ does not give a contribution to the limit. The terms

$$-l[(A - l)^{-1}\psi, \varphi] \qquad \text{and} \qquad -l[(A - l)^{-1}\varphi, \psi]$$

give contributions $[\psi, \varphi]$ and $[\varphi, \psi]$, respectively. The two remaining terms $l[\varphi, \varphi]$ and $l^2[(A - l)^{-1}\varphi), \varphi]$ are combined to

$$l[(I + l(A - l)^{-1})\varphi, \varphi] = l[A(A - l)^{-1}\varphi, \varphi] = \int_{\mathbf{R}} \frac{lt}{t - l}\, d([E(t)\varphi, \varphi]), \tag{4.10}$$

where we have used

$$l(A-l)^{-1} = -I + A(A-l)^{-1}. \tag{4.11}$$

The assumption $\varphi \in \operatorname{dom} |A|^{1/2}$ is equivalent to $\int_{\mathbf{R}} |t|\, d([E(t)\varphi,\varphi]) < \infty$. Note that

$$\left|\frac{iyt}{t-iy}\right| = \frac{y|t|}{\sqrt{t^2+y^2}} \le |t|.$$

Application of the dominated convergence theorem to (4.10) with $l = iy$, $y \to \infty$, gives the limit $-\int_{\mathbf{R}} t\, d([E(t)\varphi,\varphi])$. Next observe that

$$[U|A|^{1/2}\varphi, |A|^{1/2}\varphi] = \int_{\mathbf{R}} \frac{t}{|t|}|t|^{1/2}\, d\big([E(t)\varphi, |A|^{1/2}\varphi]\big) = \int_{\mathbf{R}} t\, d\big([E(t)\varphi,\varphi]\big),$$

which proves (4.7).

Clearly, if $Q(l) \in \mathbf{N}_0$, then γ in (4.7) is given by $\gamma = [\psi,\varphi] + [\varphi,\psi] - [A\varphi,\varphi]$. Comparing this with the operator representation (3.8) we obtain (4.8). The identity (4.11) and the representation (4.8) imply that

$$-l(Q(l)-\gamma) = [\tilde{\psi},\tilde{\psi}] - [A(A-l)^{-1}\tilde{\psi},\tilde{\psi}]. \tag{4.12}$$

The statement in (i) follows from (4.12) and the integral representation (4.2). If $Q(l) \in \mathbf{N}_{-1}$, then $\tilde{\psi} \in \operatorname{dom} |A|^{1/2}$ and

$$[A(A-l)^{-1}\tilde{\psi},\tilde{\psi}] = [(A-l)^{-1}U|A|^{1/2}\tilde{\psi}, |A|^{1/2}\tilde{\psi}].$$

Hence (4.12), (i), and (4.11) give

$$-l^2\Big(Q(l) - \gamma + \frac{m_0(\sigma)}{l}\Big) = [U|A|^{1/2}\tilde{\psi}, |A|^{1/2}\tilde{\psi}] - [A(A-l)^{-1}U|A|^{1/2}\tilde{\psi}, |A|^{1/2}\tilde{\psi}]. \tag{4.13}$$

The statement in (ii) follows from (4.13) and the integral representation (4.2). If $Q(l) \in \mathbf{N}_{-2}$, then $\tilde{\psi} \in \operatorname{dom} A$ by Proposition 4.3, and

$$[A(A-l)^{-1}U|A|^{1/2}\tilde{\psi}, |A|^{1/2}\tilde{\psi}] = [(A-l)^{-1}A\tilde{\psi}, A\tilde{\psi}],$$

and $m_1(\sigma) = [A\tilde{\psi},\tilde{\psi}]$. Hence (4.13), (ii), and (4.11) give

$$-l^3\Big(Q(l) - \gamma + \frac{m_0(\sigma)}{l} + \frac{m_1(\sigma)}{l^2}\Big) = -l[(A-l)^{-1}A\tilde{\psi}, A\tilde{\psi}]. \tag{4.14}$$

The statement in (iii) follows from (4.14) and the integral representation (4.2). This completes the proof.

5. The operator case

Let A be a selfadjoint *operator* in the Hilbert space $\mathfrak{H}$ and let $Z = \operatorname{span}\{\varphi, \psi\}$ be a one-dimensional subspace which satisfies (2.3). We will now consider Theorem 2.4 in greater detail.

First we present a suitable formulation of the definition of S and its adjoint S^*.

Lemma 5.1. *The closed symmetric operator $S = A \cap Z^*$ is given by*

$$S = \{\{f, Af\} : f \in \operatorname{dom} A,\ [Af, \varphi] - [f, \psi] = 0\}. \tag{5.1}$$

Its adjoint S^* is given by

$$S^* = \big\{\{h, A(h + c\varphi) - c\psi\} : h + c\varphi \in \operatorname{dom} A,\ c \in \mathbf{C}\big\}. \tag{5.2}$$

Proof. Since A is an operator, (5.1) is just a restatement of (2.1). Similarly, consider an arbitrary element of (2.2), i.e., an element of the form

$$\{f, g\} - c\{\varphi, \psi\}, \qquad \{f, g\} \in A,\ c \in \mathbf{C}. \tag{5.3}$$

With $h = f - c\varphi$, it follows that $f = h + c\varphi \in \operatorname{dom} A$ and that $g - c\psi = Af - c\psi = A(h + c\varphi) - c\psi$, so that the element (5.3) is equal to

$$\{h, A(h + c\varphi) - c\psi\}, \qquad h + c\varphi \in \operatorname{dom} A,\ c \in \mathbf{C}, \tag{5.4}$$

and belongs to the righthand side of (5.2).

Conversely, consider an arbitrary element in the righthand side of (5.2), i.e., an element of the form (5.4). With $f = h + c\varphi \in \operatorname{dom} A$, $c \in \mathbf{C}$, it follows that the element (5.4) is equal to (5.3) and belongs to (2.2). This completes the proof.

The form (5.2) in which the adjoint S^* is written is now used for the description of all canonical selfadjoint extensions of S. We recall from Proposition 4.1 that S is not densely defined if and only if $\varphi \in \operatorname{dom} A$, in which case $\operatorname{mul} S^* = \operatorname{span}\{A\varphi - \psi\}$.

Theorem 5.2. *The canonical selfadjoint extensions $A(\tau)$, $\tau \in \mathbf{R} \cup \{\infty\}$, of $S = A \cap Z^*$ are given by $A(0) = A$ and for $\tau \neq 0$, $1/\tau + [\psi, \varphi] \neq 0$, by*

$$A(\tau) = \Bigg\{\{h, A(h + c\varphi) - c\psi\} : h + c\varphi \in \operatorname{dom} A,\ c \in \mathbf{C}, \qquad c = \frac{[A(h + c\varphi), \varphi] - [h + c\varphi, \psi]}{1/\tau + [\psi, \varphi]}\Bigg\}, \tag{5.5}$$

while for $1/\tau + [\psi, \varphi] = 0$ *the canonical selfadjoint extension* $A(\tau)$ *is given by*

$$A(\tau) = \big\{\{h, A(h + c\varphi) - c\psi\} : h + c\varphi \in \text{dom } A,\ c \in \mathbf{C}, \\ [A(h + c\varphi), \varphi] - [h + c\varphi, \psi] = 0\big\}. \tag{5.6}$$

Proof. Consider an arbitrary element in $A(\tau)$ as given by (2.4) for $\tau \neq 0$, $1/\tau + [\psi, \varphi] \neq 0$, or by (2.5) for $1/\tau + [\psi, \varphi] = 0$. That is, consider an element of the form

$$\{f, Af\} - c\{\varphi, \psi\}. \tag{5.7}$$

If $1/\tau + [\psi, \varphi] \neq 0$, assume that $c \in \mathbf{C}$ satisfies

$$c(1/\tau + [\psi, \varphi]) = [Af, \varphi] - [f, \psi]. \tag{5.8}$$

If $1/\tau + [\psi, \varphi] = 0$, then assume that $\{f, Af\} \in S$ and note that (5.8) is still satisfied, cf. (5.1). Define $h = f - c\varphi$, then $f = h + c\varphi \in \text{dom } A$ and $g - c\psi = A(h + c\varphi) - c\psi$. Therefore (5.7) is equal to

$$\{h, A(h + c\varphi) - c\psi\}, \tag{5.9}$$

while, in addition, $c \in \mathbf{C}$ must satisfy

$$c(1/\tau + [\psi, \varphi]) = [A(h + c\varphi), \varphi] - [h + c\varphi, \psi]. \tag{5.10}$$

Hence $A(\tau)$ is contained in the righthand side of (5.5) or of (5.6), respectively.

Conversely, consider an arbitrary element in the righthand side of (5.5) with $\tau \neq 0$, $1/\tau + [\psi, \varphi] \neq 0$, or of (5.6) with $1/\tau + [\psi, \varphi] = 0$. That is, consider an element of the form (5.9) where c satisfies (5.10). Define $f = h + c\varphi$, then $f \in \text{dom } A$ and the element (5.9) has the form (5.7), while c satisfies (5.8). Note that if $1/\tau + [\psi, \varphi] = 0$, then it follows from (5.8) that $\{f, Af\} \in S$, cf. (5.1). Therefore, the righthand side of (5.5) or of (5.6) is contained in $A(\tau)$ as given by (2.4) or by (2.5), respectively. This completes the proof.

