Self-adjoint extensions of momentum operators: application of weak Weyl relations

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Abstract. By weak Weyl relations it is shown that momentum operators, \(-i\partial_x\), defined on \(C_0^\infty(\Omega)\) with some general open set \(\Omega \subset \mathbb{R}^n\) are not essentially self-adjoint but have uncountably many self-adjoint extensions.

Keywords. canonical commutation relation, CCR, Weyl relation, weak Weyl relation, momentum operator

1. Preliminaries

In this paper we are concerned with uncountably many self-adjoint extensions of momentum operators defined on open sets in \(\mathbb{R}^n\). Let us begin with considering a one dimensional momentum operator

\[ p = -i \frac{d}{dx}. \]

It is well known that \(p\) is essentially self-adjoint on \(C_0^\infty((-\infty, \infty))\), namely it has the unique self-adjoint extension. We can see however that \(p\) has no self-adjoint extension on \(C_0^\infty((0, \infty))\) but has uncountably many self-adjoint extensions on \(C_0^\infty((0, 1))\). When the dimension \(n \geq 2\), however, it is not trivial to see the essential or non-essential self-adjointness of momentum operators defined on \(C_0^\infty(\Omega)\) with open set \(\Omega\). We are then interested in self-adjoint extensions of momentum operator \(-i\partial_x\) on \(L^2(\Omega)\) with a general open set \(\Omega \subset \mathbb{R}^n\). In this paper we show a sufficient condition such that \(-i\partial_x\) is not essentially self-adjoint but has uncountably many self-adjoint extensions by using the so-called weak Weyl relations.

Let \(\mathcal{H}\) be a separable Hilbert space. Let \(H\) be a self-adjoint operator and \(T\) a symmetric operator on \(\mathcal{H}\). We say that \(\{T, H\}\) satisfies weak Weyl relation if

\[ e^{-itH} \text{Dom}(T) \subset \text{Dom}(T) \]

and

\[ T e^{-itH} \psi = e^{-itH}(T + t)\psi \]

holds for all \(\psi \in \text{Dom}(T)\) and \(t \in \mathbb{R}\), where \(\text{Dom}(A)\) denotes the domain of operator \(A\). A symmetric operator \(T\) satisfying (2) is called a time operator associated with \(H\), which is, to our best knowledge, introduced by [Sch83A, Sch83B] and drastically investigated by [Ara05]. See also [Ara99-a, Ara99-b]. If \(T\) is self-adjoint instead of symmetric, and \(\{T, H\}\) satisfies the Weyl relation

\[ e^{-isT} e^{-itH} = e^{-ist} e^{-isT} e^{-itH}, \]

then weak Weyl relation (2) can be derived from (3), but (2) does not necessarily imply (3) in general. The important facts on weak Weyl relations and Weyl relation are (1) and (2) below:

1. If \(T\) is a self-adjoint operator, then Weyl relation (3) can be derived from weak Weyl relation (2);

2. If \(\{T, H\}\) satisfies Weyl relation (3), then there exist Hilbert spaces \(\mathcal{H}_m\) and unitary operators \(U_m: \mathcal{H}_m \rightarrow L^2(\mathbb{R}), \quad 1 \leq m \leq M,\)

such that

\[ \begin{align*}
(1) & \quad \mathcal{H} = \bigoplus_{m=1}^M \mathcal{H}_m, \\
(2) & \quad T \text{ and } H \text{ are reduced to } \mathcal{H}_m, \\
(3) & \quad U_T|_{\mathcal{H}_m} U^{-1} = x \text{ and } U_H|_{\mathcal{H}_m} U^{-1} = -i \frac{d}{dx}. 
\end{align*} \]

(2) is known as von Neumann’s uniqueness theorem.

The key idea in this paper is that the momentum operator \(-i\partial_x\) can be regarded as the time operator associated with multiplication operator \(-x\). If \(-i\partial_x\) is essentially self-adjoint on \(C_0^\infty(\Omega)\) with an open set \(\Omega \subset \mathbb{R}^n\), then the pair of self-adjoint operators

\[ \left\{-i\partial_x |_{C_0^\infty(\Omega)}, -x \right\} \]

also satisfies Weyl relation. If the multiplication operator \(x\) on \(L^2(\Omega)\) is bounded, then it contradicts von Neumann’s uniqueness theorem. Thus we can conclude that \(-i\partial_x |_{C_0^\infty(\Omega)}\) is not essentially self-adjoint if \(\Omega\) is bounded. This kind of results may be already known, but our proof is new and simple. In this paper we discuss more general open sets \(\Omega\), which include unbounded sets.
2. TIME OPERATORS AND MAIN RESULTS

In this section we introduce weak Weyl relations and time operators, and prove the main theorem.

