Deficiency indices of operator polynomials in creation and annihilation operators

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We present a new method to compute deficiency indices of operators that are homogeneous polynomials in one pair of creation and annihilation operators. To this end we prove a classification theorem for special cubic forms by means of $SU(1,1)$ transformations and derive new non-selfadjointness criteria for Jacobi-like matrices. The method presented illuminates and systemizes former results of Rabsztyn.

1 Introduction

Creation and annihilation operators were originally introduced in quantum mechanics to diagonalize the harmonic oscillator and are now an indispensable tool in quantum theory being the building blocks for more complicated operators. Here we present a new method for computing the deficiency indices of symmetric operators that are homogeneous polynomials of degree three in one pair of those operators. Deficiency indices measure how far a symmetric operator (sometimes especially in physics literature also called hermitian or hermitian symmetric operator) is from being self-adjoint. To know them and, hence, to be able to decide whether or not a symmetric operator is self-adjoint is important in physical applications because different self-adjoint extensions of the same operator yield different descriptions of the system under consideration (see [10, X.1] for examples). The opposition of self-adjointness and non self-adjointness, which is important in quantum mechanics, is reflected in classical mechanics where the latter corresponds to a particle that will escape to infinity within a finite time whereas in the first case it will not (see [10, App. X.1] for a detailed discussion of this analogy and its validity).

Assume we are given a Fock representation of the canonical commutation relations (CCR), i.e. a linear operator $a : D \to \mathcal{H}$ acting along with its adjoint $a^* : D \to \mathcal{H}$ on some dense subspace $D \subset \mathcal{H}$ of a Hilbert space $\mathcal{H}$ and satisfying on D

$$aa^* - a^*a = \mathbb{1}.$$

Accessorily, there is a so-called vacuum vector $\Omega \in D$, $\Omega \neq 0$, such that $a\Omega = 0$ and $D_0 := \operatorname{span}\{(a^*)^n\Omega | n \in \mathbb{N}_0\}$ is dense in $\mathcal{H}$. From a and a^* one can build polynomials of which the harmonic oscillator $a^*a + \mathbb{1}$ is the most prominent example. It is essentially self-adjoint on D_0 as are all operators being symmetric polynomials of degree one and two. This result can be proved via the (sufficient) Carleman criterion for Jacobi matrices (see e.g. [1, p. 24]), which unfortunately fails to prove self-adjointness for degrees greater than two. Berezanski's criterion (see Theorem 3.1 below) suggests that from degree three onward self-adjointness will not be the rule. Some special cases of higher degrees have been considered thus far. The anharmonic oscillator being of degree four and serving as toy model for interacting quantum fields is proven to be self-adjoint. Various methods of proof are presented in [10, Chap. X]. For general polynomials up to degree four self-adjointness was established in the special case of semi-bounded operators by Jørgensen [5], who generalized Wouk's theorem on semi-bounded Jacobi matrices (see [13] or [1, p. 26]) to arbitrary semi-bounded operators. His result is representative in that it is based upon some positivity or semi-boundedness property. Since for degree three the operators cannot be semi-bounded at all Jørgensen's as all the other former results leaves a gap which we shall bridge by exhaustively computing the deficiency indices of the operator

$$A(\alpha_3, \alpha_1) := \alpha_3 a^3 + 3\alpha_1 a^* a^2 + 3\bar{\alpha}_1 (a^*)^2 a + \bar{\alpha}_3 (a^*)^3,\ \alpha_1, \alpha_3 \in \mathbb{C}, \tag{1}$$

on a slightly larger domain $D \supset D_0$ to be specified later. At this point we may assume without loss of generality $\alpha_1 = 1$. Our main result (see Theorem 2.3) is that each operator $A(\alpha, 1)$ can be linked to exactly one out of four normal forms

$$A(1,0), \quad A(0,1), \quad A(-3,1), \quad A(1,1) \tag{2}$$

having deficiency indices $3, 1, 1, 0$, respectively. To which normal form an operator belongs depends, basically, on the sign of the discriminant of a cubic form. Amazingly, we shall see below that the last case of a self-adjoint operator, which is the most eligible one for physicists, occurs very rarely.

To have our operator cast into its normal form we employ a special kind of unitary transformations, the so-called Bogolyubov or canonical transformations, which formally replace a and a^* according to

$$a \mapsto sa + ta^*, \quad a^* \mapsto \bar{t}a + \bar{s}a^*, \quad s, t \in \mathbb{C} \text{ with } |s|^2 - |t|^2 = 1,$$

and thus transforming the entire operator like

$$A(\alpha, 1) \mapsto A(\tilde{\alpha}_3, \tilde{\alpha}_1) + ra + \bar{r}a^*, \quad r \in \mathbb{C}, \tag{3}$$

wherein the linear terms are due to the CCR. The main part behaves like an (ordinary) cubic form

$$\alpha x^3 + 3x^2 y + 3xy^2 + \bar{\alpha} y^3, \quad x, y \in \mathbb{C},$$

under an $SU(1,1)$ transformation. The normal forms of this cubic form can be classified by means of the discriminant $D(\alpha)$ and are labeled by $D(\alpha) > 0$ and $D(\alpha) < 0$, which we call main cases, and by $D(\alpha) = 0$, the exceptional cases, which require additionally the quadratic discriminant $Q(\alpha)$.