In general it is impossible to solve the constant c in terms of A from the equation (5.5). However, since $\varphi \in \text{dom } S^*$, the condition $h + c\varphi \in \text{dom } A$ implies that $h \in \text{dom } S^*$. This observation leads to an interpretation of (5.5) in terms of triplet spaces, see [HS2]. If the Q-function $Q(l)$ of A and S is an exceptional function corresponding to the class $\mathbf{N}_1$, then it follows from Proposition 3.3 that all canonical selfadjoint extensions $A(\tau)$, $\tau \neq 0$, have Q-functions belonging to $\mathbf{N}_1$, cf. [HLS]. It is in the case where the Q-function $Q(l)$ belongs to $\mathbf{N}_1$ (or equivalently $\varphi \in \text{dom } |A|^{1/2}$), that the perturbation formula in Theorem 5.2 can be simplified. For then the limit $\gamma = \lim_{y\to\infty} Q(iy)$ exists as a real number, cf. Proposition 4.4, and in the description of all canonical selfadjoint extensions $A(\tau)$, $\tau \in \mathbf{R} \cup \{\infty\}$, of $S = A \cap Z^*$, there exists precisely one exceptional value of the parameter τ, given by $1/\tau + \gamma = 0$, for which the Q-function corresponding to $A(\tau)$ and $S = A \cap Z^*$ belongs to $\mathbf{N} \setminus \mathbf{N}_1$. In the case that $Q(l)$ belongs to $\mathbf{N}_1$, it is also possible to explicitly "solve" $c \in \mathbf{C}$ in terms of A from (5.5). Moreover, we will characterize the canonical selfadjoint extension $A(\tau)$, $1/\tau + \gamma = 0$, in terms of a "boundary condition".

Proposition 5.3. *Assume that the Q-function $Q(l)$ of $S = A \cap Z^*$ and A belongs to $\mathbf{N}_1$. Then* $\operatorname{dom} S^* \subset \operatorname{dom} |A|^{1/2}$. *All canonical selfadjoint extensions $A(\tau)$ of $S = A \cap Z^*$ are given by $A(0) = A$ and for $\tau \neq 0$, $1/\tau + \gamma \neq 0$, by*

$$A(\tau) = \Big\{ \{h, A(h + c\varphi) - c\psi\} : h + c\varphi \in \operatorname{dom} A,\ c \in \mathbf{C}, \qquad c = \frac{[U|A|^{1/2}h, |A|^{1/2}\varphi] - [h, \psi]}{1/\tau + \gamma} \Big\}, \tag{5.11}$$

while for $1/\tau + \gamma = 0$ the exceptional canonical selfadjoint extension $A(\tau)$ is given by

$$A(\tau) = \big\{ \{h, A(h + c\varphi) - c\psi\} : h + c\varphi \in \operatorname{dom} A,\ c \in \mathbf{C}, \qquad [U|A|^{1/2}h, |A|^{1/2}\varphi] - [h, \psi] = 0 \big\}. \tag{5.12}$$

Proof. Since $\varphi \in \operatorname{dom} |A|^{1/2}$, it follows from $h + c\varphi \in \operatorname{dom} A$, that $h \in \operatorname{dom} |A|^{1/2}$, as $\operatorname{dom} A \subset \operatorname{dom} |A|^{1/2}$. Hence it follows from (5.2) that $\operatorname{dom} S^* \subset \operatorname{dom} |A|^{1/2}$.

Consider an arbitrary element in $A(\tau)$ in the righthand side of (5.5) with $\tau \neq 0$, $1/\tau + [\psi, \varphi] \neq 0$, or in the righthand side of (5.6) with $1/\tau + [\psi, \varphi] = 0$. That is, consider an element of the form

$$\{h, A(h + c\varphi) - c\psi\}, \tag{5.13}$$

where $h + c\varphi \in \operatorname{dom} A$ and $c \in \mathbf{C}$ satisfies (5.10). As $\varphi \in \operatorname{dom} |A|^{1/2}$ implies that $h \in \operatorname{dom} |A|^{1/2}$, the equation (5.10) may be written as

$$c(1/\tau + [\psi, \varphi]) = c[U|A|^{1/2}\varphi, |A|^{1/2}\varphi] - c[\varphi, \psi] + [U|A|^{1/2}h, |A|^{1/2}\varphi] - [h, \psi]. \tag{5.14}$$

By Proposition 4.4 this leads to

$$c(1/\tau + \gamma) = [U|A|^{1/2}h, |A|^{1/2}\varphi] - [h, \psi]. \tag{5.15}$$

Thus we have shown that $A(\tau)$ as given by (5.5) or (5.6), is contained in the righthand side of (5.11) or of (5.12), respectively.

Conversely, consider an arbitrary element in the righthand side of (5.11) with $\tau \neq 0$, $1/\tau + \gamma \neq 0$, or of (5.12) with $1/\tau + \gamma \neq 0$. That is, consider an element of the form (5.13), where $c \in \mathbf{C}$ satisfies (5.15). Insert the expression for γ from Proposition 4.4 in (5.15). This shows that $c \in \mathbf{C}$ then satisfies (5.14). As $h + c\varphi \in \operatorname{dom} A$, the identity (5.14) is equivalent to (5.10). Hence this shows that the righthand side of (5.11) or (5.12) is contained in $A(\tau)$ as given by (5.5) or by (5.6), respectively. This completes the proof.

Another way to express the exceptional selfadjoint extension $A(\tau)$, $1/\tau+\gamma=0$, is via

$$A(\tau)=\{\{h,k\}\in S^*:[U|A|^{1/2}h,|A|^{1/2}\varphi]-[h,\psi]=0\},$$

i.e., with a "boundary condition" of the form $[U|A|^{1/2}h,|A|^{1/2}\varphi]-[h,\psi]=0$. This is similar to $S=\big\{\{h,k\}\in A:[U|A|^{1/2}h,|A|^{1/2}\varphi]-[h,\psi]=0\big\}$.

Next we will consider the case that the Q-function $Q(l)$ of $S=A\cap Z^*$ and A belongs to the class $\mathbf{N}_0$ (or equivalently that $\varphi\in\operatorname{dom}A$). In this case S is given by (3.9): $S=\big\{\{f,Af\}:f\in\operatorname{dom}A,\ [f,A\varphi-\psi]=0\big\}$. Note that S is a nondensely defined operator, due to the domain restriction. It follows from (5.2) that $\operatorname{dom}S^*\subset\operatorname{dom}A$. Furthermore, as $\varphi\in\operatorname{dom}A$ implies that $\varphi\in\operatorname{dom}|A|^{1/2}$, the following result is obtained as a special case of Proposition 5.3.

Proposition 5.4. *Assume that the Q-function $Q(l)$ of $S=A\cap Z^*$ and A belongs to $\mathbf{N}_0$. Then* $\operatorname{dom}S^*=\operatorname{dom}A$. *All canonical selfadjoint extensions $A(\tau)$ of $S=A\cap Z^*$ are given by $A(0)=A$ and for $\tau\neq0$, $1/\tau+\gamma\neq0$, by*

$$A(\tau)=\left\{\left\{h,Ah+\frac{[h,A\varphi-\psi]}{1/\tau+\gamma}(A\varphi-\psi)\right\}:h\in\operatorname{dom}A\right\}, \tag{5.16}$$

while for $1/\tau+\gamma=0$ the exceptional canonical selfadjoint extension $A(\tau)$ is given by

$$A(\tau)=\big\{\{h,Ah+c(A\varphi-\psi)\}:h\in\operatorname{dom}A,\ c\in\mathbf{C},\ [h,A\varphi-\psi]=0\big\}. \tag{5.17}$$

We explicitly state what happens when Z is spanned by an element of the form $\{0,\psi\}$, $\psi\neq0$. Clearly, Z is symmetric and $S=\big\{\{f,g\}\in A:[f,\psi]=0\big\}$. The identities (3.7) of $\chi(l)$ and (3.8) of $Q(l)$ reduce to

$$\chi(l)=-(A-l)^{-1}\psi,\qquad Q(l)=[(A-l)^{-1}\psi,\psi]\qquad(\in\mathbf{N}_0),$$

so that $\gamma=0$ and $\tau=\infty$ is the exceptional value. Recall that the Q-function $Q(l)$ changes if the pair $\{\varphi,\psi\}$ is replaced by an equivalent pair, while the function $\chi(l)$ stays the same. For $\tau\in\mathbf{R}$ the canonical selfadjoint extensions $A(\tau)$ of S are densely defined operators and when $\|\psi\|=1$, they are one-dimensional perturbations of A of the form $A(\tau)=A+\tau R$, where R denotes the orthogonal projection onto $\operatorname{mul}S^*=\operatorname{span}\{\psi\}$, see Proposition 4.1. For $\tau=\infty$ we obtain

$$A(\infty)=S\dot{+}Z=S\dot{+}\big(\{0\}\oplus\operatorname{span}\{\psi\}\big),$$

which is the unique selfadjoint extension of S which is not an operator. For finite dimensional Hilbert spaces the connection between the one-dimensional range perturbations and Kreĭn's formula is derived in [D, Chapter 6].

From the explicit expression for the canonical selfadjoint extensions $A(\tau)$ in (5.5) and (5.6) the following result is immediately clear.

Corollary 5.5. *Assume that the* Q*-function* $Q(l)$ *of* $S = A \cap Z^*$ *and* A *belongs to* $\mathbf{N} \setminus \mathbf{N}_0$. *Let* $\tau \in \mathbf{R} \cup \{\infty\}$ *and* $\tau \neq 0$. *Then* $\operatorname{dom} A(\tau) \cap \operatorname{dom} A = \operatorname{dom} S$.