**Definition 1.** (1) Let $T_1, \ldots, T_n$ and $H_1, \ldots, H_n$ be self-adjoint. We say that $(T_j, H_j)_{j=1}^n$ is Weyl relation if and only if

\[
e^{-itT_i}e^{-isH_k} = e^{-is\delta_{jk}t}e^{-isH_k}e^{-itT_j}
\]

\[
e^{-itT_i}e^{-isT_k} = e^{-isT_k}e^{-itT_j}
\]

\[
e^{-itH_j}e^{-isH_k} = e^{-isH_k}e^{-itH_j}
\]

hold for all $s, t \in \mathbb{R}$ and $j, k = 1, \ldots, n$.

(2) Let $T_1, \ldots, T_n$ be symmetric and $H_1, \ldots, H_n$ self-adjoint. We say that $(T_j, H_j)_{j=1}^n$ is weak Weyl relation if and only if

\[
e^{-itH_k}\text{Dom}(T_j) \subset \text{Dom}(T_j)
\]

and

\[
T_j e^{-itH_k} \psi = e^{-itH_k} (T_j + \delta_{jk}t) \psi, \psi \in \text{Dom}(T_j),
\]

hold for all $t \in \mathbb{R}$ and $j, k = 1, \ldots, n$.

We show some properties of Weyl relation and weak Weyl relation. Let $\mathcal{T}$ denote the closure of $T$. Let $(T_j, H_j)_{j=1}^n$ be weak Weyl relation, then also is $(\mathcal{T}_j, \mathcal{H}_j)_{j=1}^n$. As is easily seen that weak Weyl relation can be derived from Weyl relation. The converse is, however, not true. If $(T, H)$ is a weak Weyl relation, then the spectrum of $H$ is purely absolutely continuous. In particular $H$ has no eigenvalues. See [AM08-a, Gal02, Miy01]. Furthermore we can construct a time operator $T_g(H)$ associated with $g(H)$, where $g$ is some Borel measurable function, as

\[
T_g(H) = \frac{1}{2} (g(H)^{-1} T + T g(H)^{-1}),
\]

where $g = dg/dx$. See [AM08-b, HKM09] for details.

An important relationship between weak Weyl relation and Weyl relation is as follows.

**Proposition 1.** Let $(T_j, H_j)_{j=1}^n$ be weak Weyl relation and $T_1, \ldots, T_n$ self-adjoint. Then $(T_j, H_j)_{j=1}^n$ is Weyl relation.

**Proof.** See [Ara05, Proposition 2.10].

Let us define operators $\hat{x}_1, \ldots, \hat{x}_n$ and $\hat{p}_1, \ldots, \hat{p}_n$ in $L^2(\mathbb{R}^n)$. Operator $\hat{x}_j$ is the multiplication operator by $x_j$ with the domain

\[
\text{Dom}(\hat{x}_j) = \left\{ f \in L^2(\mathbb{R}^n) : \int_{\mathbb{R}^n} x_j^2 |f(x)|^2 dx < \infty \right\},
\]

and

\[
\hat{p}_j = -i\partial_{x_j}
\]

with

\[
\text{Dom}(\hat{p}_j) = H^1(\mathbb{R}^n).
\]

It is a fundamental fact that $\{\hat{x}_j, \hat{p}_j\}_{j=1}^n$ or $\{\hat{p}_j, -\hat{x}_j\}_{j=1}^n$ are Weyl relations.

**Proposition 2.** (von Neumann’s uniqueness theorem [Nen31]) Let $(T_j, H_j)_{j=1}^n$ be Weyl relation. Then there exist Hilbert spaces $\mathcal{H}_m$ and unitary operators $U_m : \mathcal{H}_m \to L^2(\mathbb{R}^m)$, $1 \leq m \leq M$, such that

(1) $\mathcal{H} = \bigoplus_{m=1}^M \mathcal{H}_m$,

(2) for each $j = 1, \ldots, n$, $T_j$ and $H_j$ are reduced to $\mathcal{H}_m$,

(3) $U_m T_j |_{\mathcal{H}_m} U_m^{-1} = \hat{x}_j$ and $U_m H_j |_{\mathcal{H}_m} U_m^{-1} = \hat{p}_j$.