In the second step we compute the deficiency indices of the normal forms. We treat the exceptional cases in the $L^2(\mathbb{R})$ representation via solving ordinary differential equations. The main cases are best understood in the $l^2(\mathbb{N}_0)$ representation where $A(\alpha_3, \alpha_1)$ becomes a band matrix and the deficiency equation is a difference equation. For $D(\alpha) > 0$ we are faced even only with a Jacobi, i.e. tridiagonal matrix, wherefore we can refer to a classical result due to Berezanski. The case $D(\alpha) < 0$ requires a new criterion. Because of the linear terms in (3) we have a tridiagonal matrix added to a larger band matrix which makes Berezanski's theorem inapplicable. We would like to remark that possibly contrary to one's intuition these linear terms cannot be considered a small perturbation to $A(\tilde{\alpha}_3, \tilde{\alpha}_1)$ whence we cannot use the Kato-Rellich theorem (see [10, Th. X.12], [12, Th. 6.1]). For even though the inequality

$$\|(ra + \bar{r}a^*)\varphi\|^2 \le \gamma \|(a^3 + (a^*)^3)\varphi\|^2 + \delta \|\varphi\|^2$$

can be proved the necessary condition $\gamma < 1$ can be ensured if and only if r is small [6].

The deficiency indices of $A(\alpha_3, \alpha_1)$ were formerly computed by Rabsztyn [8], who worked in the $L^2(\mathbb{R})$ realization by which means the deficiency equation becomes an ordinary differential equation. To examine this equation he consults the theory of asymptotic solutions instead of deriving exact solutions. However, though this reduces heavily the amount of calculations to be carried out there are a lot of cases to be distinguished, cases that have nothing to do with the normal forms above. Therefore, the actual origin of the deficiency indices is obscured and it seems to be difficult to generalize the method to higher powers in a systematic way. Contrary to this the method presented here explains the distribution of the deficiency indices in a more natural way by an algebraic criterion which can be generalized to forms of higher degree even though the computational difficulties will increase.

2 Setting and results

Let $\mathcal{H}$ be a separable complex Hilbert space. For a symmetric operator $A : D(A) \to \mathcal{H}$, $D(A) \subset \mathcal{H}$ a dense subspace, the deficiency indices (see e.g. [10, Ch. X]) are the numbers $n_\pm(z) := \dim\ker(A^* \mp z\mathbb{1})$, $\operatorname{Im} z > 0$, with A^* being the adjoint operator and $\mathbb{1}$ the identity. Since $n_\pm(z)$ is constant in the upper and lower half-plane, respectively, we may simply write $n_\pm$. A symmetric operator is essentially self-adjoint if and only if $n_\pm = 0$.

A Fock representation with one degree of freedom of the CCR in $\mathcal{H}$ is given by two operators a and a^* satisfying the following conditions:

1. $a, a^* : D \to \mathcal{H}$ with $D \subset \mathcal{H}$ being a dense subspace and $aD \subset D$ and $a^*D \subset D$.
2. a^* is the adjoint operator to a.
3. $aa^*\varphi - a^*a\varphi = \varphi$ for all $\varphi \in D$.
4. There is an $\Omega \in D$, $\Omega \neq 0$, such that $a\Omega = 0$ and $D_0 := \operatorname{span}\{(a^*)^n\Omega | n \in \mathbb{N}_0\}$ is dense in $\mathcal{H}$.

For details and generalizations see [3]. In the sequel we shall work with the Fock representation in $l^2(\mathbb{N}_0)$ and $L^2(\mathbb{R})$.

Let $\mathcal{H} = l^2(\mathbb{N}_0)$, i.e. the Hilbert space of sequences

$$c = (c_0, c_1, c_2, \ldots),\ c_n \in \mathbb{C},\ \sum_{n=0}^{\infty} |c_n|^2 < \infty.$$

Then, the operators

$$(ac)_k = \sqrt{k+1}c_{k+1}, \quad (a^*c)_k = \sqrt{k}c_{k-1},\ k \in \mathbb{N}_0 \tag{4}$$

provide a Fock representation with vacuum vector $\Omega = (1, 0, \ldots)$. Here and henceforth a negative index as in c_{-1} always requires $c_{-1} := 0$. We choose as domain of definition

$$D := \{c = (c_0, c_1, \ldots) \in l^2 \mid \forall \kappa \in \mathbb{N} : \sup_{n \in \mathbb{N}_0} n^\kappa |c_n| < \infty\}. \tag{5}$$

Lemma 2.1. *Let the symmetric k-th order difference operator $A : D \to l^2(\mathbb{N}_0)$ be given by*

$$(Ac)_n := a_n^{(0)} c_n + \sum_{j=1}^{k} (a_n^{(j)} c_{n+j} + \bar{a}_{n-j}^{(j)} c_{n-j}) \tag{6}$$

the coefficients obeying $a_n^{(j)} = O(n^\gamma)$ with some $\gamma \geq 0$. Then $D(A^*) = D^*$ where

$$D^* := \{c \in l^2(\mathbb{N}_0) | \sum_{n=0}^{\infty} |a_n^{(0)} c_n + \sum_{j=1}^{k} (a_n^{(j)} c_{n+j} + \bar{a}_{n-j}^{(j)} c_{n-j})|^2\}. \tag{7}$$

The deficiency indices of A are given by the number of linearly independent solutions to the difference equation

$$a_n^{(0)} c_n + \sum_{j=1}^{k} (a_n^{(j)} c_{n+j} + \bar{a}_{n-j}^{(j)} c_{n-j}) = \lambda c_n \tag{8}$$

that lie in $l^2(\mathbb{N}_0)$. In particular this the number of linearly independent initial conditions $(c_0, \ldots, c_{k-1})$ that yield $l^2(\mathbb{N}_0)$ solutions to (8).

Proof. Write down the quadratic form

$$(Ac, d) = \sum_{n=0}^{\infty} (a_n^{(0)} c_n + \sum_{j=1}^{k} (a_n^{(j)} c_{n+j} + \bar{a}_{n-j}^{(j)} c_{n-j})) \bar{d}_n$$

and note that because of the growth condition the order of summation may be interchanged. Thus $d \in D^*$ is only subject to the condition in (7).