The next corollary shows a completely different behaviour of the domains of the canonical selfadjoint extensions when $Q(l)$ belongs to $\mathbf{N}_0$.

Corollary 5.6. *Assume that the* Q*-function* $Q(l)$ *of* $S = A \cap Z^*$ *and* A *belongs to* $\mathbf{N}_0$. *Let* $\tau \in \mathbf{R} \cup \{\infty\}$, *then*

$$\operatorname{dom} A(\tau) = \operatorname{dom} A \text{ if } 1/\tau + \gamma \neq 0 \quad \text{and} \quad \operatorname{dom} A(\tau) = \operatorname{dom} S \text{ if } 1/\tau + \gamma = 0.$$

It follows from Corollary 5.6 that $A(\tau)$, $1/\tau + \gamma = 0$, is the only selfadjoint extension of S, which is not an operator. In fact then we have that

$$A(\tau) = S \dot{+} \big(\{0\} \oplus \operatorname{span}\{A\varphi - \psi\}\big),$$

or, equivalently,

$$A(\tau) = \big\{\{h,k\} \in S^* : [h, A\varphi - \psi] = 0\big\},$$

which is similar to

$$S = \big\{\{h,k\} \in A : [h, A\varphi - \psi] = 0\big\}.$$

Corollaries 5.5 and 5.6 show the different behaviours in the cases $Q(l) \in \mathbf{N} \setminus \mathbf{N}_0$ and $Q(l) \in \mathbf{N}_0$. If $Q(l) \in \mathbf{N}_1 \setminus \mathbf{N}_0$ the application of space triplets gives a description which is similar to Corollary 5.6. This is already apparent in the operator models for the cases $Q(l) \in \mathbf{N}_1 \setminus \mathbf{N}_0$ and $Q(l) \in \mathbf{N}_0$, see [HLS] and Section 7 of the present paper. For further details we refer to [HKS] and [HS2].

If the Q-function $Q(l)$ of $S = A \cap Z^*$ and A belongs to $\mathbf{N}_0$, then the Q-function $Q_\tau(l)$ of $A(\tau)$ and S, $1/\tau + \gamma \neq 0$, also belongs to $\mathbf{N}_0$, while for $1/\tau + \gamma = 0$ the Q-function $H(l)$ of $A(\tau)$ in (5.17) has the property that $\lim_{y\to\infty} \operatorname{Im} H(iy)/y > 0$. Likewise, if $Q(l)$ belongs to $\mathbf{N}_{-1}$ or $\mathbf{N}_{-2}$, then $Q_\tau(l)$, $1/\tau + \gamma \neq 0$, belongs to the same subclass, while for $1/\tau + \gamma = 0$ the function $H(l)$ satisfies

$$H(l) - \Big(\lim_{y\to\infty} \frac{\operatorname{Im} H(iy)}{y}\Big) l \in \mathbf{N}_1 \text{ or } \mathbf{N}_0,$$

respectively, cf. [HS1]. We relate the moments for $Q_\tau(l)$, $1/\tau + \gamma \neq 0$, to the moments for $Q(l)$. We use the notation $q = \big(\operatorname{Im} Q(\mu)\big)^2$.

Proposition 5.7. *Let the* Q*-function* $Q(l)$ *of* $S = A \cap Z^*$ *and* A *belong to* $\mathbf{N}_0$. *Then for* $1/\tau + \gamma \neq 0$ *the moments* $m_0(\sigma_\tau)$ *are given by*

$$m_0(\sigma_\tau) = \frac{(\tau^2 q + 1) m_0(\sigma)}{(\tau\gamma + 1)^2}. \tag{5.18}$$

If $Q(l) \in \mathbf{N}_{-1}$, then the moments $m_1(\sigma_\tau)$, $1/\tau + \gamma \neq 0$, are given by

$$m_1(\sigma_\tau) = \frac{(\tau^2 q + 1)\left[(\tau\gamma + 1)m_1(\sigma) + \tau m_0(\sigma)^2\right]}{(\tau\gamma+1)^3}. \tag{5.19}$$

Furthermore, if $Q(l) \in \mathbf{N}_{-2}$, then the moments $m_2(\sigma_\tau)$, $1/\tau + \gamma \neq 0$, are given by

$$m_2(\sigma_\tau) = \frac{(\tau^2 q + 1)\left[(\tau\gamma+1)^2 m_2(\sigma) + 2(\tau\gamma+1)\tau m_1(\sigma)m_0(\sigma) + \tau^2 m_0(\sigma)^3\right]}{(\tau\gamma+1)^4}. \tag{5.20}$$

Proof. Assume that $Q(l) \in \mathbf{N}_0$. It follows from (3.17) that for $\tau\gamma + 1 \neq 0$ the limit $\gamma_\tau = \lim_{y\to\infty} Q_\tau(iy)$ exists as a real number and is given by

$$\gamma_\tau = \frac{\gamma - \tau q}{\tau\gamma + 1}.$$

Then a simple calculation shows that

$$-iy\big(Q_\tau(iy) - \gamma_\tau\big) = \frac{-iy\big(Q(iy) - \gamma\big)(\tau^2 q + 1)}{(\tau\gamma+1)\big(\tau Q(iy) + 1\big)}.$$

Taking limits and using (i) of Proposition 4.4 gives (5.18). Next assume that $Q(l) \in \mathbf{N}_{-1}$ and use the identity:

$$\begin{aligned} &-(iy)^2\Big(Q_\tau(iy) - \gamma_\tau + \frac{m_0(\sigma_\tau)}{iy}\Big) \\ &= \frac{\big(-(iy)^2[Q(iy) - \gamma + m_0(\sigma)/iy](\tau\gamma+1) - (iy)[Q(iy) - \gamma]\tau m_0(\sigma)\big)(\tau^2 q + 1)}{(\tau\gamma+1)^2\big(\tau Q(iy) + 1\big)}. \end{aligned}$$

Hence, taking limits and using (i) and (ii) of Proposition 4.4 gives (5.19). Now assume that $Q(l) \in \mathbf{N}_{-2}$. A straightforward calculation shows that

$$\begin{aligned} -(iy)^3\Big(Q_\tau(iy) - \gamma_\tau + \frac{m_0(\sigma_\tau)}{iy} + \frac{m_1(\sigma_\tau)}{(iy)^2}\Big) \\ = -\frac{(iy)^3[Q(iy) - \gamma + m_0(\sigma)/iy + m_1(\sigma)/(iy)^2](\tau^2 q + 1)(\tau\gamma+1)^2}{(\tau\gamma+1)^3\big(\tau Q(iy) + 1\big)} \\ - \frac{(iy)^2[Q(iy) - \gamma + m_0(\sigma)/iy](\tau^2 q + 1)(\tau\gamma+1)\tau m_0(\sigma)}{(\tau\gamma+1)^3\big(\tau Q(iy) + 1\big)} \\ - \frac{(iy)[Q(iy) - \gamma](\tau^2 q + 1)[(\tau\gamma+1)\tau m_1(\sigma) + \tau^2 m_0(\sigma)^2]}{(\tau\gamma+1)^3\big(\tau Q(iy) + 1\big)}. \end{aligned}$$

Again by taking limits and using (i), (ii), and (iii) of Proposition 4.4 yields (5.20). This completes the proof.

6. The multivalued case

Let A be a selfadjoint *relation* in the Hilbert space $\mathfrak{H}$ and let $Z = \operatorname{span}\{\varphi, \psi\}$ be a one-dimensional subspace which satisfies (2.3). We may assume, without loss of generality, that $\operatorname{mul} A$ is one-dimensional and that S is a closed symmetric operator. For this case we will consider Theorem 2.4 in greater detail.

Let $A = A_s \oplus A_\infty$ be a selfadjoint relation whose multivalued part $\operatorname{mul} A$ is one-dimensional, so that

$$\mathfrak{H} = (\mathfrak{H} \ominus \operatorname{mul} A) \oplus \operatorname{mul} A.$$

Recall that $\operatorname{dom} A = \operatorname{dom} A_s$ is dense in $\mathfrak{H} \ominus \operatorname{mul} A$. Choose a unit vector in $\operatorname{mul} A$ and identify $\mathfrak{H} = (\mathfrak{H} \ominus \operatorname{mul} A) \oplus \operatorname{mul} A$ with $\mathfrak{H} = (\mathfrak{H} \ominus \operatorname{mul} A) \oplus \mathbf{C}$ in the obvious way. We use vector notation for the elements in this last Hilbert space. Hence we may write

$$A = \left\{ \left\{ \begin{pmatrix} h \\ 0 \end{pmatrix}, \begin{pmatrix} A_s h \\ u \end{pmatrix} \right\} : h \in \operatorname{dom} A_s,\ u \in \mathbf{C} \right\}. \tag{6.1}$$

Now let $Z = \operatorname{span}\{\varphi, \psi\}$ be any one-dimensional subspace in $\mathfrak{H}^2$; it is equivalent to the subspace $\operatorname{span}\{\varphi, P\psi\}$. Hence, without loss of generality, we may assume that

$$Z = \operatorname{span} \left\{ \begin{pmatrix} \varphi_0 \\ \delta \end{pmatrix}, \begin{pmatrix} \psi_0 \\ 0 \end{pmatrix} \right\}, \tag{6.2}$$

with elements $\varphi_0, \psi_0 \in \mathfrak{H} \ominus \operatorname{mul} A$ and $\delta \in \mathbf{C}$.