In particular Spec$(T_j) = \text{Spec}(H_j) = \mathbb{R}$.

The next lemma is a criterion to show non-essential self-adjointness of a time operator.

**Lemma 1.** Let $(T_j, H_j)_{j=1}^n$ be weak Weyl relation with Spec$(H_j) \neq \mathbb{R}$ for some $j = 1, \ldots, n$. Then $T_j$ is not essentially self-adjoint.

**Proof.** Suppose that $T_j$ is essentially self-adjoint. Then $(\mathcal{T}_j, \mathcal{H}_j)$ is Weyl relation by Proposition 1. However this contradicts Proposition 2 since Spec$(H_j) \neq \mathbb{R}$. Therefore $T_j$ is not essentially self-adjoint.

Let $\Omega$ be an open subset in $\mathbb{R}^n$. Let $x_j$ be the multiplication operator by $x_j$ with

\[
\text{Dom}(x_j) = \left\{ f \in L^2(\Omega) : \int_{\Omega} x_j^2 |f(x)|^2 dx < \infty \right\},
\]

and $p_j = -i\partial_{x_j}$ with

\[
\text{Dom}(p_j) = C_0^\infty(\Omega).
\]

Let $f, g \in C_0^\infty(\Omega)$. Since we know that

\[
(f, p_j g)_{L^2(\Omega)} = (f, p_j g)_{L^2(\mathbb{R}^n)} = (p_j f, g)_{L^2(\mathbb{R}^n)} = (p_j f, g)_{L^2(\Omega)},
\]

$p_j$ is symmetric and then closable.

**Lemma 2.** Let $\Omega$ be an open subset in $\mathbb{R}^n$. Then $(\mathcal{T}_j, -x_j)_{j=1}^n$ is weak Weyl relation on $L^2(\Omega)$.

**Proof.** Since $e^{itx_j}$ leaves $C_0^\infty(\Omega)$ invariant and

\[
p_k e^{itx_j} f = e^{itx_j} (p_k + \delta_{jk} t) f
\]

for $f \in C_0^\infty(\Omega)$ by a direct calculation, $(p_j, -x_j)_{j=1}^n$ is weak Weyl relation on $L^2(\Omega)$. Hence $(\mathcal{T}_j, -x_j)_{j=1}^n$ is also weak Weyl relation.

We define the class $\mathcal{O}_j$ of open subsets in $\mathbb{R}^n$. Let $\pi_j : \mathbb{R}^n \to \mathbb{R}$ be the projection defined by $\pi_j(x) = x_j$. We define $\mathcal{O}_j$ by

\[
\mathcal{O}_j = \left\{ \Omega \subset \mathbb{R}^n \mid \Omega \text{ is an open subset and } \pi_j(\Omega) \neq \mathbb{R} \right\}
\]

for $j = 1, \ldots, n$.

**Theorem 1.** Let $\Omega \in \mathcal{O}_j$. Then $p_j$ is not essentially self-adjoint on $C_0^\infty(\Omega)$. 

Proof. Note that \( \text{Spec}(x_j) = \overline{\pi_j(\Omega)} \neq \mathbb{R} \) for \( \Omega \in \mathcal{O} \). Assume that \( p_j \) is essentially self-adjoint. Then \( \{p_j, -x_j\} \) is weak Weyl relation by Lemma 2. In particular, \( \{p_j, -x_j\} \) is also Weyl relation. It however contradicts Lemma 1 since \( \text{Spec}(x_j) \neq \mathbb{R} \). Hence \( p_j \) is not essentially self-adjoint.

Let \( \mathcal{O} \) be the set of open subsets \( \Omega \) in \( \mathbb{R}^n \) such that \( \overline{\Omega} \neq \mathbb{R}^n \).

**Theorem 2.** Let \( \Omega \in \mathcal{O} \). Then at least one momentum operator is not essentially self-adjoint on \( C_0^\infty(\Omega) \).

Proof. Assume that all the momentum operators \( p_j \) are essentially self-adjoint. Then \( \{p_j, -x_j\} \) is Weyl relation. Thus the joint distribution of \( \{x_1, \ldots, x_n\} \) has to be \( \mathbb{R}^n \) by Theorem 1, but is indeed \( \overline{\Omega} \). Then at least one momentum operator is not essentially self-adjoint.

