Generation of semigroup for symmetric matrix Schrödinger operators in $L^p$-spaces

A. Maichine

Received: 25 January 2018 / Accepted: 6 June 2018 / Published online: 16 July 2018
© Springer Science+Business Media, LLC, part of Springer Nature 2018

Abstract
In this paper we prove that the symmetric matrix Schrödinger operator $\text{div}(Q\nabla u) - Vu$ generates an analytic semigroup when, for every $x \in \mathbb{R}^d$, $V(x) = (v_{ij}(x))$ is a semi-definite positive and symmetric matrix, the diffusion matrix $Q(\cdot)$ is supposed to be strongly elliptic and bounded and the potential $V$ satisfies the weak condition $v_{ij} \in L^1_{\text{loc}}(\mathbb{R}^d)$, for all $i, j \in \{1, \ldots, m\}$. We also determine the positivity and compactness of the semigroup.

Keywords Schrödinger operator · Matrix potential · Sesquilinear forms · Beurling–Deny criterion

1 Introduction
Parabolic systems with unbounded coefficients have become an interesting topic thanks to their application in the study of several phenomena that come from several sciences such as economics, physics, chemistry, etc. The semigroup theory allows solving autonomous linear parabolic systems by studying the properties of the associated second order differential operator; the so-called vector-valued elliptic operator. In the case of absence of a drift term, one obtains a Schrödinger operator with matrix potential which we call, in this paper, matrix Schrödinger operator. Such operators have the general form $A = \text{div}(Q\nabla \cdot) - V$, where $Q$ and $V$ are, respectively, the diffusion and potential matrices. The matrix Schrödinger operator appears, in non-relativistic mechanical quantum, as the Hamiltonian for a system of interacting adsorbate and substrate atoms. The entries of the potential matrix $V$ represent the inter-particle elec-
trical interactions; namely, electron–electron repulsions, electron–nuclear attractions and nuclear–nuclear repulsions, see [11,12].

Recently, in [6], the authors have considered a matrix Schrödinger operator of type $\mathbb{A}$ and they have shown, by application of a noncommutative version of the Dore-Venni theorem, the generation of a semigroup in $L^p(\mathbb{R}^d, \mathbb{R}^m)$, $p \in (1, \infty)$, under smoothness and growth assumptions on $Q$ and $V$. Further properties of the semigroup like compactness and positivity have been investigated. Afterward, in [7], similar results as in [6] have been obtained for matrix potentials with diagonal entries of polynomial growth. Moreover, kernel estimates for the associated semigroup have been investigated and the asymptotic distribution of eigenvalues of the matrix Schrödinger operator has been established.

In this article we associate a sesquilinear form, in $L^2(\mathbb{R}^d, \mathbb{C}^m)$, to the matrix Schrödinger operator $\mathcal{A}u = (\text{div}(Q\nabla u_j))_j - Vu$, $u = (u_1, \ldots, u_m)$, where $V = (v_{ij})_{1 \leq i, j \leq m}$ is a symmetric matrix-valued function. As in the scalar case, see [2, Section 1.8], and under the weakest condition $v_{ij} \in L^1_{\text{loc}}(\mathbb{R}^d)$, $i, j \in \{1, \ldots, m\}$, we prove that $\mathcal{A}$ admits a dissipative self-adjoint realization in $L^2(\mathbb{R}^d, \mathbb{C}^m)$ and we extrapolate its associated semigroup to the spaces $L^p(\mathbb{R}^d, \mathbb{C}^m)$, using a vectorial version of 'Beurling–Deny’ criterion of $L^\infty$-contractivity. We also investigate on some properties of the semigroup.

This article is structured as follow: in Sect. 2 we study the associated form to $\mathcal{A}$ and show that $\mathcal{A}$ has a self-adjoint realization $\mathcal{A}$ that generates an analytic strongly continuous semigroup $\{T(t)\}_{t \geq 0}$ in $L^2(\mathbb{R}^d, \mathbb{C}^m)$. In Sect. 3, we apply a ’Beurling–Deny’ criterion type, see [9, Theorem 2], to establish $L^\infty$-contractivity of the semigroup $\{T(t)\}_{t \geq 0}$ and thus extrapolate it to $L^p(\mathbb{R}^d, \mathbb{C}^m)$. Section 4 is devoted to characterize positivity, study compactness of the semigroup and analyze the spectrum of $\mathcal{A}$.

Notation Throughout this paper we adopt the following notation: $d, m \in \mathbb{N}$, $K = \mathbb{R}$ or $K = \mathbb{C}$, $(\cdot, \cdot)$ the inner-product of $K^j$, $j = d, m$. $L^p(\mathbb{R}^d, K^m)$, $1 < p < \infty$, denotes the vectorial Lebesgue space endowed with the norm

$$
\| \cdot \|_p : f = (f_1, \ldots, f_m) \mapsto \| f \|_p := \left( \int_{\mathbb{R}^d} \left( \sum_{j=1}^m |f_j|^2 \right)^{\frac{p}{2}} dx \right)^{\frac{1}{p}}.
$$

$H^1(\mathbb{R}^d)$ refers to the classical Sobolev space of order 1 over $L^2(\mathbb{R}^d)$. $H^1(\mathbb{R}^d, \mathbb{R}^m)$ is the vectorial Sobolev space constituted of vectorial function $f = (f_1, \ldots, f_m)$ such that $f_j \in H^1(\mathbb{R}^d)$, for all $j \in \{1, \ldots, m\}$. We note that all the derivatives are considered in the distribution sense. For $y = (y_1, \ldots, y_m) \in \mathbb{R}^m$, we write $y \geq 0$ if $y_j \geq 0$ for all $j \in \{1, \ldots, m\}$. For $r > 0$, $B(r) = \{ x \in \mathbb{R}^d : |x| < 1 \}$ denotes the euclidean open ball of $\mathbb{R}^d$ of center 0 and radius $r$. $\chi_E$ is the characteristic function of the set $E$.