The first statement concerning the deficiency indices follows immediately from the first part of the lemma. The second statement is a consequence of the fact that we can choose exactly $c_0, \ldots, c_{k-1}$ as initial values in (8) (note $c_j = 0$ for $j < 0$). □

Under certain conditions the Fock representation of the CCR is unique up to unitary transformations [7, § 4.14], [3, Th. 1.4]. We can conversely exploit this fact to construct a unitary transform by putting

$$b := sa + ta^*, \ b^* := \bar{t}a + \bar{s}a^*$$

with $s, t \in \mathbb{C}$, $|s|^2 - |t|^2 = 1$. Note that s and t are chosen in such a way that b and b^* satisfy the CCR. Now it is crucial that there is $\tilde{\Omega} \in D$, $\tilde{\Omega} \neq 0$, obeying $b\tilde{\Omega} = 0$. This was one of the reasons why we wanted a and a^* to act on D in (5) instead of just D_0. We thus have the following

Theorem 2.2. *The Bogolyubov or canonical transform* $U(s,t) : \mathcal{H} \to \mathcal{H}$ *depending on two parameters* $s, t \in \mathbb{C}$ *with* $|s|^2 - |t|^2 = 1$ *is a unitary operator, which maps* D *into itself and transforms* a *and* a^* *according to*

$$U(s,t)aU(s,t)^* = sa + ta^*, \; U(s,t)a^*U(s,t)^* = \bar{t}a + \bar{s}a^*.$$

Finally, we describe the Fock representation in $L^2(\mathbb{R})$ with underlying Hilbert space $\mathcal{H} = L^2(\mathbb{R})$. Taking the Hermite functions as a basis for $L^2(\mathbb{R})$ yields a Hilbert space isomorphism between $L^2(\mathbb{R})$ and $l^2(\mathbb{N}_0)$ (see [9, Appendix to V.3]) whereby everything carries over from $l^2(\mathbb{N}_0)$ to $L^2(\mathbb{R})$ without further ado. In particular $D = \mathcal{S}(\mathbb{R})$, the Schwartz space, and

$$a = \frac{1}{\sqrt{2}}(x + \frac{d}{dx}), \quad a^* = \frac{1}{\sqrt{2}}(x - \frac{d}{dx}). \tag{9}$$

Now everything is at hand to formulate our main result, the following classification for the deficiency indices of $A(\alpha_3, \alpha_1)$, which exactly mirrors the classification of cubic forms in Theorem A.4.

Theorem 2.3. *For* $\alpha_1 = 0$ *we have* $n_\pm = 3$*. For* $\alpha_1 \neq 0$ *put* $\alpha := \alpha_3\bar{\alpha}_1/\alpha_1$ *and let* $D(\alpha) := 27(-|\alpha|^4 + 6|\alpha|^2 - 4(\alpha + \bar{\alpha}) + 3)$ *be the cubic and* $Q(\alpha) := 4(1-\alpha)$ *be the quadratic discriminant. Then* $A(\alpha_3, \alpha_1)$ *has the following deficiency indices:*

1. $D(\alpha) < 0$: $n_\pm = 3$.
2. $D(\alpha) > 0$: $n_\pm = 1$.
3. $D(\alpha) = 0$, $Q(\alpha) \neq 0$: $n_\pm = 1$.
4. $D(\alpha) = Q(\alpha) = 0$: $n_\pm = 0$.

When $D(\alpha) \neq 0$ *the corresponding cases are referred to as main cases otherwise as exceptional cases.*

Proof. First of all we see by applying $U(-1,0)$ that $n_+ = n_-$. For $\alpha_1 = 0$ the statement then follows from Proposition 3.2. Assume now $\alpha_1 \neq 0$. By dint of $U(\bar{\alpha}_1/|\alpha_1|, 0)$ we conclude that $A(\alpha_3\bar{\alpha}_1/\alpha_1^2, 1)$ has the same deficiency indices as $A(\alpha_3, \alpha_1)$. Due to the CCR

$$U(s,t)A(\alpha,1)U(s,t) = A(\tilde{\alpha}_3, \alpha_1) + ra + \bar{r}a^*$$

where the cubic part of the operator behaves like the ordinary cubic form

$$\alpha x^3 + 3x^2y + 3xy^2 + \bar{\alpha}y^3$$

under a map from $SU(1,1)$. Hence, Theorem A.4 in the appendix shows that $A(\alpha, 1)$ is unitarily equivalent to exactly one of the operators

$$A(1,0) + ra + \bar{r}a^*, \quad A(0,1) + ra + \bar{r}a^*, \quad A(-3,1) + ra + \bar{r}a^*, \quad A(1,1) + ra + \bar{r}a^*$$

whose deficiency indices are given in Propositions 3.2, 3.4, 4.1, 4.2. □

The interested reader may want to draw a picture showing the curve $D(\alpha) = 0$ by himself to visualize the regions of the deficiency indices.

3 Deficiency indices: main cases

We start with $D(\alpha) > 0$. The operator to be considered is $A(0,1) + ra + \bar{r}a^*$ whose deficiency equation in $l^2(\mathbb{N}_0)$ reads

$$\sqrt{n+1}(n+r)c_{n+1} + \sqrt{n}(n-1+\bar{r})c_{n-1} = \lambda c_n, \quad n \in \mathbb{N}_0, \tag{10}$$

which can be treated by a classical result due to Berezanski (see [2, p. 507] or [1, p. 26]).

Theorem 3.1 (Berezanski). *Let $b_n \in \mathbb{R}$ and $a_n \in \mathbb{C}$, $n \in \mathbb{N}_0$, such that*

$$|b_n| \leq M < \infty,\ n \in \mathbb{N}_0 \text{ and } a_n \neq 0,\ |a_{n-1}||a_{n+1}| \leq |a_n|^2,\ n \geq n_0,\ \sum_{n=n_0}^{\infty} \frac{1}{|a_n|} < \infty$$

with $M \geq 0$ and some $n_0 \in \mathbb{N}_0$. Then c defined by $c_0 := 1$ and

$$a_n c_{n+1} + b_n c_n + \bar{a}_{n-1} c_{n-1} = \lambda c_n, \quad n \geq 0,$$

is in $l^2(\mathbb{N}_0)$ for all $\lambda \in \mathbb{C}$.