The following corollary is immediate.

**Corollary 1.** Let \( \Omega \in \mathcal{O} \). Then for all \( \Omega \) in \( \mathbb{R}^{n-1} \) such that \( \overline{\Omega} = \mathbb{R} \times K \).

**Theorem 3.** Let \( \Omega \) be simple. Then each momentum operator \( p_j, j = 1, \ldots, n \), is not essentially self-adjoint on \( C_0^\infty(\Omega) \).

Proof. By Theorem 2 at least one momentum operator is not essentially self-adjoint. Since all the momentum operators are unitarily equivalent by the symmetry, each \( p_j \) is not essentially self-adjoint on \( C_0^\infty(\Omega) \).

### 3. Generalizations

We can extend Theorems 1 and 2 mentioned in the previous section. We say that an open set \( \Omega \) is simple if and only if there is no open set \( K \subset \mathbb{R}^{n-1} \) such that \( \Omega = \mathbb{R} \times K \).

**Theorem 3.** Let \( \Omega \) be simple. Then each momentum operator \( p_j, j = 1, \ldots, n \), is not essentially self-adjoint on \( C_0^\infty(\Omega) \).

Proof. Let \( 1 \leq j \leq n \) be fixed. Then there exists a parallel transformation \( T \) on \( \mathbb{R}^n \) such that

\[
O = (0, \ldots, 0) \notin T\Omega \tag{7}
\]

and

\[
X_j = (0, \ldots, 0, t) \in T\Omega
\]

with some \( t \). Without loss of generality we may reset \( T\Omega = \Omega \). The distance between \( \Omega \) and the origin \( O \) is denoted by \( \delta > 0 \). Let \( \delta > \epsilon > 0 \) be such that

\[
B_\epsilon(X_j) \subset \Omega \tag{9}
\]

where \( B_\epsilon(X_j) \) denotes the open ball centered at \( X_j \) with radius \( \epsilon \). \( (9) \) can be possible by \( (8) \) for sufficiently small \( \epsilon \).

Now we define the self-adjoint operator \( D \) on \( L^2(\Omega) \) by

\[
D = \sum_{j=1}^n x_j^2 \tag{10}
\]

Thus it follows that

\[
(f, Df)_{L^2(\Omega)} \geq \delta^2 \|f\|_{L^2(\Omega)}^2
\]

for all \( f \in C_0^\infty(\Omega) \). Let \( \phi \in C_0^\infty(\mathbb{R}^n) \) be such that \( \text{supp}\phi \subset B_\epsilon(0) \). See Fig. 1. With \( t \in \mathbb{R} \), the parallel transform of \( \phi \) in the \( X_j \)-direction is denoted by \( \phi_t \):

\[
\phi_t(x) = \phi((x_1, \ldots, x_j - t, \ldots, x_n)), \quad x \in \Omega,
\]

we see that \( \phi_t \in L^2(\Omega) \) by \( (9) \). Suppose that \( p_j \) is essentially self-adjoint on \( C_0^\infty(\Omega) \) and we denote the closure of \( p_j \) by \( P_j \). Thus it follows that

\[
\langle e^{i\alpha P_j} \phi_t, D e^{i\alpha P_j} \phi_t \rangle_{L^2(\Omega)} \geq \delta^2 \|\phi\|_{L^2(\mathbb{R}^n)}^2. \tag{11}
\]

Now we compute the left hand side of \( (11) \). Since \( P_j \) is self-adjoint, \( \{P_j, -x_j\} \) is not only weak Weyl relation but also Weyl relation. Then

\[
e^{-i\alpha P_j} e^{ix_j} e^{-i\alpha P_j} = e^{-i\alpha P_j} (x_j + s)
\]

From this the weak Weyl relation
follows. Thus

\begin{equation}
 x_j^2 e^{-isP_j} = e^{-isP_j} (x_j + s)^2 \tag{12}
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\end{equation}
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on \( C^\infty_0(\Omega) \). Inserting \(-s\) into \( s \) in (12), we have

\begin{equation}
 x_j^2 e^{-isP_j} = e^{-isP_j} (x_j - s)^2 \tag{13}
\end{equation}

and

\[ e^{-isP_j} D e^{isP_j} = x_j^2 + \cdots + (x_j - s)^2 + \cdots + x_n^2 \]

on \( C^\infty_0(\Omega) \). Inserting this into the left-hand side of (11) and setting \( t = s \), we have

\[ \text{LHS} (11) = \int_{\mathcal{B}_i(0)} |\phi(x)|^2 \left( \sum_{j=1}^n x_j^2 \right) dx \leq \epsilon^2 ||\phi||^2_{L^2(\mathbb{R}^n)}. \]