## 2 Generation of the semigroup in $L^2$

Throughout we assume the following hypotheses
2.1 Hypotheses

(a) Let $Q : \mathbb{R}^d \to \mathbb{R}^{d \times d}$ be a symmetric matrix-valued function. Assume that there exist positive numbers $\eta_1$ and $\eta_2$ such that
\[
\eta_1 |\xi|^2 \leq \langle Q(x)\xi, \xi \rangle \leq \eta_2 |\xi|^2, \quad x, \xi \in \mathbb{R}^d. \tag{2.1}
\]

(b) Let $V : \mathbb{R}^d \to \mathbb{R}^{m \times m}$ be a matrix-valued operator such that $v_{ij} = v_{ji} \in L^1_{\text{loc}}(\mathbb{R}^d)$ for all $i, j \in \{1, \ldots, m\}$ and
\[
\langle V(x)\xi, \xi \rangle \geq 0, \quad x \in \mathbb{R}^d, \xi \in \mathbb{R}^m. \tag{2.2}
\]

We introduce, for $x \in \mathbb{R}^d$, the inner-product $\langle \cdot, \cdot \rangle_{Q(x)}$ given, for $y, z \in \mathbb{C}^d$, by
\[
\langle y, z \rangle_{Q(x)} := \langle Q(x)y, z \rangle \quad \text{and its associated norm } |z|_{Q(x)} := \sqrt{\langle Q(x)z, z \rangle}, \quad z \in \mathbb{C}^d.
\]

2.2 The $L^2$-sesquilinear form

Let us define the sesquilinear form
\[
a(f, g) := \int_{\mathbb{R}^d} \sum_{j=1}^m \langle Q(x)\nabla f_j(x), \nabla g_j(x) \rangle dx + \int_{\mathbb{R}^d} \langle V(x)f(x), g(x) \rangle dx, \tag{2.3}
\]
for $f, g \in D(a)$, where $D(a)$, the domain of $a$, is defined by
\[
D(a) = \{ f = (f_1, \ldots, f_m) \in H^1(\mathbb{R}^d, \mathbb{C}^m) : \int_{\mathbb{R}^d} \langle V(x)f(x), f(x) \rangle dx < +\infty \}. \tag{2.4}
\]

We endow $D(a)$ with the norm
\[
\|f\|_a = \left( \|f\|_{H^1(\mathbb{R}^d, \mathbb{C}^m)}^2 + \int_{\mathbb{R}^d} \langle V(x)f(x), f(x) \rangle dx \right)^{1/2} = \left( \|f\|_{L^2(\mathbb{R}^d, \mathbb{C}^m)}^2 + \sum_{j=1}^m \|\nabla f_j\|_{L^2(\mathbb{R}^d, \mathbb{C}^m)}^2 + \int_{\mathbb{R}^d} \langle V(x)f(x), f(x) \rangle dx \right)^{1/2}.
\]

We now give some properties of $a$

**Proposition 2.1** Assume Hypotheses 2.1 are satisfied. Then,

(i) $a$ is densely defined, i.e., $D(a)$ is dense in $L^2(\mathbb{R}^d, \mathbb{R}^m)$.

(ii) $a$ is accretive.

(iii) $a$ is continuous, i.e., exists $M > 0$ such that
\[
|a(f, g)| \leq M \|f\|_a \|g\|_a, \quad f, g \in D(a).
\]
(iv) $a$ is closed i.e., $(D(a), \| \cdot \|_a)$ is a complete space.

**Proof**

(i) It is obvious that $C_c^\infty(\mathbb{R}^d, \mathbb{R}^m) \subset D(a)$. Hence, $D(a)$ is dense in $L^2(\mathbb{R}^d, \mathbb{R}^m)$.

(ii) **Accretivity** For $f \in D(a)$ one has

$$
\text{Re } a(f) = \int_{\mathbb{R}^d} \sum_{j=1}^m |Q^{1/2}(x) \nabla f_j(x)|^2 \, dx + \int_{\mathbb{R}^d} \text{Re } \langle V(x) f(x), f(x) \rangle \, dx \geq 0.
$$

(iii) **Continuity** Let $f, g \in D(a)$. By application of Cauchy–Schwartz and Young inequalities one gets

$$
|a(f, g)| \leq \eta_2 \sum_{j=1}^m \int_{\mathbb{R}^d} |\nabla f_j(x)| |\nabla g_j(x)| \, dx
$$

$$
+ \int_{\mathbb{R}^d} |\langle V(x)^{1/2} f(x), V(x)^{1/2} g(x) \rangle| \, dx
$$

$$
\leq \eta_2 \sum_{j=1}^m \|\nabla f_j\| \|\nabla g_j\| + \left( \int_{\mathbb{R}^d} |V(x)^{1/2} f(x)|^2 \, dx \right)^{1/2}
$$

$$
\times \left( \int_{\mathbb{R}^d} |V(x)^{1/2} g(x)|^2 \, dx \right)^{1/2}
$$

$$
\leq \eta_2 \left( \sum_{j=1}^m \|\nabla f_j\|_2^2 \right)^{1/2} \left( \sum_{j=1}^m \|\nabla g_j\|_2^2 \right)^{1/2}
$$

$$
+ \left( \int_{\mathbb{R}^d} \langle V(x) f(x), f(x) \rangle \, dx \right) \left( \int_{\mathbb{R}^d} \langle V(x) g(x), g(x) \rangle \, dx \right)
$$

$$
\leq (1 + \eta_2) \|f\|_a \|g\|_a.
$$

(iv) **Closedness** Let $(f_n)_{n \in \mathbb{N}} \subset D(a)$ be a Cauchy sequence in $(D(a), \| \cdot \|_a)$. Then,

$$
\|f_n - f_l\|_{H^1(\mathbb{R}^d, \mathbb{R}^m)} + \int_{\mathbb{R}^d} \langle V(x)(f_n(x) - f_l(x)), (f_n(x) - f_l(x)) \rangle \, dx \xrightarrow{n,l \to \infty} 0,
$$