If A is a selfadjoint relation whose multivalued part is one-dimensional, then $S = A \cap Z^*$ is a closed symmetric relation and $\operatorname{mul} S$ is at most one-dimensional. We now consider a suitable formulation of the definition of S and its adjoint S^*.

Lemma 6.1. *Let A be a selfadjoint relation as in* (6.1) *and let Z be a one-dimensional subspace as in* (6.2)*. Then the closed symmetric relation $S = A \cap Z^*$ is given by*

$$S = \left\{ \left\{ \begin{pmatrix} f \\ 0 \end{pmatrix}, \begin{pmatrix} A_s f \\ u \end{pmatrix} \right\} : f \in \operatorname{dom} A_s,\ u\bar{\delta} = [f, \psi_0] - [A_s f, \varphi_0],\ u \in \mathbf{C} \right\}. \tag{6.3}$$

Its adjoint S^* is given by

$$S^* = \left\{ \left\{ \begin{pmatrix} h \\ -c\delta \end{pmatrix}, \begin{pmatrix} A_s(h + c\varphi_0) - c\psi_0 \\ v \end{pmatrix} \right\} : h + c\varphi_0 \in \operatorname{dom} A_s,\ c, v \in \mathbf{C} \right\}. \tag{6.4}$$

Proof. The identity (6.3) follows from the definition $S = A \cap Z^*$ and the special form (6.1) and (6.2) of A and Z, respectively. In order to prove (6.4), let

$$\left\{ \begin{pmatrix} h \\ -c\delta \end{pmatrix}, \begin{pmatrix} k \\ v \end{pmatrix} \right\}, \qquad h, k \in \mathfrak{H} \ominus \text{mul } A,\ c, v \in \mathbf{C},$$

be an element of S^*. Then for all $f \in \text{dom } A_s$ we have

$$\left\langle \left\{ \begin{pmatrix} h \\ -c\delta \end{pmatrix}, \begin{pmatrix} k \\ v \end{pmatrix} \right\}, \left\{ \begin{pmatrix} f \\ 0 \end{pmatrix}, \begin{pmatrix} A_s f \\ u \end{pmatrix} \right\} \right\rangle = 0,$$

with $u\bar{\delta} = [f, \psi_0] - [A_s f, \varphi_0]$. This is equivalent to

$$[k + c\psi_0, f] - [h + c\varphi_0, A_s f] = 0, \qquad f \in \text{dom } A_s.$$

Hence $h + c\varphi_0 \in \text{dom } A_s$ and $A_s(h + c\varphi_0) = k + c\psi_0$. Therefore, S^* is contained in the righthand side of (6.4).

Conversely, assume that $h + c\varphi_0 \in \text{dom } A_s$. Then for every $f \in \text{dom } A_s$ with $u\bar{\delta} = [f, \psi_0] - [A_s f, \varphi_0]$ we have

$$\left\langle \left\{ \begin{pmatrix} h \\ -c\delta \end{pmatrix}, \begin{pmatrix} A_s(h + c\varphi_0) - c\psi_0 \\ v \end{pmatrix} \right\}, \left\{ \begin{pmatrix} f \\ 0 \end{pmatrix}, \begin{pmatrix} A_s f \\ u \end{pmatrix} \right\} \right\rangle$$
$$= [A_s(h + c\varphi_0), f] - [h + c\varphi_0, A_s f] = 0.$$

Hence the righthand side of (6.4) is contained in S^*. This completes the proof.

Note that

$$\left[\begin{pmatrix} \psi_0 \\ 0 \end{pmatrix}, \begin{pmatrix} \varphi_0 \\ \delta \end{pmatrix} \right] = [\psi_0, \varphi_0]. \tag{6.5}$$

From (6.1) and (6.2) it follows that $Z \subset A$ if and only if $\delta = 0$ and $\{\varphi_0, \psi_0\} \in A_s$. Hence the condition (2.3) is equivalent to

$$\delta \neq 0 \qquad \text{or} \qquad \{\varphi_0, \psi_0\} \notin A_s. \tag{6.6}$$

Clearly, if $\delta = 0$ and $\{\varphi_0, \psi_0\} \notin A_s$ it follows from (6.3) that mul S is one-dimensional, and reduction to $\mathfrak{H} \ominus \text{mul } S$ gives us the situation considered in the previous section. (Note that this case occurs if $\varphi \in \text{dom } A$.) On the other hand, it follows from (6.3) that if $\delta \neq 0$ then S is an operator. Therefore we will assume in the rest of this section that

$$\delta \neq 0, \tag{6.7}$$

which is equivalent to (2.3) and S being an operator. In a similar manner as before, the form (6.4) in which the adjoint S^* is written is now used for the description of all canonical selfadjoint extensions of S.

Theorem 6.2. *Let A be a selfadjoint relation given by* (6.1)*, let the one-dimensional subspace Z be given by* (6.2) *and assume* (6.7)*. Then the Q-function $Q(l)$ of $S = A \cap Z^*$ and A satisfies*

$$\lim_{y\to\infty} \frac{\operatorname{Im} Q(iy)}{y} = |\delta|^2. \tag{6.8}$$

The canonical selfadjoint extensions $A(\tau)$, $\tau \in \mathbf{R} \cup \{\infty\}$, of $S = A \cap Z^*$ are given by $A(0) = A$ and for $\tau \neq 0$ by

$$\begin{aligned} A(\tau) = \Big\{ \Big\{ \begin{pmatrix} h \\ -c\delta \end{pmatrix}, \begin{pmatrix} A_s(h + c\varphi_0) - c\psi_0 \\ u \end{pmatrix} \Big\} &: h + c\varphi_0 \in \operatorname{dom} A_s, \\ c, u \in \mathbf{C}, u\bar{\delta} = c(1/\tau + [\psi_0, \varphi_0]) - [A_s(h + c\varphi_0), \varphi_0] &+ [h + c\varphi_0, \psi_0] \Big\}. \end{aligned} \tag{6.9}$$

Proof. It follows from (4.1) that $Q(l)$ satisfies (6.8). In order to prove (6.9) we apply Theorem 2.4. Consider an arbitrary element in $A(\tau)$ as given by (2.4) for $\tau \neq 0$, $1/\tau + [\psi_0, \varphi_0] \neq 0$, or by (2.5) for $1/\tau + [\psi_0, \varphi_0] = 0$, cf. (6.5). That is, consider an element of the form

$$\Big\{ \begin{pmatrix} f \\ 0 \end{pmatrix}, \begin{pmatrix} A_s f \\ u \end{pmatrix} \Big\} - c \Big\{ \begin{pmatrix} \varphi_0 \\ \delta \end{pmatrix}, \begin{pmatrix} \psi_0 \\ 0 \end{pmatrix} \Big\}. \tag{6.10}$$

If $1/\tau + [\psi_0, \varphi_0] \neq 0$, assume that $c \in \mathbf{C}$ satisfies

$$\begin{aligned} c(1/\tau + [\psi_0, \varphi_0]) &= \Big\langle \Big\{ \begin{pmatrix} f \\ 0 \end{pmatrix}, \begin{pmatrix} A_s f \\ u \end{pmatrix} \Big\}, \Big\{ \begin{pmatrix} \varphi_0 \\ \delta \end{pmatrix}, \begin{pmatrix} \psi_0 \\ 0 \end{pmatrix} \Big\} \Big\rangle \\ &= [A_s f, \varphi_0] - [f, \psi_0] + u\bar{\delta}. \end{aligned} \tag{6.11}$$

If $1/\tau + [\psi_0, \varphi_0] = 0$, then assume that

$$\begin{pmatrix} f \\ 0 \end{pmatrix} \in \operatorname{dom} S.$$

Note that then (6.11) is still satisfied due to (6.3). Define $h = f - c\varphi_0$, then $h + c\varphi_0 = f \in \operatorname{dom} A_s$ and $A_s f - c\psi_0 = A_s(h + c\varphi_0) - c\psi_0$. Therefore the element (6.10) has the form

$$\Big\{ \begin{pmatrix} h \\ -c\delta \end{pmatrix}, \begin{pmatrix} A_s(h + c\varphi_0) - c\psi_0 \\ u \end{pmatrix} \Big\}, \tag{6.12}$$

where c must satisfy

$$c(1/\tau + [\psi_0, \varphi_0]) = [A_s(h + c\varphi_0), \varphi_0] - [h + c\varphi_0, \psi_0] + u\bar{\delta}. \tag{6.13}$$

Hence $A(\tau)$ is contained in the righthand side of (6.9).

Conversely, consider an arbitrary element in the righthand side of (6.9) with $\tau \neq 0$. That is, consider an element of the form (6.12) where $c \in \mathbf{C}$ satisfies (6.13). Define $f = h + c\varphi_0$, then $f \in \operatorname{dom} A_s$ and the element (6.12) has the form (6.10). Moreover (6.11) is satisfied. Note that if $1/\tau + [\psi_0, \varphi_0] = 0$, then it follows from (6.11) and (6.3), that

$$\left\{ \begin{pmatrix} f \\ 0 \end{pmatrix}, \begin{pmatrix} A_s f \\ u \end{pmatrix} \right\} \in S.$$

Therefore, the righthand side of (6.9) is contained in the righthand side of (2.4) or of (2.5), respectively. This completes the proof.