This theorem can be applied immediately to our situation.

Proposition 3.2. *The sequence defined by (10) is in $l^2(\mathbb{N}_0)$. In particular, for all $r \in \mathbb{C}$ the operator $A(0,1) + ra + \bar{r}a^*$ has deficiency indices $(1,1)$.*

Proof. Here $a_n = \sqrt{n+1}(n+r)$ and $b_n = 0$ whence a simple application of the inequality of the geometric and the arithmetic mean shows the assumptions of Theorem 3.1 being satisfied. Setting $k = 1$ and $c_0 = 1$ in Lemma 2.1 and using (10) prove the proposition. □

We turn to the case $D(\alpha) < 0$ with the corresponding operator $A(1,0) + ra + \bar{r}a^*$ having in $l^2(\mathbb{N}_0)$ the deficiency equation

$$\sqrt{(n+1)(n+2)(n+3)}c_{n+3} + r\sqrt{n+1}c_{n+1} + \bar{r}\sqrt{n}c_{n-1} + \sqrt{n(n-1)(n-2)}c_{n-3} = \lambda c_n. \tag{11}$$

We abbreviate

$$a_n := \sqrt{(n+1)(n+2)(n+3)}, \quad b_n := r\sqrt{n+1}, \quad n \in \mathbb{N}_0. \tag{12}$$

To begin with we introduce the auxiliary quantities e_n via

$$a_n e_{n+3} = a_{n-3} e_{n-3}, \quad n \geq 3, \quad e_0 = \cdots = e_5 = 1. \tag{13}$$

We need the asymptotics of e_n.

Lemma 3.3. *There are constants $K_j > 0$, $j = 0, \ldots, 5$, such that*

$$e_{6k+j} = \frac{K_j}{(k+1)^{3/4}} + O\left(\frac{1}{(k+1)^{7/4}}\right), \quad k \in \mathbb{N}_0, \quad j = 0, \ldots, 5.$$

Proof. From the recursion formula (13) one can derive an explicit representation of the e_n. Then Stirling's formula yields the asymptotics. $\square$

We put

$$c_n = \tau_n e_n d_n \quad \text{with} \quad \tau_{6k+j} = \tau_j, \; j = 0, \ldots, 5 \tag{14}$$

and τ_j to be fixed below. Inserting this into (11) yields:

$$d_{n+3} + \beta_n d_{n+1} - \gamma_n d_n + \delta_n d_{n-1} + d_{n-3} = 0 \tag{15}$$

where we have abbreviated

$$\beta_n := \frac{b_n \tau_{n+1} e_{n+1}}{a_{n+3} \tau_{n+3} e_{n+3}}, \quad \gamma_n := \frac{\lambda \tau_n e_n}{a_{n-3} \tau_{n-3} e_{n-3}}, \quad \delta_n := \frac{\bar{b}_{n-1} \tau_{n-1} e_{n-1}}{a_{n-3} \tau_{n-3} e_{n-3}}. \tag{16}$$

From the above lemma we conclude

$$\left| \frac{\tau_n e_n}{\tau_{n-3} e_{n-3}} \right| \leq M < \infty \tag{17}$$

for $n \geq 3$ and, having chosen $\tau_0, \ldots, \tau_5$ appropriately,

$$\frac{\tau_{n+1} e_{n+1}}{\tau_{n+3} e_{n+3}} = 1 + O\left(\frac{1}{n}\right), \quad \frac{\tau_{n-1} e_{n-1}}{\tau_{n-3} e_{n-3}} = 1 + O\left(\frac{1}{n}\right) \tag{18}$$

as $n \to \infty$. From (18) and (17) we know

$$\beta_n, \delta_n = O\left(\frac{1}{n}\right), \quad \gamma_n = O\left(\frac{1}{n^{3/2}}\right).$$

By introducing

$$S_n := \begin{pmatrix} 0 & -\beta_n & \gamma_n & -\delta_n & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

and $y_n := (d_{n+2}, \ldots, d_{n-3})^T$ we can write (15) in matrix form

$$y_{n+1} = S_n y_n. \tag{19}$$

Now consider

$$y_{n+6} = S_{n+5} S_{n+4} S_{n+3} S_{n+2} S_{n+1} S_n y_n \tag{20}$$

instead of (19) and decompose the matrix product into

$$y_{n+6} = V_n' y_n + W_n' y_n$$

where

$$V_n' := \begin{pmatrix} -1 & 0 & \beta_{n+5} & 0 & \delta_{n+5} & 0 \\ 0 & -1 & 0 & \beta_{n+4} & 0 & \delta_{n+4} \\ -\delta_{n+3} & 0 & -1 & 0 & \beta_{n+3} & 0 \\ 0 & -\delta_{n+2} & 0 & -1 & 0 & \beta_{n+2} \\ -\beta_{n+1} & 0 & -\delta_{n+1} & 0 & -1 & 0 \\ 0 & -\beta_n & 0 & -\delta_n & 0 & -1 \end{pmatrix}$$

contains the terms up to order $1/n$ and W_n' the remaining products. We can further simplify V_n' by replacing $\beta_n, \ldots, \beta_{n+5}$ and $\delta_n, \ldots, \delta_{n+5}$ to first order by $\bar{r}/n$:

$$y_{n+6} = (-\mathbb{1} + \frac{1}{n} V) y_n + W_n y_n \tag{21}$$

with the skew-symmetric matrix

$$V := \begin{pmatrix} 0 & 0 & r & 0 & \bar{r} & 0 \\ 0 & 0 & 0 & r & 0 & \bar{r} \\ -\bar{r} & 0 & 0 & 0 & r & 0 \\ 0 & -\bar{r} & 0 & 0 & 0 & r \\ -r & 0 & -\bar{r} & 0 & 0 & 0 \\ 0 & -r & 0 & -\bar{r} & 0 & 0 \end{pmatrix}.$$