which yields

$$
\begin{align*}
& \begin{cases} 
 f_n - f_l \xrightarrow{n,l \to \infty} 0 \text{ in } H^1(\mathbb{R}^d, \mathbb{R}^m) \\
 \int_{\mathbb{R}^d} |V^{1/2}(f_n - f_l)|^2 \xrightarrow{n,l \to \infty} 0
\end{cases}.
\end{align*}
$$
Hence, \((f_n)_{n \in \mathbb{N}}\) and \((V^{1/2} f_n)_{n \in \mathbb{N}}\) are Cauchy sequences respectively in \(H^1(\mathbb{R}^d, \mathbb{C}^m)\) and \(L^2(\mathbb{R}^d, \mathbb{C}^m)\). Therefore

\[
\begin{aligned}
  f_n & \to f \quad \text{in} \quad H^1(\mathbb{R}^d, \mathbb{C}^m) \\
  V^{1/2} f_n & \to g \quad \text{in} \quad L^2(\mathbb{R}^d, \mathbb{C}^m)
\end{aligned}
\]

The pointwise convergence of subsequences implies that

\[
V^{1/2} f = g \in L^2(\mathbb{R}^d, \mathbb{C}^m).
\]

Then \(f \in D(a)\) and

\[
a(f_n - f) = \|f_n - f\|_{H^1(\mathbb{R}^d, \mathbb{C}^m)}^2 + \int_{\mathbb{R}^d} |V^{1/2}(x)(f_n - f)(x)|^2 \, dx \to 0, \quad n \to \infty,
\]

which ends the proof.

Now define

\[
A f := \text{div}(Q \nabla f) - V f = (\text{div}(Q \nabla f_j))_{1 \leq j \leq m} - V f. \quad (2.5)
\]

Thanks to Proposition 2.1 and applying [8, Proposition 1.22] and the well-known Lumer-Phillips theorem, [3, Chap-II, Theorem 3.15], one obtains.

**Corollary 2.2** A admits a realization \(A\) in \(L^2(\mathbb{R}^d, \mathbb{C}^m)\) that generates a bounded strongly continuous semigroup \((T(t))_{t \geq 0}\) which is analytic in the open right half plane of \(C\). Moreover, \(A\) is self-adjoint and \(-A\) is the linear operator associated to the form \(a\).

**Remark 2.3** The form method does not apply for non symmetric potentials. In fact, in [6, Example 3.5], it has been proved that the semigroup associated to a matrix Schrödinger operator with matrix potential

\[
V(x) = \begin{pmatrix} 0 & -x \\ x & 0 \end{pmatrix}, \quad x \in \mathbb{R},
\]

is not analytic. Otherwise, we show by straightforward computation that the continuity property of the form \(a\) fails when one takes instead of a symmetric potential the above antisymmetric one \(V\). Indeed, let \(\varphi \in C_c^\infty(\mathbb{R}^d)\) such that \(\chi_{B(1)} \leq \varphi \leq \chi_{B(2)}\). Consider, for \(n \geq 1\),

\[
f_n(x) = \frac{\varphi(x/n)}{\sqrt{1 + |x|^2}} e_1 \quad \text{and} \quad g_n(x) = \frac{\varphi(x/n)}{\sqrt{1 + |x|^2}} e_2.
\]
where \( \{ e_1, e_2 \} \) is the canonical basis of \( \mathbb{R}^2 \). Since \( V = -V^* \) then \( \langle V(x)\xi, \xi \rangle = 0 \), for all \( \xi \in \mathbb{R}^2 \). Thus

\[
a(f_n) = a(g_n) = \int_{\mathbb{R}} \left( -\frac{\varphi(x/n)}{(1 + |x|^2)^2} x + \frac{1}{n} \frac{1}{\sqrt{1 + |x|^2}} \nabla \varphi(x/n) \right)^2 dx
\]

and

\[
|a(f_n, g_n)| = \int_{\mathbb{R}^d} \frac{|x|}{(1 + |x|^2)^2} \varphi(x/n) dx.
\]

If the continuity property -Proposition 2.1 (iii)- of the form were satisfied, then there will exist \( C > 0 \) such that

\[
|a(f_n, g_n)| \leq C \| f_n \|_a \| g_n \|_a = C (\| f_n \|_{L^2(\mathbb{R}, \mathbb{R}^2)}^2 + a(f_n)).
\]

By the Lebesgue dominated convergence theorem one can let \( n \) tends to \( \infty \) and obtains

\[
\int_{\mathbb{R}} \frac{|x|}{1 + |x|^2} dx \leq C \left( \int_{\mathbb{R}^d} \frac{|x|^2}{(1 + |x|^2)^2} dx + \int_{\mathbb{R}^d} \frac{1}{1 + |x|^2} dx \right) < \infty.
\]

However, the integral of the left-hand side is infinite.

### 3 Extension to \( L^p \)

In this section we will show that \( \mathcal{A} \) has a \( L^p \)-realization which generates a holomorphic semigroup in \( L^p(\mathbb{R}^d, \mathbb{C}^m) \), \( 1 < p < \infty \). In order to do so we prove that, for every \( t > 0 \), the restriction \( T(t)|_{L^2 \cap L^\infty} \) of \( T(t) \) to \( L^2(\mathbb{R}^d, \mathbb{C}^m) \cap L^\infty(\mathbb{R}^d, \mathbb{C}^m) \) can be extended to a bounded operator \( T_p(t) \) in \( L^p(\mathbb{R}^d, \mathbb{C}^m) \), \( 2 < p < \infty \). Then, we show that \( (T_p(t))_{t \geq 0} \) is strongly continuous. Moreover, since \( (T(t))_{t \geq 0} \) is self-adjoint, the semigroups \( (T_p(t))_{t \geq 0} \), for \( p \in (1, 2) \) will obtained by duality arguments. For this aim it suffices that \( (T(t))_{t \geq 0} \) satisfy the following \( L^\infty \)-contractivity property:

\[
\| T_2(t) f \|_{\infty} \leq \| f \|_{\infty}, \quad \forall f \in L^2(\mathbb{R}^d, \mathbb{R}^m) \cap L^\infty(\mathbb{R}^d, \mathbb{R}^m).
\]