Note that in Theorem 6.2 the relation $A(0) = A$ is the only canonical selfadjoint extension of $S = A \cap Z^*$, which is not an operator. All the other extensions $A(\tau)$, $\tau \in \mathbf{R} \cup \{\infty\}$, $\tau \neq 0$, are (densely defined) selfadjoint operators, which can also be immediately seen from (6.9). Moreover, it can be seen from (6.3) that $\operatorname{dom} A = \operatorname{dom} S$, cf. Proposition 4.1; comparing (6.4) and (6.9) we see that $\operatorname{dom} S^* = \operatorname{dom} A(\tau)$ for all $\tau \neq 0$, cf. Proposition 5.4. The Q-function $Q(l)$ of S and A is an exceptional function corresponding to the class $\mathbf{N}_0$; all selfadjoint extensions $A(\tau)$, $\tau \neq 0$, in (6.9) have a Q-function in $\mathbf{N}_0$. Recall that if we normalize $Q(l)$ and $Q_\tau(l)$ by $\operatorname{Re} Q(\mu) = 0$ and $\operatorname{Re} Q_\tau(\mu) = 0$ for some $\mu \in \mathbf{C} \setminus \mathbf{R}$, then the functions $Q(l)$ and $Q_\tau(l)$ are related by (3.17).

We can use this model to interpret some results concerning $\mathbf{N}_{-1}$ and $\mathbf{N}_{-2}$ functions, cf. [HS1]. Now the operator part A_s plays an important role in the descriptions. Moreover, we will present some transformation formulas for the corresponding moments in terms of the exceptional extension.

Using the special form (6.1) and (6.2) of A and Z, respectively, and rearranging terms in (3.3), we obtain

$$Q(l) - |\delta|^2 l = l[\varphi_0, \varphi_0] + [(A_s - l)^{-1}(l\varphi_0 - \psi_0), \bar{l}\varphi_0 - \psi_0]. \tag{6.14}$$

In the Hilbert space $(\mathfrak{H} \ominus \operatorname{mul} A)^2$ we introduce the, at most one-dimensional, subspace Z_0 by

$$Z_0 = \operatorname{span}\{\varphi_0, \psi_0\}. \tag{6.15}$$

We define the symmetric operator S_0 in the Hilbert space $\mathfrak{H} \ominus \operatorname{mul} A$ by $S_0 = A_s \cap Z_0^*$, i.e.,

$$S_0 = \big\{ \{f, A_s f\} : f \in \operatorname{dom} A_s,\ [A_s f, \varphi_0] - [f, \psi_0] = 0 \big\}. \tag{6.16}$$

Note that

$$S_0 = S \cap (\mathfrak{H} \ominus \operatorname{mul} A)^2.$$

If $Z_0 \subset A_s$, then we have the degenerate case where $S_0 = A_s$, and it follows from (6.14) that

$$Q(l) = |\delta|^2 l + [\varphi_0, \psi_0]. \tag{6.17}$$

Now we assume that $Z_0 = \operatorname{span}\{\varphi_0, \psi_0\}$ is one-dimensional and that

$$A_s \cap \operatorname{span}\{\varphi_0, \psi_0\} = \{0, 0\}. \tag{6.18}$$

Then S_0 is a closed symmetric operator in $\mathfrak{H} \ominus \operatorname{mul} A$ with defect numbers $(1, 1)$. By comparing the righthand side of (6.14) with (3.4), we obtain the following result.

Lemma 6.3. *The function $Q(l) - |\delta|^2 l$ is the Q-function of S_0 and A_s. It belongs to $\mathbf{N}_1$ or to $\mathbf{N}_0$ if and only if $\varphi_0 \in \operatorname{dom} |A_s|^{1/2}$ or $\varphi_0 \in \operatorname{dom} A_s$, respectively.*

The following result is obtained from [HS1, Propositions 3.2 and 4.2].

Corollary 6.4. *The Q-function $Q(l)$ of $S = A \cap Z^*$ and A is an exceptional function corresponding to $\mathbf{N}_{-1}$ or $\mathbf{N}_{-2}$, if and only if $\varphi_0 \in \operatorname{dom} |A_s|^{1/2}$ or $\varphi_0 \in \operatorname{dom} A_s$, respectively. In these cases the Q-functions of the selfadjoint extensions $A(\tau)$, $\tau \neq 0$, in* (6.9) *belong to $\mathbf{N}_{-1}$ or $\mathbf{N}_{-2}$, respectively.*

The expression for $A(\tau)$, $\tau \neq 0$, in (6.9) can be simplified in each of these cases, cf. Propositions 5.3 and 5.4. We will not pursue this, but instead, we will express the corresponding moments in terms of $Q(l)$. We observe that if $Q(l) - |\delta|^2 l \in \mathbf{N}_1$, then there exists a real limit

$$\eta = \lim_{y \to \infty} \big(Q(iy) - |\delta|^2 iy\big), \tag{6.19}$$

and that if $Q(l) - |\delta|^2 l \in \mathbf{N}_0$, then

$$\begin{aligned} m_0 &= \sup_{y>0} y \operatorname{Im}(Q(iy) - |\delta|^2 iy) = \lim_{y \to \infty} -iy\big(Q(iy) - |\delta|^2 iy - \eta\big) \\ &= \int_{\mathbf{R}} d\varrho(t) < \infty, \end{aligned} \tag{6.20}$$

and is positive, since we have assumed that $Q(l) - |\delta|^2 l$ does not reduce to a real constant. Denote the spectral function of $Q_\tau(l)$ (cf. the integral representation (4.2)) by $\sigma_\tau(t)$. Again we use the notation $q = \big(\operatorname{Im} Q(\mu)\big)^2$.

Proposition 6.5. *Let $\tau \in \mathbf{R} \cup \{\infty\}$, $\tau \neq 0$. The moments $m_0(\sigma_\tau)$ are given by*

$$m_0(\sigma_\tau) = \frac{\tau^2 q + 1}{\tau^2 |\delta|^2}. \tag{6.21}$$

If $Q(l) - |\delta|^2 l$ belongs to $\mathbf{N}_1$, then the moments $m_1(\sigma_\tau)$ are given by

$$m_1(\sigma_\tau) = -\frac{(\tau^2 q + 1)(\tau\eta + 1)}{\tau^3 |\delta|^4}. \tag{6.22}$$

Moreover, if $Q(l) - |\delta|^2 l$ belongs to $\mathbf{N}_0$, then the moments $m_2(\sigma_\tau)$ are given by

$$m_2(\sigma_\tau) = \frac{(\tau^2 q + 1)[(\tau\eta + 1)^2 + \tau^2 |\delta|^2 m_0]}{\tau^4 |\delta|^6}. \tag{6.23}$$

Proof. Clearly, $\lim_{y \to \infty} Q_\tau(iy) = 1/\tau$ and hence

$$iy(Q_\tau(iy) - 1/\tau) = -\frac{\tau^2 q + 1}{1/iy\big(\tau^2 Q(iy) + \tau\big)}.$$

Taking limits and using (6.8) and (i) of Proposition 4.4 gives (6.21). Now assume that $Q(l) - |\delta|^2 l$ belongs to $\mathbf{N}_{-1}$ and use the identity:

$$(iy)^2 \left(Q_\tau(iy) - \frac{1}{\tau} + \frac{\tau^2 q + 1}{iy\tau^2 |\delta|^2} \right) = iy \left(\frac{(\tau^2 q + 1)\big(\tau(Q(iy) - |\delta|^2 iy) + 1\big)}{\tau^2 |\delta|^2 \big(\tau Q(iy) + 1\big)} \right).$$

Hence, taking limits and using (6.8), (6.19), and (ii) of Proposition 4.4 gives (6.22). Now assume that $Q(l) - |\delta|^2 l$ belongs to $\mathbf{N}_0$ and use the identity:

$$\begin{aligned} (iy)^3 \left(Q(iy) - \frac{1}{\tau} + \frac{\tau^2 q + 1}{iy\tau^2 |\delta|^2} - \frac{(\tau^2 q + 1)(\tau\eta + 1)}{(iy)^2 \tau^3 |\delta|^4} \right) \\ = iy \left(\frac{(\tau^2 q + 1) iy \big(Q(iy) - |\delta|^2 iy - \eta\big) \tau^2 |\delta|^2}{\big(\tau Q(iy) + 1\big) \tau^3 |\delta|^4} \right) \\ - iy \left(\frac{(\tau^2 q + 1)(\tau\eta + 1)\big(\tau\big(Q(iy) - |\delta|^2 iy\big) + 1\big)}{\big(\tau Q(iy) + 1\big) \tau^3 |\delta|^4} \right). \end{aligned}$$

Again by taking limits and using (6.8), (6.19), (6.20), and (iii) of Proposition 4.4 yields (6.23). This completes the proof.