The correcting terms are contained in $W_n = (W_n^{jk})_{j,k=1,\ldots,6}$ and obey

$$W_n^{jk} = O\left(\frac{1}{n^{3/2}}\right), \quad j,k = 1, \ldots, 6. \tag{22}$$

Now we can prove the following

Proposition 3.4. *For all $r \in \mathbb{C}$ and all initial values c_0, c_1, c_2 every solution to* (11) *is in $l^2(\mathbb{N}_0)$. In particular, the operator $A(1,0) + ra + \bar{r}a^*$ has deficiency indices* $(3,3)$.

Proof. Because of the asymptotics of e_n in Lemma 3.3 it suffices to show that the d_n in (14) are bounded. To this end we prove boundedness of y_n in the euclidean norm $\|\cdot\|_2$ on $\mathbb{C}^6$. We have from (21)

$$\|y_{n+6}\|_2 \leq \|(-\mathbb{1} + \frac{1}{n} V) y_n\|_2 + \|W_n y_n\|_2.$$

Now note that V has purely imaginary eigenvalues and can be diagonalized by a unitary matrix U, $V = U^* \Delta U$. We obtain:

$$\|V_n y_n\|_2 = \|U^*(-\mathbb{1} + \frac{1}{n}\Delta) U y_n\|_2 \leq \left(1 + \frac{\rho}{2}\frac{1}{n^2}\right) \|y_n\|$$

with some $\rho \geq 0$. The second norm may be estimated with less care:

$$\|W_n y_n\|_2 \leq \frac{K}{n^{3/2}} \|y_n\|_2$$

with some constant $K > 0$ resulting from (22). We thus have:

$$\|y_{n+6}\|_2 \leq \left(1 + \frac{\rho}{2}\frac{1}{n^2} + \frac{K}{n^{3/2}}\right) \|y_n\|_2$$

wherefrom we derive inductively:

$$\|y_{6(k+1)+3}\|_2 \leq \prod_{l=0}^{k} \left(1 + \frac{\rho}{2}\frac{1}{(6l+3)^2} + \frac{K}{(6l+3)^{3/2}}\right) \|y_3\|_2.$$

The product converges because the corresponding series do.

We apply Lemma 2.1 to (11) by putting $k = 3$ and choose for c_0, c_1, c_2 the surely linearly independent vectors

$$(1,0,0), \quad (0,1,0), \quad (0,0,1)$$

wherewith the proposition is proven. $\square$

4 Deficiency indices: exceptional cases

We start with the case $D(\alpha) = 0$, $Q(\alpha) \neq 0$. It will turn out to be more convenient to apply beforehand the Bogolyubov transformation $U(i,0)$. Putting $\lambda = i\mu$, $\mu \in \mathbb{R}$, we arrive at the deficiency equation

$$\left(a^3 + a^* a^2 - (a^*)^2 a - (a^*)^3 + \frac{r}{3}a - \frac{\bar{r}}{3}a^*\right)\varphi = \frac{\mu}{3}\varphi, \tag{23}$$

which in $L^2(\mathbb{R})$ reads

$$-x^2 \frac{d}{dx}\varphi + \frac{1}{2}\left(1 - \frac{r+\bar{r}}{6}\right)\frac{d}{dx}\varphi - \left(1 + \frac{r-\bar{r}}{12}\right)x\varphi = -\frac{\mu}{3\sqrt{2}}\varphi. \tag{24}$$

We choose $\mu = -3\sqrt{2}$ and put

$$F := \frac{1}{2}\left(1 - \frac{\operatorname{Re} r}{3}\right), \; G := \frac{\operatorname{Im} r}{6}$$

whence,

$$(F - x^2)\varphi' - (iG + 1)x\varphi = \varphi. \tag{25}$$

Any weak solution to (25) is a strong solution except, possibly, a finite number of isolated singularities (see e.g. [4, XIII.2]). In other words we obtain the complete solution by combining the strong solutions on the intervals having boundary points at the singularities. Since we are allowed to choose zero as solution on some (not all) of these intervals it is possible to gain more than one linearly independent weak solution notwithstanding the equation being of order one. To have the complete solution in $L^2(\mathbb{R})$ we must determine which of the partial solutions are in $L^2(\mathbb{R})$.

Proposition 4.1. *Equation* (25) *has exactly one linearly independent square integrable (weak) solution. In particular, the operator* $A(-3,1) + ra + \bar{r}a^*$ *has deficiency indices* $(1,1)$.

Proof. The formal solution u of (25) is given through

$$(\ln\varphi)' = \frac{1 + (iG+1)x}{F - x^2} =: v(x).$$

In computing the primitive function of v we distinguish the cases $F < 0, F > 0$, and $F = 0$. For the sake of simplicity we shall henceforth suppress without loss of generality the constants of integration.

$F < 0$. Since $|F| = -F$,

$$\begin{aligned}\int v(x)\,dx &= -\int \frac{1}{|F| + x^2}\,dx - (iG+1)\int \frac{x}{|F|+x^2}\,dx \\ &= -\frac{1}{\sqrt{|F|}}\arctan\frac{x}{\sqrt{|F|}} - \frac{1}{2}(iG+1)\ln(|F|+x^2).\end{aligned}$$

We obtain

$$\varphi(x) = \exp\left(-\frac{1}{\sqrt{|F|}}\arctan\frac{x}{\sqrt{|F|}}\right)\exp\left(-\frac{iG}{2}\ln(|F|+x^2)\right)\frac{1}{(|F|+x^2)^{1/2}} \tag{26}$$

wherein the first two factors are bounded on $\mathbb{R}$ and the third factor is square integrable which shows the statement.