A characterization of (3.1) via the associated form is given by E.M. Ouhabaz in [9, Theorem2]. According to this characterization, (3.1) holds true if the following is satisfied

**Proposition 3.1** Let \( f \in H^1(\mathbb{R}^d, \mathbb{R}^m) \) and set \( \text{sign}(f) := \frac{f}{|f|} \chi_{\{f \neq 0\}} \). Then,

(i) \( f \in D(a) \) implies \( (1 \wedge |f|)\text{sign}(f) \in D(a) \);

(ii) for every \( f \in D(a) \), one has

\[
a((1 \wedge |f|)\text{sign}(f)) \leq a(f).
\]
Now we proceed to prove the above proposition. As a first step, we establish the assertion (i) of the above proposition in the following lemma.

**Lemma 3.2** (a) Assume \( f \in H^1(\mathbb{R}^d, \mathbb{R}^m) \). Then, \(|f| \in H^1(\mathbb{R}^d)\) and

\[
\nabla |f| = \frac{\sum_{j=1}^{m} f_j \nabla f_j}{|f|} \chi_{\{f \neq 0\}}. \tag{3.2}
\]

(b) Let \( f \in D(a) \). Then \((1 \wedge |f|) \text{sign}(f) \in D(a)\). In particular,

\[
\nabla ((1 \wedge |f|) \text{sign}(f))_j = \frac{1 + \text{sign}(1 - |f|)}{2} \frac{f_j}{|f|} \chi_{\{f \neq 0\}} \nabla |f| + \frac{1 \wedge |f|}{|f|} \left( \nabla f_j - \frac{f_j}{|f|} \nabla |f| \right) \chi_{\{f \neq 0\}}, \tag{3.3}
\]

for every \( j \in \{1, \ldots, m\} \).

**Proof** (a) Let \( f \in H^1(\mathbb{R}^d, \mathbb{R}^m) \). Define, for \( \varepsilon > 0 \), \( f_\varepsilon = \left( \sum_{j=1}^{m} f_j^2 + \varepsilon^2 \right)^{1/2} - \varepsilon \).

One has

\[
0 \leq f_\varepsilon = \frac{|f|^2}{\left( \sum_{j=1}^{m} f_j^2 + \varepsilon^2 \right)^{1/2} + \varepsilon} \leq |f|. 
\]

Hence, by dominated convergence theorem \( f_\varepsilon \xrightarrow{\varepsilon \to 0} |f| \) in \( L^2(\mathbb{R}^d) \). On the other hand, \( f_\varepsilon \in H^1_{\text{loc}}(\mathbb{R}^d) \) and

\[
\nabla f_\varepsilon = \frac{\sum_{j=1}^{m} f_j \nabla f_j}{\left( \sum_{j=1}^{m} f_j^2 + \varepsilon^2 \right)^{1/2} \xrightarrow{\varepsilon \to 0} |f|} \chi_{\{f \neq 0\}}. 
\]

Again, the dominated convergence theorem yields \(|f| \in H^1(\mathbb{R}^d)\) and (3.2).

(b) Let \( f \in D(a) \) i.e., \( f \in H^1(\mathbb{R}^d, \mathbb{R}^m) \) and \( V^{1/2} f \in L^2(\mathbb{R}^d, \mathbb{R}^m) \). One has

\[
\int_{\mathbb{R}^d} \langle V(x)(1 \wedge |f|) \text{sign}(f), (1 \wedge |f|) \text{sign}(f) \rangle dx \\
\leq \int_{\{f \neq 0\}} \left( \frac{1 \wedge |f|}{|f|} \right)^2 \langle V(x) f(x), f(x) \rangle dx \\
\leq \int_{\mathbb{R}^d} \langle V(x) f(x), f(x) \rangle dx < \infty.
\]

Now remains to show that \((1 \wedge |f|) \text{sign}(f) \in H^1(\mathbb{R}^d, \mathbb{R}^m)\). Set
\[ Pf := (1 \wedge |f|) \text{sign}(f) = (1 \wedge |f|) \frac{f}{|f|} \chi_{\{f \neq 0\}}, \]

and

\[ P_\varepsilon f := (1 \wedge |f|) \frac{f}{|f| + \varepsilon} = \frac{1 + |f| - |1 - |f||}{2} \frac{f}{|f| + \varepsilon}, \]

for \( \varepsilon > 0 \). One has

\[
\begin{aligned}
|P_\varepsilon f| &\leq (1 \wedge |f|) \leq |f| \\
P_\varepsilon f &\longrightarrow Pf \quad \text{a.e.},
\end{aligned}
\]

which implies that \( P_\varepsilon f \rightarrow Pf \) in \( L^2(\mathbb{R}^d, \mathbb{R}^m) \) as \( \varepsilon \rightarrow 0 \).