Finally, we will consider the linear fractional transform of $H(l) = Q(l) - |\delta|^2 l$. It is the Q-function of S_0 and A_s. Assume that it is normalized by $\operatorname{Re} H(\mu) = 0$. Then for each $\tau \in \mathbf{R} \cup \{\infty\}$ the Nevanlinna function $H_\tau(l)$ is defined by

$$H_\tau(l) = \frac{H(l) - \tau\big(\operatorname{Im} H(\mu)\big)^2}{\tau H(l) + 1}, \qquad \tau \in \mathbf{R} \cup \{\infty\}. \tag{6.24}$$

It is the Q-function of S_0 and the canonical selfadjoint extension $A_0(\tau)$ of S_0 in $\mathfrak{H} \ominus \operatorname{mul} A$, defined by

$$\begin{aligned} A_0(\tau) = \Big\{ &\{h, A_s(h + c\varphi_0) - c\psi_0\} : \; h + c\varphi_0 \in \operatorname{dom} A_s, \; c \in \mathbf{C}, \\ & c = \frac{[A_s(h + c\varphi_0), \varphi_0] - [h + c\varphi_0, \psi_0]}{1/\tau + [\psi_0, \varphi_0]} \Big\}, \end{aligned} \tag{6.25}$$

while for $1/\tau + [\psi_0, \varphi_0] = 0$ the canonical selfadjoint extension $A_0(\tau)$ is given by

$$\begin{aligned} A_0(\tau) = \big\{ &\{h, A_s(h + c\varphi_0) - c\psi_0\} : \; h + c\varphi_0 \in \operatorname{dom} A_s, \; c \in \mathbf{C}, \\ & [A_s(h + c\varphi_0), \varphi_0] - [h + c\varphi_0, \psi_0] = 0 \big\}. \end{aligned} \tag{6.26}$$

Note that $A(\tau)$ and $A_0(\tau)$ are related by

$$A_0(\tau) = \big\{ \{Pf, g\} : \{f, g\} \in A(\tau), \; g \in \mathfrak{H} \ominus \operatorname{mul} A \big\},$$

and that

$$A(\tau) \cap (\mathfrak{H} \ominus \operatorname{mul} A)^2 = S_0, \qquad \tau \neq 0.$$

7. Multiplication operators

In this section we consider a real-valued nondecreasing function ρ on $\mathbf{R}$ and associate with this function the Hilbert space $L^2(d\rho)$. Multiplication by the independent variable:

$$\mathscr{M}_\rho = \big\{ \{f, g\} \in \big(L^2(d\rho)\big)^2 : g = tf \big\},$$

is a densely defined selfadjoint operator, cf. [AG]. We will consider either this selfadjoint operator $\mathscr{M}_\rho$ in the Hilbert space $L^2(d\rho)$, or the selfadjoint relation

$$\mathscr{M}_\rho \oplus (\{0\} \oplus \mathbf{C}),$$

in the Hilbert space $L^2(d\rho) \oplus \mathbf{C}$. In each of these cases we will consider a symmetric restriction with defect numbers $(1, 1)$ and describe its selfadjoint extensions.

The operator case. Let $\mathfrak{H} = L^2(d\rho)$ and $A = \mathscr{M}_\rho$. Let $Z = \operatorname{span}\{\varphi, \psi\}$ be a one-dimensional subspace of $\mathfrak{H}^2$ which satisfies (2.3). Define the function ω by $\omega(t) = t\varphi(t) - \psi(t)$. The function ω does not vanish on $\mathbf{R}$ because of (2.3). Note that the function ω remains the same if the pair $\{\varphi, \psi\}$ is replaced by an equivalent pair. Moreover, pairs producing the same ω are equivalent. The function ω does not necessarily belong to $L^2(d\rho)$. In fact, we have

$$\varphi \in \operatorname{dom} |A|^{1/2} \quad \text{if and only if} \quad \varphi\bar{\omega} \in L^1(d\rho) \tag{7.1}$$
$$\text{if and only if} \quad \int_{\mathbf{R}} \frac{|\omega(t)|^2}{|t|+1}\, d\rho(t) < \infty,$$

and

$$\varphi \in \operatorname{dom} A \quad \text{if and only if} \quad \int_{\mathbf{R}} |\omega(t)|^2\, d\rho(t) < \infty. \tag{7.2}$$

Clearly, the conditions $\varphi \in \operatorname{dom} A$ and $A\varphi - \psi \in \operatorname{dom} |A|^{1/2}$ are equivalent to $\sqrt{|t|+1}\,\omega(t) \in L^2(d\rho)$ and the conditions $\varphi \in \operatorname{dom} A$ and $A\varphi - \psi \in \operatorname{dom} A$ are equivalent to $(|t|+1)\,\omega(t) \in L^2(d\rho)$.

For each $f \in \operatorname{dom} A$ the function $f\bar{\omega}$ is in $L^1(d\rho)$ and we denote the integral $\int_{\mathbf{R}} f\overline{\omega}\, d\rho$ by $[f, \omega]$, abusing the notation for the inner product in $L^2(d\rho)$. Observe that for each $f \in \operatorname{dom} A$

$$\langle \{f, Af\}, \{\varphi, \psi\} \rangle = [f, \omega]. \tag{7.3}$$

Let $h \in L^2(d\rho)$ and $c \in \mathbf{C}$, then clearly

$$th + c\omega \in L^2(d\rho) \quad \text{if and only if} \quad h + c\varphi \in \operatorname{dom} A. \tag{7.4}$$

Hence, in this case $(h + c\varphi)\overline{\omega}$ belongs to $L^1(d\rho)$ and the integral $\int_{\mathbf{R}} (h + c\varphi)\overline{\omega}\, d\rho$ is thus denoted by $[h + c\varphi, \omega]$.

We now express $S = A \cap Z^*$, S^* and the corresponding null spaces of $S^* - l$ in terms of the function ω. The following lemma is a restatement of (5.1), (5.2) and (3.1).

Lemma 7.1. *The symmetric operator S is given by*

$$S = \big\{ \{f, tf\} : f \in \operatorname{dom} \mathscr{M}_\rho,\ [f, \omega] = 0 \big\}. \tag{7.5}$$

The adjoint relation S^* is given by

$$S^* = \big\{ \{h, th + c\omega\} : c \in \mathbf{C},\ h, th + c\omega \in L^2(d\rho) \big\}. \tag{7.6}$$

In particular, S is not densely defined if and only if $\omega \in L^2(d\rho)$, in which case $\operatorname{mul} S^* = \operatorname{span}\{\omega\}$. *The null space* $\ker(S^* - l)$ *is spanned by*

$$\chi(l) = \frac{\omega}{t - l}, \qquad l \in \mathbf{C} \setminus \mathbf{R}. \tag{7.7}$$

We describe all canonical selfadjoint extensions of S by means of Theorem 5.2, applied to the case that $\mathfrak{H} = L^2(d\rho)$ and $A = \mathscr{M}_\rho$. Our description is in terms of restrictions of the adjoint S^* in (7.6).

Proposition 7.2. *All canonical selfadjoint extensions $A(\tau)$ of $S = A \cap Z^*$ are given by $A(0) = A$ and for $\tau \neq 0$ and $1/\tau + [\psi, \varphi] \neq 0$, by*

$$A(\tau) = \left\{ \{h, th + c\omega\} : c \in \mathbf{C},\ h, th + c\omega \in L^2(d\rho),\ c = \frac{[h + c\varphi, \omega]}{1/\tau + [\psi, \varphi]} \right\}. \tag{7.8}$$

If $1/\tau + [\psi, \varphi] = 0$, then $A(\tau)$ is given by

$$A(\tau) = \big\{ \{h, th + c\omega\} : c \in \mathbf{C},\ h, th + c\omega \in L^2(d\rho),\ [h + c\varphi, \omega] = 0 \big\}. \tag{7.9}$$

We now assume that $Q(l) \in \mathbf{N}_1$ and formulate the counterpart of Proposition 5.3 for the multiplication operator on $L^2(d\rho)$. Recall from Proposition 4.4 that the exceptional value τ corresponding to $Q(l)$ is given by $1/\tau + \gamma = 0$. For $h \in L^2(d\rho)$ for which $h\bar{\omega} \in L^1(d\rho)$, we denote the integral $\int_{\mathbf{R}} h\overline{\omega}\, d\rho$ by $[h, \omega]$, abusing the notation for the inner product in $L^2(d\rho)$. The case $Q(l) \in \mathbf{N}_0$ gives the same formal results.

Proposition 7.3. *Assume that $Q(l)$ belongs to $\mathbf{N}_1$. Then all canonical selfadjoint extensions $A(\tau)$ of $S = A \cap Z^*$ are given by $A(0) = A$ and for $\tau \neq 0$ and $1/\tau + \gamma \neq 0$, by*

$$\begin{aligned} A(\tau) = \Big\{ \{h, th + \frac{1}{1/\tau + \gamma}[h, \omega]\, \omega\} :& \\ h \in L^2(d\rho),\ h\bar{\omega} \in L^1(d\rho),\ th + \frac{1}{1/\tau + \gamma}[h, \omega]\, \omega \in L^2(d\rho) \Big\}.& \end{aligned} \tag{7.10}$$

These extensions are all operators. If $1/\tau + \gamma = 0$, then the exceptional canonical selfadjoint extension $A(\tau)$ is given by

$$\begin{aligned} A(\tau) = \big\{ \{h, th + c\,\omega\} :& \\ h \in L^2(d\rho),\ h\bar{\omega} \in L^1(d\rho),\ [h, \omega] = 0,\ th + c\,\omega \in L^2(d\rho) \big\}.& \end{aligned} \tag{7.11}$$

The extension $A(\tau)$, $1/\tau + \gamma = 0$, is not an operator if and only if $\omega \in L^2(d\rho)$, in which case $\operatorname{mul} S^* = \operatorname{span}\{\omega\}$.