$F > 0$. The function in front of φ' has two distinct real zeros. Firstly for $|x| < \sqrt{F}$:

$$\int \frac{1}{F - x^2}\,dx = \frac{1}{2\sqrt{F}}\ln\frac{\sqrt{F}+x}{\sqrt{F}-x} \quad \text{and} \quad \int \frac{x}{F-x^2}\,dx = -\frac{1}{2}\ln(F - x^2).$$

The solution thus is

$$\varphi(x) = \left(\frac{\sqrt{F}+x}{\sqrt{F}-x}\right)^{\frac{1}{2\sqrt{F}}}\exp\left(-\frac{iG}{2}\ln(F-x^2)\right)\frac{1}{(F-x^2)^{1/2}}. \tag{27}$$

Because of $F - x^2 > 0$ the second factor has absolute value 1. We conclude

$$|\varphi(x)|^2 = \frac{(\sqrt{F}+x)^{1/\sqrt{F}}}{(\sqrt{F}-x)^{1/\sqrt{F}}}\frac{1}{(\sqrt{F}-x)(\sqrt{F}+x)} = \frac{(\sqrt{F}+x)^{(1/\sqrt{F})-1}}{(\sqrt{F}-x)^{(1/\sqrt{F})+1}}.$$

Since φ is not square integrable at $x \nearrow \sqrt{F}$ this part must not contribute to the solution

$$\varphi(x) = 0 \text{ for } -\sqrt{F} < x < \sqrt{F}.$$

For $x > \sqrt{F}$ we use

$$\int \frac{x}{x^2 - F}\, dx = \frac{1}{2}\ln(x^2 - F) \quad \text{and} \quad \int \frac{1}{x^2 - F}\, dx = \frac{1}{2\sqrt{F}} \ln \frac{x - \sqrt{F}}{x + \sqrt{F}}$$

to compute the primitive function of v:

$$\varphi(x) = \left(\frac{x + \sqrt{F}}{x - \sqrt{F}}\right)^{\frac{1}{2\sqrt{F}}} \exp\left(\frac{-iG}{2}\ln(x^2 - F)\right) \frac{1}{(x^2 - F)^{1/2}} \tag{28}$$

having absolute value

$$|\varphi(x)|^2 = \frac{(x + \sqrt{F})^{(1/\sqrt{F})-1}}{(x - \sqrt{F})^{(1/\sqrt{F})+1}}$$

whence φ is not square integrable at $x \searrow \sqrt{F}$ and the corresponding part of the solution must vanish:

$$\varphi(x) = 0 \text{ for } x > \sqrt{F}.$$

We arrive at the square integrable part $x < -\sqrt{F}$. The solution here is also given by (28). However, the first factor behaves differently. To see why we write $x = -y, y > 0$. Then $y > \sqrt{F}$:

$$|\varphi(x)|^2 = \left(\frac{-y + \sqrt{F}}{-y - \sqrt{F}}\right)^{1/\sqrt{F}} \frac{1}{(y - \sqrt{F})(y + \sqrt{F})} = \frac{(y - \sqrt{F})^{(1/\sqrt{F})-1}}{(y + \sqrt{F})^{(1/\sqrt{F})+1}}.$$

Because of $1/\sqrt{F} - 1 > -1$ this function is square integrable for $y > \sqrt{F}$.

The only square integrable weak solution to (25) is thus given by

$$\varphi(x) = \begin{cases} 0 & \text{for } x \geq -\sqrt{F} \\ (28) & \text{for } x < -\sqrt{F} \end{cases}$$

$F = 0$. Both zeros in the singular part of (25) coincide whence there can be at most two linearly independent weak solutions. We have

$$\int v(x)\, dx = -(iG + 1)\ln|x| + \frac{1}{x}.$$

We obtain the solution

$$\varphi(x) = \exp(-iG\ln|x|)\frac{1}{|x|}\exp\left(\frac{1}{x}\right)\ ,\ x \neq 0, \tag{29}$$

and moreover:

$$|\varphi(x)|^2 = \frac{1}{x^2} e^{2/x}.$$

One sees immediately that $|\varphi|^2$ is integrable only at $x \nearrow 0$ whence the weak solution of (25) in $L^2(\mathbb{R})$ is given by

$$\varphi(x) = \begin{cases} 0 & \text{for } x \geq 0 \\ (29) & \text{for } x < 0 \end{cases}$$

This completes the proof. $\square$

We conclude with the case $D(\alpha) = Q(\alpha) = 0$ for which the result can be given without any effort.

Proposition 4.2. *The operator $A(1,1)$ has deficiency indices* $(0,0)$.

Proof. We have

$$A(1,1) = a^3 + 3a^*a^2 + 3(a^*)^2 a + (a^*)^3 = (a + a^*)^3 - 3(a + a^*).$$

In our $L^2(\mathbb{R})$ representation $a + a^*$ is just multiplication by x up to factor whence $A(1,1)$ too is a multiplication operator and, thus, essentially self-adjoint on D. $\square$

A Cubic forms and their normal forms

We want to reduce the cubic form

$$\alpha x^3 + 3xy^2 + 3x^2 y + \bar{\alpha} y^3, \ x, y \in \mathbb{C}, \ \alpha \in \mathbb{C}, \tag{30}$$

to certain normal forms by means of a linear map $B \in SU(1,1)$, i.e.

$$B = \begin{pmatrix} s & t \\ \bar{t} & \bar{s} \end{pmatrix}, \quad \det B = 1. \tag{31}$$

We know from algebra that we can do this by finding a fractional linear transformation:

$$z \mapsto hz = \frac{sz + t}{\bar{t}z + \bar{s}} \tag{32}$$

having the same coefficients s and t as B and acting on the polynomial associated to (30)

$$p_\alpha(z) := \alpha z^3 + 3z^2 + 3z + \bar{\alpha}. \tag{33}$$

We indicate the relationship between h and B by writing $h \sim B$. Note, that this correspondence is unique only up to a factor. For each $B \in SU(1,1)$ the corresponding h is an element of the automorphism group $Aut(X_+)$ of the unit disc $X_+ := \{z \in \mathbb{C} | |z| < 1\}$. Moreover, the sets

$$X_0 := \{z \in \mathbb{C} | |z| = 1\}, \quad X_- := \{z \in \mathbb{C} | |z| > 1\} \tag{34}$$

are left invariant by those transformations. Since the action of h on p_α is uniquely determined by the action on the zeros we need some information on these zeros.