Thus \( \epsilon^2 ||\phi||^2_{L^2(\mathbb{R}^n)} \geq \delta^2 ||\phi||^2_{L^2(\mathbb{R}^n)} \). See Fig. 2. This contradicts the \( \epsilon < \delta \) and then \( p_j \) is not essentially self-adjoint. \( \square \)

**Theorem 4.** Let \( \Omega = \mathbb{R}^m \times K \subseteq \mathcal{E} \), where \( K \) is simple. Then \( p_1, \ldots, p_m \) are essentially self-adjoint on \( C^\infty_0(\Omega) \) but \( p_{m+1}, \ldots, p_n \) are not essentially self-adjoint.

**Proof.** Under the identification \( L^2(\Omega) = L^2(\mathbb{R}^m) \otimes L^2(K) \), \( p_j = p_{ij} \otimes 1, j = 1, \ldots, m \), are essentially self-adjoint on \( C^\infty_0(\Omega) \). While \( p_j, m + 1 \leq j \leq n \), are not essentially self-adjoint by Theorem 3. \( \square \)

Now we investigate the existence of self-adjoint extensions of momentum operators defined in \( L^2(\Omega) \). Let \( R_j : \mathbb{R}^n \to \mathbb{R}^n \) be the reflection defined by replacing the \( j \)th coordinate \( x_j \) with \( -x_j \). Let \( \theta_{\text{sym}, j} \) be defined by

\[ \theta_{\text{sym}, j} = \{ \Omega \in \mathcal{E} | R_j \Omega = \Omega \}, \quad j = 1, \ldots, n. \]

**Corollary 2.** Let \( \Omega \in \theta_{\text{sym}, j} \) and suppose that \( p_j \) is not essentially self-adjoint. Then uncountably many self-adjoint extensions of \( p_j | C^\infty_0(\Omega) \) exist.

**Proof.** Let \( P_j = p_{ij} | C^\infty_0(\Omega) \). Let \( C_j : L^2(Q) \to L^2(Q) \) be the antilinear map defined by

\[ (C_j f)(x) = \overline{f(R_j x)}, \]

where \( \overline{f} \) denotes the complex conjugate of \( f \). We can see that \( C_j : C^\infty_0(\Omega) \to C^\infty_0(\Omega) \) and \( C_j p_j C_j \) on \( C^\infty_0(\Omega) \), then a limiting argument yields that \( C_j \text{Dom}(P_j) \subset \text{Dom}(P_j) \) and \( C_j P_j = P_j C_j \) on \( \text{Dom}(P_j) \). From this it follows that \( p_j \) has equal deficiency indices by von Neumann’s theorem [RS2, Theorem X.3]. Since \( P_j \) is not self-adjoint, the deficiency indices of \( P_j \) is \( (m, m) \) with \( m \geq 1 \). Hence \( P_j \) has uncountably many self-adjoint extensions. \( \square \)

**Example 1.** (1) Let \( \Omega = \mathbb{R}^n \setminus \mathcal{B}_i(0) \). Then each \( p_j, \ j = 1, \ldots, n, \) is not essentially self-adjoint and has uncountably many self-adjoint extensions, since \( \Omega \in \cap_{j=1}^n \theta_{\text{sym}, j} \). Refer to see [Hir00].

(2) Let \( \Omega = \mathcal{B}_r(0) \). Then each \( p_j, j = 1, \ldots, n, \) is not essentially self-adjoint and has uncountably many self-adjoint extensions, since \( \Omega \in \cap_{j=1}^n \theta_{\text{sym}, j} \).

(3) Let

\[ \Omega_+ = \{(x, y) \in \mathbb{R}^2 | -1 < xy < 1 \}, \]

\[ \Omega_- = \{(x, y) \in \mathbb{R}^2 | 1 < xy, xy < -1 \}. \]

Then \( p_j, j = 1, 2, \) are not essentially self-adjoint on \( C^\infty_0(\Omega_\pm) \) but have uncountably many self-adjoint extensions, since \( \Omega_\pm \in \cap_{j=1,2} \theta_{\text{sym}, j} \).

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