The Q-function $Q(l)$ of S and A in (3.3) has an integral representation in terms of the measure $d\rho$. It is given by

$$Q(l) = [\psi, \varphi] + [\varphi, \psi] + \int_{\mathbf{R}} \Big(\frac{|\omega(t)|^2}{t - l} - t|\varphi(t)|^2 \Big)\, d\rho(t). \tag{7.12}$$

Observe that the function $t|\varphi|^2$ acts as a regularizing factor, which ensures the integrability of the integrand in (7.12). To see (7.12), observe that it follows from the definition of ω that

$$\frac{|\omega|^2}{t - l} - t|\varphi|^2 = l|\varphi|^2 - \varphi\overline{\psi} - \psi\overline{\varphi} + \frac{(l\varphi - \psi)(l\overline{\varphi} - \overline{\psi})}{t - l}.$$

Since φ and ψ belong to $L^2(d\rho)$ and $(t-l)^{-1}$ is bounded for $t \in \mathbf{R}$ it is clear that the righthand side belongs to $L^1(d\rho)$. Hence the integral in (7.12) is well-defined and the identity in (7.12) for $Q(l)$ follows from rewriting (3.4). We can characterize the Q-function $Q(l)$ in terms of the function $\omega(t)$ as follows:

(i) $Q(l)$ belongs to $\mathbf{N}_1$ if and only if $\omega(t)/\sqrt{|t|+1}$ belongs to $L^2(d\rho)$,
(ii) $Q(l)$ belongs to $\mathbf{N}_0$ if and only if $\omega(t)$ belongs to $L^2(d\rho)$,
(iii) $Q(l)$ belongs to $\mathbf{N}_{-1}$ if and only if $\sqrt{|t|+1}\,\omega(t)$ belongs to $L^2(d\rho)$,
(iv) $Q(l)$ belongs to $\mathbf{N}_{-2}$ if and only if $(|t|+1)\,\omega(t)$ belongs to $L^2(d\rho)$.

In these cases (7.12) can be rewritten as

$$Q(l) = \gamma + \int_{\mathbf{R}} \frac{|\omega(t)|^2}{t-l}\, d\rho(t). \tag{7.13}$$

In Proposition 1.4 we have given necessary and sufficient conditions for the existence of a Q-function in $\mathbf{N}_0$ or $\mathbf{N}_{-2}$, in terms of the symmetric operator S. In the present case of a multiplication operator on $L^2(d\rho)$ we obtain

(a) the function $Q(l)$ belongs to $\mathbf{N}_0$ if and only if $\operatorname{dom} S$ is not dense in $L^2(d\rho)$,
(b) the function $Q(l)$ belongs to $\mathbf{N}_{-2}$ if and only if $\operatorname{dom} A = \operatorname{dom} S + \operatorname{span}\{\omega\}$.

It is now possible to obtain similar results for the classes $\mathbf{N}_1$ and $\mathbf{N}_{-1}$. For this purpose, we define the Hilbert space $L^2_+(d\rho) \subset L^2(d\rho)$ as follows

$$L^2_+(d\rho) = L^2\big((|t|+1)d\rho\big).$$

Then $\operatorname{dom} A \subset L^2_+(d\rho)$ and $\operatorname{dom} A$ is dense in this Hilbert space. In addition we define the Hilbert space $L^2_+(S)$ as the closure of $\operatorname{dom} S$ in the space $L^2_+(d\rho)$.

Proposition 7.4. *We have*

(i) *the function* $Q(l)$ *belongs to* $\mathbf{N}_1$ *if and only if* $\operatorname{dom} S$ *is not dense in* $L^2_+(d\rho)$,
(ii) *the function* $Q(l)$ *belongs to* $\mathbf{N}_{-1}$ *if and only if* $L^2_+(d\rho) = L^2_+(S) + \operatorname{span}\{\omega\}$.

Proof. We prove (i) by showing that $\operatorname{dom} S$ is not dense in $L^2_+(d\rho)$ if and only if $\omega/\sqrt{|t|+1} \in L^2(d\rho)$. If $\omega/\sqrt{|t|+1} \in L^2(d\rho)$, then $h \in \operatorname{dom} S$ means that

$$0 = \int_{\mathbf{R}} h(t)\overline{\omega(t)}\, d\rho(t) = \int_{\mathbf{R}} h(t)\frac{\overline{\omega(t)}}{|t|+1}(|t|+1)\, d\rho(t).$$

Since $\omega/(|t|+1) \in L^2_+(d\rho)$ we conclude that $\operatorname{dom} S$ is not dense in $L^2_+(d\rho)$.

For the converse statement we assume that there exists a nontrivial $g_0 \in L^2_+(d\rho)$, such that for all $h \in \operatorname{dom} S$

$$\int_{\mathbf{R}} h(t)\overline{g_0(t)}(|t|+1)\, d\rho(t) = 0.$$

Since $\mathrm{dom}\, A$ is dense in $L^2_+(d\rho)$ there exists an element $f_0 \in \mathrm{dom}\, A$ for which

$$c_0 = \int_{\mathbf{R}} f_0(t)\overline{g_0(t)}(|t|+1)\, d\rho(t) \neq 0.$$

Clearly f_0 does not belong to $\mathrm{dom}\, S$. We define c_1 and $\omega_0(t)$ by

$$c_1 = \int_{\mathbf{R}} f_0(t)\overline{\omega(t)}\, d\rho(t), \qquad \omega_0(t) = \omega(t)/(|t|+1).$$

It follows that for every $f \in \mathrm{dom}\, A$

$$\int_{\mathbf{R}} f(t)\big(c_1\overline{g_0(t)} - c_0\overline{\omega_0(t)}\,\big)(|t|+1)\, d\rho(t) = 0, \tag{7.14}$$

as this is clear for $f = f_0$ and for $f \in \mathrm{dom}\, S$, and $\mathrm{dom}\, A$ is the span of f_0 and $\mathrm{dom}\, S$. Let Δ be a compact subinterval of $\mathbf{R}$. Let f be any function in $L^2_\Delta(d\rho)$ and extend f to all of $\mathbf{R}$ by setting it equal to zero outside Δ. Then $f \in \mathrm{dom}\, A$ and, hence, it follows from (7.14) that

$$\int_{\Delta} f(t)\big(c_1\overline{g_0(t)} - c_0\overline{\omega_0(t)}\,\big)(|t|+1)\, d\rho(t) = 0.$$

Therefore we conclude that $c_1\overline{g_0(t)} - c_0\overline{\omega_0(t)} = 0$ in Δ almost everywhere with respect to the measure $(|t|+1)d\rho(t)$. Note that here $\omega_0(t) = \big(t\varphi(t)-\psi(t)\big)/(|t|+1)$, restricted to Δ, belongs to $L^2_\Delta\big((|t|+1)d\rho\big)$. Since Δ is arbitrary we conclude that $c_1\overline{g_0(t)} - c_0\overline{\omega_0(t)} = 0$ almost everywhere with respect to $(|t|+1)d\rho(t)$. Now $c_0 \neq 0$ forces $\omega_0 \in L^2_+(d\rho)$, which is equivalent to $\omega/\sqrt{|t|+1} \in L^2(d\rho)$.

We prove (ii) by showing that $L^2_+(d\rho) = L^2_+(S) + \mathrm{span}\,\{\omega\}$ if and only if $\sqrt{|t|+1}\,\omega \in L^2(d\rho)$. If $\sqrt{|t|+1}\,\omega \in L^2(d\rho)$, then $\omega \in L^2_+(d\rho)$ and certainly $\omega/(|t|+1) \in L^2_+(d\rho)$. Moreover, in the sense of $L^2_+(d\rho)$ we have the orthogonal decomposition

$$\mathrm{dom}\, A = \mathrm{dom}\, S\, [+]\, \mathrm{span}\left\{\frac{\omega}{|t|+1}\right\}.$$

This implies that

$$L^2_+(d\rho) = L^2_+(S)\, [+]\, \mathrm{span}\left\{\frac{\omega}{|t|+1}\right\}.$$

Now $\omega \in L^2_+(d\rho)$ and $\omega \notin L^2_+(S)$, imply $L^2_+(d\rho) = L^2_+(S) + \mathrm{span}\,\{\omega\}$. The converse statement is obvious. This completes the proof.

We make some comments about the usual Riesz–Herglotz integral representation. For simplicity we assume that ω does not vanish on a set of positive $d\rho$-measure, and we associate with the measure $d\rho$ and the function ω a measure $d\sigma$ by $d\sigma = |\omega|^2 \, d\rho$. Since the function $\chi(i)$ belongs to $L^2(d\rho)$ (cf. Lemma 7.1), it follows that the measure $d\sigma$ satisfies the integrability condition

$$\int_{\mathbf{R}} \frac{d\sigma(t)}{t^2+1} < \infty. \tag{7.15}$$

In terms of the measure $d\sigma$, the function $Q(l)$ in (7.12) has the integral representation

$$Q(l) = \alpha + \int_{\mathbf{R}} \Big(\frac{1}{t-l} - \frac{t}{t^2+1} \Big) \, d\sigma(t),$$

where $\alpha \in \mathbf{R}$ is given by

$$\begin{aligned}\alpha = & \int_{\mathbf{R}} \frac{t}{t^2+1} \big(|\psi(t)|^2 - |\varphi(t)|^2 \big) \, d\rho(t) \\ & + \int_{\mathbf{R}} \frac{1}{t^2+1} \varphi(t)\overline{\psi(t)} \, d\rho(t) + \int_{\mathbf{R}} \frac{1}{t^2+1} \psi(t)\overline{\varphi(t)} \, d\rho(t).\end{aligned}$$