Lemma A.1. *Let $\alpha \in \mathbb{C} \setminus \{0\}$ and z_1, z_2, z_3 be the zeros of p_α. Then either $|z_j| = 1$, $j = 1, 2, 3$, or $|z_1| = 1$, $|z_2| \neq 0$, $z_3 = 1/\bar{z}_2$ up to permutations.*

Proof. Since $\alpha \neq 0$ we have $z_j \neq 0$. We note that along with z also $1/\bar{z}$ is a zero of p_α:

$$p_\alpha(\frac{1}{\bar{z}}) = \alpha \frac{1}{\bar{z}^3} + 3\frac{1}{\bar{z}^2} + 3\frac{1}{\bar{z}} + \bar{\alpha} = \frac{1}{\bar{z}^3}(\overline{\bar{\alpha} + 3z + 3z^2 + \alpha z^3}) = 0.$$

Furthermore, Vieta's theorem tells us $z_1 z_2 z_3 = -\bar{\alpha}/\alpha$ whence $|z_1||z_2||z_3| = 1$. When the first case does not hold we may assume without loss of generality $|z_2| \neq 1$ and hence $z_2 \neq 1/\bar{z}_2$. Then,

$$1 = |z_1||z_2|\frac{1}{|\bar{z}_2|} = |z_1|$$

which proves the lemma. □

To decide which case holds we look at the discriminant $D(\alpha)$ of p_α (see e.g. [11, p. 102]):

$$D(\alpha) := \alpha^4 W(\alpha)^2, \quad W(\alpha) := (z_1 - z_2)(z_1 - z_3)(z_2 - z_3). \tag{35}$$

$D(\alpha)$ can be expressed solely by the coefficients of p_α:

$$D(\alpha) = 27(-|\alpha|^4 + 6|\alpha|^2 - 4(\alpha + \bar{\alpha}) + 3) \in \mathbb{R}. \tag{36}$$

Proposition A.2. *Let $\alpha \in \mathbb{C} \setminus \{0\}$ and let z_1, z_2, z_3 be the zeros of p_α. Then:*

1. *$D(\alpha) \leq 0$: All zeros lie on the unit circle X_0. When $D(\alpha) = 0$ there are multiple zeros.*

2. *$D(\alpha) > 0$: We have $|z_1| = 1$ and $|z_2| < 1$, $z_3 = 1/\bar{z}_2$ up to permutations.*

Proof. Since $z_j \neq 0$ we may write

$$W(\alpha) = z_1 z_2 z_3 \left(\frac{z_1}{z_3} - \frac{z_1}{z_2} + \frac{z_3}{z_2} - \frac{z_2}{z_3} + \frac{z_2}{z_1} - \frac{z_3}{z_1} \right).$$

1) Let $|z_j| = 1$, i.e. $1/z_j = \bar{z}_j$:

$$W(\alpha) = -\frac{\bar{\alpha}}{\alpha}(z_1\bar{z}_3 - \bar{z}_1 z_3 + \bar{z}_1 z_2 - z_1\bar{z}_2 + \bar{z}_2 z_3 - z_2\bar{z}_3) = -\frac{\bar{\alpha}}{\alpha}2i\,\mathrm{Im}(z_1\bar{z}_3 + \bar{z}_1 z_2 + \bar{z}_2 z_3). \tag{37}$$

Hence,

$$D(\alpha) = -4|\alpha|^4(\mathrm{Im}(z_1\bar{z}_3 + \bar{z}_1 z_2 + \bar{z}_2 z_3))^2 \leq 0.$$

2) When not all z_j lie on the unit circle then by Lemma A.1 $1/z_1 = \bar{z}_1$, $z_3 = 1/\bar{z}_2$, and

$$W(\alpha) = -\frac{\bar{\alpha}}{\alpha}(2\,\mathrm{Re}(z_1(\bar{z}_2 - \bar{z}_3)) + |z_3|^2 - |z_2|^2).$$

Hence,

$$D(\alpha) = |\alpha|^4(2\,\mathrm{Re}(z_1(\bar{z}_2 - \bar{z}_3)) + |z_3|^2 - |z_2|^2)^2 > 0$$

because by Lemma A.1 $D(\alpha) = 0$ can only occur in Case 1. $\square$

To obtain normal forms for p_α we transform its zeros to special points.

Proposition A.3. *1) Assume $|z_1| = 1$ and $0 < |z_2| < 1$. Then there is an $h \in Aut(X_+)$ such that*

$$h(z_1) = -1, \quad h(z_2) = 0, \quad h(z_3) = \infty. \tag{38}$$

2) Let $z_1, z_2, z_3 \in X_0$ be pairwise different points. Then there is an $h \in Aut(X_+)$ such that

$$h(z_1) = -1, \quad h(z_2) = \vartheta, \quad h(z_3) = \bar{\vartheta} \quad \text{with } \vartheta := e^{i\pi/3} = (1+\sqrt{3})/2 \tag{39}$$

after z_j having been renumbered suitably.