On the other hand, \( P_\varepsilon f \in H^1_{\text{loc}}(\mathbb{R}^d, \mathbb{R}^m) \) and

\[
\nabla(P_\varepsilon f)_j = \nabla \left( \frac{1 + |f| - |1 - |f||}{2} \frac{f_j}{|f| + \varepsilon} \right) = \frac{1 + |f| - |1 - |f||}{2} \left( \nabla f_j - \frac{f_j}{|f| + \varepsilon} \nabla|f| \right)
\]

\[
+ \frac{1}{2 |f| + \varepsilon} \left( \nabla|f| + \text{sign}(1 - |f|) \nabla|f| \right)
\]

\[
= \frac{1 \wedge |f|}{|f| + \varepsilon} \left( \nabla f_j - \frac{f_j}{|f| + \varepsilon} \nabla|f| \right)
\]

\[
+ \frac{1}{2 |f| + \varepsilon} (1 + \text{sign}(1 - |f|)) \nabla|f|.
\]

Hence,

\[
\lim_{\varepsilon \to 0} \nabla(P_\varepsilon f)_j = \frac{1 \wedge |f|}{|f|} \left( \nabla f_j - \frac{f_j}{|f|} \nabla|f| \right) \chi_{\{f \neq 0\}}
\]

\[
+ \frac{1}{2 |f|} (1 + \text{sign}(1 - |f|)) \chi_{\{f \neq 0\}} \nabla|f|,
\]

and

\[
|\nabla(P_\varepsilon f)_j| \leq \frac{1 \wedge |f|}{|f|} (|\nabla f_j| + |\nabla|f||) + |\nabla|f|| \leq |\nabla f_j| + 2|\nabla|f|| \in L^2(\mathbb{R}^d).
\]

By the dominated convergence theorem we conclude that \( Pf = \lim_{\varepsilon \to 0} P_\varepsilon f \in H^1(\mathbb{R}^d, \mathbb{R}^m) \), and

\( \Box \) Springer
\[
\n\nabla (Pf)_j := \lim_{\varepsilon \to 0} \nabla (P_{\varepsilon}f)_j \\
= \frac{1 \wedge |f|}{|f|} \left( \nabla f_j - \frac{f_j}{|f|} \nabla |f| \right) \chi_{\{f \neq 0\}} \\
+ \frac{1}{2} \frac{f_j}{|f|} (1 + \text{sign}(1 - |f|)) \chi_{\{f \neq 0\}} \nabla |f|.
\]

In the following we state another lemma where we prove (ii) of Proposition 3.1

**Lemma 3.3** Let \( f \in D(a) \). Then

\[
a((1 \wedge |f|)\text{sign}(f)) \leq a(f).
\] (3.4)

**Proof** Let \( f \in D(a) \). One has,

\[
\alpha_f := \langle Q \nabla ((1 \wedge |f|)\text{sg}(f)), \nabla ((1 \wedge |f|)\text{sign}(f)) \rangle \\
= \sum_{j=1}^{m} \left| \frac{1 \wedge |f|}{|f|} \left( \nabla f_j - \frac{f_j}{|f|} \nabla |f| \right) \chi_{\{f \neq 0\}} \right| \\
+ \frac{1}{2} \frac{f_j}{|f|} (1 + \text{sign}(1 - |f|)) \chi_{\{f \neq 0\}} \nabla |f|_Q^2 \\
= \frac{(1 + \text{sign}(1 - |f|))^2}{4} \chi_{\{f \neq 0\}} \nabla |f|_Q^2 \\
+ \frac{(1 \wedge |f|)^2}{|f|^2} \chi_{\{f \neq 0\}} \sum_{j=1}^{m} \left| \nabla f_j - \frac{f_j}{|f|} \nabla |f| \right|_Q^2 \\
+ (1 + \text{sign}(1 - |f|)) \frac{1 \wedge |f|}{|f|} \chi_{\{f \neq 0\}} \sum_{j=1}^{m} \langle Q \nabla |f|, (\nabla f_j - \frac{f_j}{|f|} \nabla |f|) f_j \rangle \\
= \frac{(1 + \text{sign}(1 - |f|))^2}{4} \chi_{\{f \neq 0\}} \nabla |f|_Q^2 \\
+ \frac{(1 \wedge |f|)^2}{|f|^2} \chi_{\{f \neq 0\}} \left( \sum_{j=1}^{m} \langle Q \nabla f_j, \nabla f_j \rangle + \nabla |f|_Q^2 - \langle \nabla |f|_Q^2, \frac{\nabla |f|}{|f|} \rangle \right) \\
+ (1 + \text{sign}(1 - |f|)) \frac{1 \wedge |f|}{|f|} \chi_{\{f \neq 0\}} \\
\times \left( \frac{1}{2} \langle Q \nabla |f|, \nabla |f|_Q^2 \rangle - |f| \langle Q \nabla |f|, \nabla |f| \rangle \right) \\
= \frac{(1 + \text{sign}(1 - |f|))^2}{4} \chi_{\{f \neq 0\}} \nabla |f|_Q^2
\]
+ \frac{(1 \wedge |f|)^2}{|f|^2} \chi_{|f| \neq 0} \left( \sum_{j=1}^{m} \langle Q \nabla f_j, \nabla f_j \rangle - |\nabla f||^2_Q \right)
= \left( \frac{(1 + \text{sign}(1 - |f|))^2}{4} - \frac{(1 \wedge |f|)^2}{|f|^2} \right) \chi_{|f| \neq 0} |\nabla f||^2_Q
+ \frac{(1 \wedge |f|)^2}{|f|^2} \chi_{|f| \neq 0} \sum_{j=1}^{m} \langle Q \nabla f_j, \nabla f_j \rangle.

Discussing the cases $|f| < 1$, $|f| = 1$ and $|f| > 1$, one can easily see that

$$\frac{(1 + \text{sign}(1 - |f|))^2}{4} - \frac{(1 \wedge |f|)^2}{|f|^2} \leq 0.$$ 

Thus,

$$\alpha_f \leq \frac{(1 \wedge |f|)^2}{|f|^2} \chi_{|f| \neq 0} \sum_{j=1}^{m} \langle Q \nabla f_j, \nabla f_j \rangle
\leq \sum_{j=1}^{m} \langle Q \nabla f_j, \nabla f_j \rangle.$$ 

Integrating over $\mathbb{R}^d$, one gets

$$a_0((1 \wedge |f|)\text{sign}(f)) := \int_{\mathbb{R}^d} \langle Q \nabla ((1 \wedge |f|)\text{sign}(f)), \nabla ((1 \wedge |f|)\text{sign}(f)) \rangle \, dx
\leq \int_{\mathbb{R}^d} \sum_{j=1}^{m} \langle Q \nabla f_j, \nabla f_j \rangle \, dx := a_0(f).$$

Therefore,

$$a((1 \wedge |f|)\text{sign}(f)) = a_0((1 \wedge |f|)\text{sign}(f))
+ \int_{\mathbb{R}^d} \langle V(x)(1 \wedge |f|)\text{sign}(f), (1 \wedge |f|)\text{sign}(f) \rangle \, dx
\leq a_0(f) + \int_{\mathbb{R}^d} \langle Vf, f \rangle \, dx = a(f).$$

As a consequence of the statement of Proposition 3.1, one gets.