It follows from (7.12) that the function $Q(l)$ belongs to $\mathbf{N}_1$, $\mathbf{N}_0$, $\mathbf{N}_{-1}$, $\mathbf{N}_{-2}$ if and only if

$$\int_{\mathbf{R}} \frac{d\sigma(t)}{|t|+1} < \infty, \qquad \int_{\mathbf{R}} d\sigma(t) < \infty,$$
$$\int_{\mathbf{R}} (|t|+1) \, d\sigma(t) < \infty, \qquad \text{or} \qquad \int_{\mathbf{R}} (t^2+1) \, d\sigma(t) < \infty,$$

respectively, cf. [HS1]. In [HLS] an operator model was constructed involving the Hilbert space $L^2(d\sigma)$ and multiplication by the independent variable $\mathscr{M}_\sigma$ in that space. Let ι be the mapping that assigns to each function f on $\mathbf{R}$ a function of the form f/ω. Note that $\iota\omega = \mathbf{1}$. Then ι provides an isometric isomorphism between $L^2(d\rho)$ and $L^2(d\sigma)$; in addition the selfadjoint operators $\mathscr{M}_\rho$ and $\mathscr{M}_\sigma$ are isometrically isomorphic under ι. The symmetric operator S in $L^2(d\rho)$ given by (7.5) is isometrically isomorphic to the symmetric operator $\big\{ \{f, g\} \in \mathscr{M}_\sigma : [f, \mathbf{1}] = 0 \big\}$. If $\omega(t) = 1$, then the two measures coincide: $d\sigma = d\rho$ and ι is the identity mapping. If we start with a measure $d\rho$ which satisfies

$$\int_{\mathbf{R}} \frac{d\rho(t)}{t^2+1} < \infty,$$

then we can choose φ and ψ in $L^2(d\rho)$ such that $\omega = \mathbf{1}$. Take any $\psi \in L^2(d\rho)$, which behaves like $-1 + O(t)$ near 0. Then the function φ defined by $\varphi(t) = (\psi(t)+1)/t$ belongs to $L^2(d\rho)$. As we mentioned before any other pair giving the same $\omega = \mathbf{1}$ is equivalent to this choice.

The above descriptions are all stated in terms of the function $\omega(t)$, which does not necessarily belong to the Hilbert space $L^2(d\rho)$. However, if for instance $Q(l)$ belongs to $\mathbf{N}_1$, then $\omega(t)$ belongs to the Hilbert space $L^2_-(d\rho)$, where $L^2_-(d\rho)$ is the L^2 space with measure $d\rho(t)/(|t|+1)$, which contains the original Hilbert space $L^2(d\rho)$ as a proper dense subset. Its dual is the Hilbert space $L^2_+(d\rho)$, which is contained in the original Hilbert space $L^2(d\rho)$. The inner product of the Hilbert space $L^2(d\rho)$ can be extended to serve as a duality between these spaces. The results in the present section act as models for the interpretation of the previous results by means of specific triplets of Hilbert spaces. In general, this program is carried out for the case that $Q(l)$ belongs to $\mathbf{N}_1$ in [HKS] and for the case that $Q(l)$ satisfies less restrictive conditions in [HS2].

The multivalued case. Let $\mathfrak{H} = L^2(d\rho) \oplus \mathbf{C}$ and define $A = \mathscr{M}_\rho \oplus (\{0\} \oplus \mathbf{C})$. Let $Z \subset \mathfrak{H}^2$ be defined by

$$Z = \operatorname{span}\left\{ \begin{pmatrix} \varphi_0 \\ \delta \end{pmatrix}, \begin{pmatrix} \psi_0 \\ 0 \end{pmatrix} \right\},$$

with elements $\varphi_0, \psi_0 \in L^2(d\rho)$ and $\delta \in \mathbf{C}$. We assume that (6.7) is satisfied, which is equivalent to (2.3) and S being an operator. Define the function ω_0 by $\omega_0(t) = t\varphi_0(t) - \psi_0(t)$. The following lemma is just a translation of (6.3), (6.4) and (3.1).

Lemma 7.5. *The closed symmetric operator $S = A \cap Z^*$ is given by*

$$S = \left\{ \left\{ \begin{pmatrix} f \\ 0 \end{pmatrix}, \begin{pmatrix} tf \\ u \end{pmatrix} \right\} : f \in \operatorname{dom} \mathscr{M}_\rho,\ u\bar{\delta} + [f, \omega_0] = 0 \right\}. \tag{7.16}$$

Its adjoint S^* is given by

$$S^* = \left\{ \left\{ \begin{pmatrix} h \\ -c\delta \end{pmatrix}, \begin{pmatrix} th + c\omega_0 \\ v \end{pmatrix} \right\} : th + c\omega_0 \in L^2(d\rho),\ c, v \in \mathbf{C} \right\}. \tag{7.17}$$

The null space $\ker(S^* - l)$ *is spanned by*

$$\chi(l) = \begin{pmatrix} \omega_0/(t-l) \\ \delta \end{pmatrix}, \qquad l \in \mathbf{C} \setminus \mathbf{R}. \tag{7.18}$$

As before, the form (7.17) is now used for the description of all canonical selfadjoint extensions of S, cf. Theorem 6.2.

Proposition 7.6. *The canonical selfadjoint extensions $A(\tau)$, $\tau \in \mathbf{R} \cup \{\infty\}$, of $S = A \cap Z^*$ are given by $A(0) = A$ and for $\tau \neq 0$ by*

$$\begin{aligned} A(\tau) = \Bigg\{ \left\{ \begin{pmatrix} h \\ -c\delta \end{pmatrix}, \begin{pmatrix} th + c\omega_0 \\ u \end{pmatrix} \right\} &: th + c\omega_0 \in L^2(d\rho),\ c, u \in \mathbf{C}, \\ & u\bar{\delta} = c(1/\tau + [\psi_0, \varphi_0]) - [h + c\varphi_0, \omega_0] \Bigg\}. \end{aligned} \tag{7.19}$$

We give an integral representation of the Q-function $Q(l)$ in terms of the measure $d\rho$ and the constant δ in (6.2). It follows from (6.8) and (6.14) that the Q-function $Q(l)$ in (3.3) of $S = A \cap Z^*$ and A is given by

$$Q(l) = [\psi_0, \varphi_0] + [\varphi_0, \psi_0] + |\delta|^2 l + \int_{\mathbf{R}} \Big(\frac{|\omega_0(t)|^2}{t-l} - t|\varphi_0(t)|^2 \Big)\, d\rho(t). \tag{7.20}$$

The function $H(l) = Q(l) - |\delta|^2 l$ can be further characterized in terms of the function ω_0 by means of (6.14):
(i) $H(l)$ belongs to $\mathbf{N}_1$ if and only if $\omega_0(t)/\sqrt{|t|+1}$ belongs to $L^2(d\rho)$,
(ii) $H(l)$ belongs to $\mathbf{N}_0$ if and only if $\omega_0(t)$ belongs to $L^2(d\rho)$
If $H(l) \in \mathbf{N}_1$, then

$$H(l) = \gamma_0 + \int_{\mathbf{R}} \frac{|\omega_0(t)|^2}{t-l}\, d\rho(t), \tag{7.21}$$

where $\gamma_0 = [\psi_0, \varphi_0] + [\varphi_0, \psi_0] - [t\varphi_0, \varphi_0]$. In this case the conditions in (7.19) of Proposition 7.6:

$$th + c\omega_0 \in L^2(d\rho), \qquad u\bar{\delta} = c(1/\tau + [\psi_0, \varphi_0]) - [h + c\varphi_0, \omega_0],$$

are equivalent to

$$h\bar{\omega}_0 \in L^1(d\rho), \qquad u\bar{\delta} = c(1/\tau + \gamma_0) - [h, \omega_0].$$

Note that it follows from (7.17) that $\binom{0}{1}$ spans mul S^*. Moreover, we see directly from (7.17) that $\omega_0 \in L^2(d\rho)$ if and only if $\binom{0}{1} \in$ dom S^*. Hence, we have proved $H(l) \in \mathbf{N}_0$ if and only if mul $S^* \subset$ dom S^*. We have mentioned in Corollary 6.4, that $H(l) \in \mathbf{N}_0$ if and only if $Q_\tau(l) \in \mathbf{N}_{-2}$ for $\tau \neq 0$, cf. Proposition 1.4. Similar comments are valid when $H(l) \in \mathbf{N}_1$, in which case again space triplets are needed.

Also in this case it is possible to reduce the integral representation to the usual Riesz–Herglotz representation. Assume for simplicity that ω_0 does not vanish on a set of positive $d\rho$-measure. Then we associate with the measure $d\rho$ and the function ω_0 the measure $d\sigma_0$, $d\sigma_0 = |\omega_0|^2\, d\rho$. The measure $d\sigma_0$ satisfies the integrability condition

$$\int_{\mathbf{R}} \frac{d\sigma_0(t)}{t^2+1} < \infty,$$

cf. (7.18), and the Q-function $Q(l)$ in (7.20) has the integral representation

$$Q(l) = \alpha + \beta l + \int_{\mathbf{R}} \Big(\frac{1}{t-l} - \frac{t}{t^2+1} \Big)\, d\sigma(t), \tag{7.22}$$

where $\beta = |\delta|^2$ and $\alpha \in \mathbf{R}$ is given by

$$\alpha = \int_{\mathbf{R}} \frac{t}{t^2+1} \left(|\psi_0(t)|^2 - |\varphi_0(t)|^2 \right) d\rho(t) + \int_{\mathbf{R}} \frac{1}{t^2+1} \varphi_0(t) \overline{\psi_0(t)} \, d\rho(t) + \int_{\mathbf{R}} \frac{1}{t^2+1} \psi_0(t) \overline{\varphi_0(t)} \, d\rho(t).$$

Again, an isometric isomorphism between the various spaces and operators can be made explicit.

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