Proof. 1) Note $z_3 = 1/\bar{z}_2$. A transformation satisfying (38) can be written down immediately:

$$hz = -\frac{z - z_2}{z - 1/\bar{z}_2}\frac{z_1 - 1/\bar{z}_2}{z_1 - z_2} = \frac{z - z_2}{-\bar{z}_2 z + 1}\frac{z_1\bar{z}_2 - 1}{z_1 - z_2}.$$

We check that h has the form required. Because of $|z_1| = 1$ we see

$$\left|\frac{z_1\bar{z}_2 - 1}{z_1 - z_2}\right| = \left|\frac{z_1\bar{z}_2 - z_1\bar{z}_1}{z_1 - z_2}\right| = 1$$

whence there is a $\tau \in [0, 2\pi[$ such that

$$\frac{z_1\bar{z}_2 - 1}{z_1 - z_2} = e^{i\tau}.$$

Thus,

$$h(z) = \frac{z - z_2}{-\bar{z}_2 z + 1}e^{i\tau} = \frac{e^{i\tau/2}z - e^{i\tau/2}z_2}{-e^{-i\tau/2}\bar{z}_2 z + e^{-i\tau/2}}$$

has the correct form and the determinant being $1-|z_2|^2>0$ because of $|z_2|<1$. Hence we have $(1-|z_2|^2)^{1/2}\in\mathbb{R}$.

2) We are seeking a transformation h satisfying (39). To begin with the transformation h_1 given by

$$h_1 \sim \begin{pmatrix} z_2-z_3 & z_1(z_3-z_2) \\ z_2-z_1 & z_3(z_1-z_2) \end{pmatrix} =: M_1$$

maps

$$h_1(z_1)=0, \quad h_1(z_2)=1, \quad h_1(z_3)=\infty.$$

Analogously h_2,

$$h_2 \sim \begin{pmatrix} -\vartheta & -\bar{\vartheta} \\ \bar{\vartheta} & \vartheta \end{pmatrix} =: M_2$$

maps

$$h_2(\vartheta)=0, \quad h(-1)=1, \quad h_2(\bar{\vartheta})=\infty.$$

Then $h:=h_2^{-1}h_1$ is an appropriate candidate. Because of $h_2^{-1}\sim -M_2$ computing M_1M_2 and getting rid of the products z_1z_2, z_1z_3, z_2z_3 with the aid of Vieta's theorem yield:

$$\begin{aligned} h_2h_1^{-1} &\sim \frac{1}{\alpha^2}\begin{pmatrix} \alpha(-\bar{\vartheta}z_1+(\vartheta+\bar{\vartheta})z_2-\vartheta z_3) & \bar{\alpha}(\vartheta\bar{z}_3-(\vartheta+\bar{\vartheta})\bar{z}_2+\bar{\vartheta}\bar{z}_1) \\ \alpha(\vartheta z_1-(\vartheta+\bar{\vartheta})z_2+\bar{\vartheta}z_3) & \bar{\alpha}(-\bar{\vartheta}\bar{z}_3+(\vartheta+\bar{\vartheta})\bar{z}_2-\vartheta\bar{z}_1) \end{pmatrix} \\ &=: \frac{1}{\alpha^2}M. \end{aligned}$$

The matrix M generates $h_2h_1^{-1}$ as well as M/α^2. We compute $\det M$. Because of $\vartheta^3=1$ we have:

$$-\det M_2 = -\vartheta^2+\bar{\vartheta}^2 = \bar{\vartheta}-\vartheta = -2i\operatorname{Im}\vartheta = -i\sqrt{3}.$$

Furthermore,

$$\det M_1 = (z_2-z_3)(z_2-z_1)(z_1-z_3) = -W(\alpha) = 2i\frac{\bar{\alpha}}{\alpha}\operatorname{Im}(z_1\bar{z}_3+\bar{z}_1z_2+\bar{z}_2z_3)$$

where we used (37). Hence,

$$\det M = -\det M_2\det M_1 = 2\sqrt{3}|\alpha|\operatorname{Im}(z_1\bar{z}_2+\bar{z}_1z_2+\bar{z}_2z_3).$$

By renumbering the z_j we can always ensure $\operatorname{Im}(z_1\bar{z}_3+\bar{z}_1z_2+\bar{z}_2z_3)>0$ whence $\sqrt{\det M}\in\mathbb{R}$. Then $M/\sqrt{\det M}$ satisfies (31). □

When the discriminant vanishes there are two possible cases. First, we have one single and one twofold zero. This case can be treated by Proposition A.3. A simple polynomial is:

$$p_\alpha(z) = z^3-z^2-z+1. \tag{40}$$

We can map the zeros z_1 and z_2 to -1 and ϑ. The same holds for our prescribed image points -1 and 1. The statement then follows from the group structure of $Aut(X_+)$.

When there is a threefold zero p_α already has its normal form since in this case $\alpha = 1$ which follows from the quadratic discriminant vanishing (see [11, p. 102]):

$$4(1 - \alpha) = 0.$$

Hence $\alpha = 1$. We summarize our results for the cubic form (30).

Theorem A.4. *Let* $D(\alpha) = 27(-|\alpha|^4 + 6|\alpha|^2 - 4(\alpha + \bar{\alpha}) + 3)$ *be the cubic and* $Q(\alpha) = 4(1 - \alpha)$ *be the quadratic discriminant of the cubic form* (30). *Then, there is a* $SU(1,1)$ *map that maps* (30) *to one of the following normal forms:*

1. $D(\alpha) < 0$: $x^3 + y^3$.
2. $D(\alpha) > 0$: $x^2y + xy^2$.
3. $D(\alpha) = 0$, $Q(\alpha) \neq 0$: $x^3 - x^2y - xy^2 + y^3$.
4. $D(\alpha) = Q(\alpha) = 0$, *i.e.* $\alpha = 1$: $x^3 + 3x^2y + 3xy^2 + y^3$.

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