**Corollary 3.4** The semigroup $\{T(t)\}_{t \geq 0}$ is $L^\infty$-contractive.

Now, we are able to state our main theorem of this section.
Theorem 3.5  Let $1 < p < \infty$ and assume Hypotheses 2.1. Then, $A$ admits a realization $A_p$ in $L^p(\mathbb{R}^d, \mathbb{C}^m)$ that generates a bounded strongly continuous semigroup $(T_p(t))_{t \geq 0}$. Moreover, $(T_p(t))_{t \geq 0}$ is analytic in the sector of angle $\frac{\pi}{p}$ if $p > 2$; it is analytic in the sector of angle $\frac{\pi}{p}$ if $1 < p < 2$ where $1/p + 1/p' = 1$.

Proof  Let $2 < p < \infty$. According to Corollaries 2.2 and 3.4, $(T(t))_{t \geq 0}$ is self-adjoint and $L^\infty$-contractive. Hence, by the Riesz-Thorin interpolation theorem, $(T(t))_{t \geq 0}$ admits a unique bounded extension $(T_p(t))_{t \geq 0}$ to $L^p(\mathbb{R}^d, \mathbb{C}^m)$; this extension is analytic in the sector of angle $\frac{\pi}{p}$, cf. [4, Theorem 2.9]. Moreover, for every $f \in L^2(\mathbb{R}^d, \mathbb{C}^m) \cap L^\infty(\mathbb{R}^d, \mathbb{C}^m)$,

$$
\|T(t)f - f\|_p \leq \|T(t)f - f\|_2^\theta \|T(t)f\|^{1-\theta} \leq 2^{1-\theta}\|f\|_\infty^{1-\theta}\|T(t)f - f\|_2^\theta,
$$

where $\theta = \frac{2}{p}$. This shows how $(T_p(t))_{t \geq 0}$ is strongly continuous.

Concerning the case $1 < p < 2$, we prove by duality that $\|T(t)f\|_1 \leq \|f\|_1$, for every $t > 0$, and similarly, we obtain an analytic extrapolation of $(T(t))_{t \geq 0}$ which is strongly continuous. $\square$

Remark 3.6  We can extrapolate the semigroup $(T(t))_{t \geq 0}$ to a strongly continuous one in $L^1(\mathbb{R}^d, \mathbb{C}^m)$. It is an easier consequence of consistency and $L^p$-contractivity of $(T(t))_{t \geq 0}$, see [10].

4 Further properties of the semigroup

In this section we study positivity and compactness of $(T(t))_{t \geq 0}$ and the spectrum of $A$. We start by the positivity

4.1 Positivity

In this subsection we give necessary and sufficient condition for positivity of the semigroup $(T(t))_{t \geq 0}$. We use the form characterization of the invariance of convex subsets via semigroups. For this purpose we introduce

$$
C^+ := \{ f = (f_1, \ldots, f_m) \in L^2(\mathbb{R}^d, \mathbb{R}^m) : f \geq 0 \text{ a.e.} \}.
$$

$C^+$ is a closed convex subset of $L^2(\mathbb{R}^d, \mathbb{R}^m)$. The projection $P_+$ on $C^+$ is given by

$$
P_+f := f^+ = (f_j \wedge 0)_{1 \leq j \leq m}, \quad \forall f \in L^2(\mathbb{R}^d, \mathbb{R}^m).
$$

One knows that the projection on a closed convex subsets of a Banach space is uniquely defined and it is easy to check that $P_+$, defined above, is the right one for $C^+$. We recall that $(T(t))_{t \geq 0}$ is positive if, and only if, $f \in L^2(\mathbb{R}^d, \mathbb{R}^m)$ and $f \geq 0$ imply $T(t)f \geq 0$, for every $t > 0$. The form characterization of positivity is given by [9, Theorem 3 (iii)] as follow
Proposition 4.1 \((T(t))_{t \geq 0}\) is a positive semigroup if, and only if, \(f^+ \in D(a)\) for all \(f \in D(a)\) and \(a(f^+, f^-) \leq 0\), where \(f^- = f - P_+ f = ((-f_j) \wedge 0)_{1 \leq j \leq m}\).

By application of [9, Theorem 3 (iii)] we get the following characterization of positivity of \((T(t))_{t \geq 0}\) in term of entries of the potential matrix \(V\).

Theorem 4.2 The semigroup \((T(t))_{t \geq 0}\) is positive if and only if \(v_{ij} \leq 0\), for all \(i \neq j \in \{1, \ldots, m\}\).

Proof Suppose that \((T(t))_{t \geq 0}\) is positive. Let \(i \neq j \in \{1, \ldots, m\}\) and consider \(f = \varphi(e_i - e_j)\) where \(0 \leq \varphi \in C^\infty_c(\mathbb{R}^d)\) to be arbitrarily chosen. One has \(f^+ = \varphi e_i\), \(f^- = \varphi e_j\) and \(\langle Q \nabla f^+, \nabla f^- \rangle = 0\). Applying Proposition 4.1 one obtains

\[
0 \geq a(f^+, f^-) = \sum_{k=1}^{m} \int_{\mathbb{R}^d} \langle Q \nabla u^+_k, \nabla f^-_k \rangle dx + \int_{\mathbb{R}^d} \langle \nabla f^+, f^- \rangle dx = \int_{\mathbb{R}^d} v_{ij} \varphi^2 dx,
\]

for every \(0 \leq \varphi \in C^\infty_c(\mathbb{R}^d)\). This yields \(v_{ij} \leq 0\) a.e. Conversely, assume that the off-diagonal entries \(v_{ij}, i \neq j\), are less than or equal to 0 and let \(f \in D(a)\). Let us show first that \(f^+ \in D(a)\). According to [5, Lemma 7.6] one has, \(\nabla f^+_k = \chi_{\{f_k > 0\}} \nabla f_k\) and \(\nabla f^-_k = \chi_{\{f_k < 0\}} \nabla f_k\), hence \(f^+ \in H^1(\mathbb{R}^d, \mathbb{R}^m)\) and \(\langle Q \nabla f^+_k, \nabla f^-_k \rangle = 0\). On the other hand,

\[
\langle Vf, f \rangle = \langle V(f^+ - f^-), (f^+ - f^-) \rangle = \langle Vf^+, f^+ \rangle + \langle Vf^-, f^- \rangle - 2 \langle Vf^+, f^- \rangle = \langle Vf^+, f^+ \rangle + \langle Vf^-, f^- \rangle - 2 \sum_{i,j=1}^{m} v_{ij} f^+_i f^-_j
\]

\[
\geq \langle Vf^+, f^+ \rangle + \langle Vf^-, f^- \rangle \geq \langle Vf^+, f^+ \rangle.
\]

Thus \(\int_{\mathbb{R}^d} \langle Vf^+, f^+ \rangle dx \leq \int_{\mathbb{R}^d} \langle Vf, f \rangle dx < \infty\). Consequently \(f^+ \in D(a)\). Moreover,

\[
a(f^+, f^-) = \sum_{k=1}^{m} \int_{\mathbb{R}^d} \langle Q \nabla f^+_k, \nabla f^-_k \rangle dx + \int_{\mathbb{R}^d} \langle Vf^+, f^- \rangle dx = \int_{\mathbb{R}^d} \sum_{i,j=1}^{m} v_{ij} f^+_i f^-_j dx
\]
\[
= \int_{\mathbb{R}^d} \sum_{i=1}^{m} v_{ii} f_i^+ f_i^- \, dx + \int_{\mathbb{R}^d} \sum_{i \neq j} v_{ij} f_i^+ f_j^- \, dx
= \int_{\mathbb{R}^d} \sum_{i \neq j} v_{ij} f_i^+ f_j^- \, dx \leq 0.
\]

4.2 Compactness

In this subsection we give a necessary condition for compactness of the resolvent of the operator $A$ in $L^2(\mathbb{R}^d, \mathbb{R}^m)$ and we give counter example when the condition is not satisfied. Our assumption is that the smallest eigenvalue $\mu(x)$ of $V(x)$ blow up at infinity, which we rewrite as follows:

There exists $\mu : \mathbb{R}^d \to \mathbb{R}^+$ locally integrable such that $\lim_{|x| \to \infty} \mu(x) = +\infty$, and

\[
(V(x)\xi, \xi) \geq \mu(x)|\xi|^2, \quad \forall \xi \in \mathbb{R}^m, \forall x \in \mathbb{R}^d. \tag{4.1}
\]

**Proposition 4.3** Assume that (4.1) is satisfied. Then, $T_p(t)$ is compact in $L^p(\mathbb{R}^d, \mathbb{C}^m)$, for every $t > 0$. Consequently, the spectrum of $A_p$ is independent of $p \in (1, \infty)$, countable and consists of negative eigenvalues that accumulate at $-\infty$.

**Proof** It suffices to prove $D(a)$ is compactly embedded in $L^2(\mathbb{R}^d, \mathbb{C}^m)$. Indeed, this implies that $A$ has a compact resolvent and, by analyticity, $T(t)$ is compact in $L^2(\mathbb{R}^d, \mathbb{R}^m)$, for every $t > 0$. The compactness in $L^p(\mathbb{R}^d, \mathbb{C}^m)$, $1 < p < \infty$, follows by [2, Theorem 1.6.1] and the $p$-independence of the spectrum by [2, Corollary 1.6.2].

Now, let us consider the ‘diagonal’ sesquilinear form

\[
a_{\mu}(f, g) = \int_{\mathbb{R}^d} \sum_{j=1}^{m} (Q(x)\nabla f_j(x), \nabla g_j(x)) \, dx + \int_{\mathbb{R}^d} \sum_{j=1}^{m} \mu(x) f_j(x) g_j(x) \, dx,
\]

with domain

\[
D(a_{\mu}) = \{ f \in H^1(\mathbb{R}^d, \mathbb{C}^m) : \int_{\mathbb{R}^d} \sum_{j=1}^{m} \mu(x)|f_j(x)|^2 \, dx < +\infty \}.
\]

Since $\lim_{|x| \to \infty} \mu(x) = +\infty$, one has $D(a_{\mu})$ is compactly embedded in $L^2(\mathbb{R}^d, \mathbb{C}^m)$, see [2, Chapter 4]. On the other hand, (4.1) implies $D(a) \subseteq D(a_{\mu})$ and $a_{\mu}(f) \leq a(f)$ for all $f \in D(a)$. Thus, $D(a)$ is continuously embedded in $D(a_{\mu})$. It follows that the embedding $D(a) \hookrightarrow L^2(\mathbb{R}^d, \mathbb{C}^m)$ is compact. Now, the discreteness of the spectrum follows by the spectral mapping theorem, since $A$ has a compact resolvent. \[\square\]

**Example 4.4** Here we give a counter-example where Proposition 4.3 cannot apply and the compactness result fails even if all entries of the matrix potential blow up at infinity.
We even have a spectrum which is not punctual. Let us consider the following two-size matrix-valued function

\[ x \mapsto V(x) := v(x) \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = v(x)J, \]

where \( v \in L^1_{\text{loc}}(\mathbb{R}^d) \) is a nonnegative function such that \( \lim_{|x| \to \infty} v(x) = +\infty \). \( V \) is symmetric and satisfies (2.2). \( V \) can be written as follow

\[ V(x) = P^{-1} \begin{pmatrix} 2v(x) & 0 \\ 0 & 0 \end{pmatrix} P, \]

where \( P := \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \). The Schrödinger operator \( A \) with \( Q = I_2 \) becomes

\[ A = \Delta - V = P^{-1} \begin{pmatrix} \Delta - 2v(x) & 0 \\ 0 & \Delta \end{pmatrix} P. \]

Since the Laplacian operator \( \Delta \) has no compact resolvent on \( L^2(\mathbb{R}^d) \), thus the matrix operator

\[ \begin{pmatrix} \Delta - 2v(x) & 0 \\ 0 & \Delta \end{pmatrix} \]

has no compact resolvent. Then so is \( A \).

Furthermore, the spectrum of \( A \) is continuous. In fact, \( \sigma(A) = \sigma(\Delta) \cup \sigma(\Delta - 2v) = ] - \infty, 0[. \) However, the punctual spectrum \( \sigma_p(A) = \sigma(\Delta - 2v) \) is countable.

Such potentials can be constructed even for higher dimensions : \( m \geq 3 \). One can consider \( V(x) = v(x)J_m \) where \( v \) is any nonnegative locally integrable function that blow up at infinity and \( J_m \) a symmetric semi-definite positive \((m \times m)\)-matrix having 0 as eigenvalue. For instance, one can choose

\[ J_m = \begin{pmatrix} m - 1 & -1 & \cdots & -1 \\ -1 & m - 1 & \cdots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ -1 & \cdots & -1 & m - 1 \end{pmatrix}. \]

**Remark 4.5** Under the condition (4.1) which guaranties the compactness of the resolvent of \( A \), one can get more information about the spectrum \( \sigma(A) \) of \( A \) by application of the min-max principle. Indeed, let \( \mu, v : \mathbb{R}^d \to \mathbb{R}^+ \) be locally integrable such that \( \mu \) blows up at infinity and

\[ \mu(x)|\xi|^2 \leq \langle V(x)\xi, \xi \rangle \leq v(x)|\xi|^2, \quad (4.2) \]

\( \blacksquare \) Springer
for every \( x \in \mathbb{R}^d \) and \( \xi \in \mathbb{R}^m \). Denote by \( \{ \lambda_1 < \lambda_2 < \ldots \} \) the increasing sequence of eigenvalues of \( -A \). By \( \{ \lambda_1^\mu < \lambda_2^\mu < \ldots \} \) we denote the eigenvalues of the scalar operator \( -(\text{div}(Q \nabla \cdot) - \mu) \) in \( L^2(\mathbb{R}^d) \). We use the same notation for \( \nu \). According to the min-max principle, one has \( \lambda_n^\nu \leq \lambda_n \leq \lambda_n^\mu \), for all \( n \in \mathbb{N} \).

We recall that the min-max principle is a way to express eigenvalues of an operator via its associated form, see [1, Chapter IV]. The min-max formula applied to \( A \) yields

\[
\lambda_n = \max_{F_1, \ldots, F_{n-1} \in H} \inf \{ a(f) : f \in \{ F_1, \ldots, F_{n-1} \} \perp \cap D(a) \text{ with } \| f \| = 1 \}.
\]

Acknowledgements The author would like to thank Markus Kunze for suggesting the reference [9] which contains the vectorial Deny–Beurling criterion of \( L^\infty \)-contractivity. He is also grateful to the referee for valuable comments and suggestions.

References

1. Courant, R., Hilbert, D.: Methods of Mathematical Physics, vol. 1. Interscience Publishers, New York (1953)
2. Davies, E.B.: Heat Kernels and Spectral Theory. Cambridge University Press, Cambridge (1989)
3. Engel, K.J., Nagel, R.: One-Parameter Semigroups for Linear Evolution Equations. Springer, New York (2000)
4. Favini, A., Goldstein, G.R., Goldstein, J.A., Obrecht, E., Romanelli, S.: Elliptic operators with general Wentzell boundary conditions, analytic semigroups and the angle concavity theorem. Math. Nachr. 283(4), 504–521 (2010)
5. Gilbarg, D., Trudinger, N.: Elliptic Partial Differential Equations of Second Order. Springer, New York (1983)
6. Kunze, M., Lorenzi, L., Maichine, A., Rhandi, A.: \( L^p \)-theory for Schrödinger systems. arXiv:1705.03333
7. Maichine, A., Rhandi, A.: On a polynomial scalar perturbation of a Schrödinger system in \( L^p \)-spaces. J. Math. Anal. Appl. 466, 655–675 (2018)
8. Ouhabaz, E.M.: Analysis of Heat Equations on Domains. London Math. Soc. Monogr. Ser., vol. 31. Princeton Univ. Press, Princeton (2004)
9. Ouhabaz, E.M.: \( L^p \) contraction semigroups for vector valued functions. Positivity 3, 83–93 (1999)
10. Voigt, J.: One-parameter semigroups acting simultaneously on different \( L_p \)-spaces. Bull. Soc. R. Sci. Liège 61, 465–470 (1992)
11. Worth, G.A., Robbb, M.A., Lasorne, B.: Solving the time-dependent Schrödinger equation for nuclear motion in one step: direct dynamics of non-adiabatic systems. Mol. Phys. 106(16–18), 2077–2091 (2008). https://doi.org/10.1080/00268970802172503
12. Wodtke, A.M., Tully, J.C., Auerbach, D.J.: Electronically non-adiabatic interactions of molecules at metal surfaces: can we trust the Born–Oppenheimer approximation for surface chemistry? Int. Rev. Phys. Chem. 23(4), 513–539 (2004). https://doi.org/10.1080/01442350500037521