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Spectral Inclusion Properties of Unbounded Hamiltonian Operators*

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Abstract In this paper, the authors investigate the spectral inclusion properties of the quadratic numerical range for unbounded Hamiltonian operators. Moreover, some examples are presented to illustrate the main results.

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1 Introduction

For a system in quantum mechanics, quantum field theory and elasticity theory, the physical reasoning may give a formal expression of its Hamiltonian. It is, in general, a partial differential operator in an appropriate functional space, and we say "formal" when the domain of the Hamiltonian is not specified. It is usually easy to find a dense domain on which the formal Hamiltonian is well-defined (see [11]).

Let X be an infinite dimensional complex Hilbert space. The Hamiltonian operator is given by the following densely-defined closed block-operator matrix:

$$H = \begin{pmatrix} A & B \\ C & -A^* \end{pmatrix}, \quad \mathcal{D}(H) = (\mathcal{D}(A) \cap \mathcal{D}(C)) \oplus (\mathcal{D}(B) \cap \mathcal{D}(-A^*)), \tag{1.1}$$

where A is closed and B, C are self-adjoint in X. In particular, if $A = 0$ (resp. $C = 0$), we call H off-diagonal (resp. upper triangular); while we call H non-negative if B and C are non-negative operators.

Clearly, the Hamiltonian operator H satisfies $JH \subset (JH)^*$, $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$. The Hamiltonian operator, however, is not symplectic self-adjoint in general, i.e., $(JH)^* \neq JH$, for it might be difficult to find a general approach to compute the adjoint of unbounded operator matrices,

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when there are rows or columns with more than one unbounded entry. In fact, a Hamiltonian operator is symplectic self-adjoint if and only if its adjoint coincides with its formal adjoint. It is well-known that the symplectic self-adjoint operator matrix H has some good spectral properties as follows (see [1]). (i) The union of the point spectrum $\sigma_p(H)$ and the residual spectrum $\sigma_r(H)$ is symmetric with respect to the imaginary axis, and $\sigma_r(H)$ contains no point symmetric with respect to the imaginary axis. Then, we further have that $\sigma_r(H) = \emptyset$ if and only if $\sigma_p(H)$ is symmetric with respect to the imaginary axis. (ii) The continuous spectrum $\sigma_c(H)$, and therefore the spectrum $\sigma(H)$ and the resolvent set $\rho(H)$ are all symmetric with respect to the imaginary axis. These spectral properties have important applications in the numerical computation of Hamiltonian systems, and in the completeness of the eigenfunction system of symplectic self-adjoint operator matrices (see [14]).

The invariant subspaces of Hamiltonian operators and solutions of the corresponding Riccati equations were studied in [8]. In [7], Kurina G. A. investigated the invertibility of non-negative Hamiltonian operators with bounded off-diagonal entries, and Wu D. and Chen A. [15] extended the results to the unbounded cases with diagonal and off-diagonal domains. In [9], Langer H., Markus A. S., Matsaev V. I. and Tretter C. introduced the concept of the quadratic numerical range, which may be used to give enclosures for the spectrum of block operator matrices. The numerical range of an operator may be used for studying spectral properties of operators. However, the numerical range is not defined with respect to the block structure of operator matrices, and thus the lost information of the entries may lead to the loss of some related properties. The quadratic numerical range is always contained in the numerical range.

It has been shown that, for bounded operator matrices, the closure of the quadratic numerical range contains their spectrum. But, it is not the case for unbounded block operator matrices, even when we only consider the approximate point spectrum. In fact, the approximate point spectrum of an unbounded linear operator in a Hilbert space is contained in the closure of the numerical range. In [13], Tretter C. proved the analogue of this inclusion for the quadratic numerical range for diagonally dominant and for off-diagonally dominant block operator matrices of order 0. In this paper, we make use of the particular block structure of the unbounded Hamiltonian operators to consider the spectral inclusion properties of unbounded Hamiltonian operators by the quadratic numerical range.

The present paper is organized as follows. In Section 2, we state some basic concepts. In Section 3.1, the off-diagonally Hamiltonian operator is considered; the upper triangular case is investigated in Section 3.2; in Section 3.3, we show the spectral inclusion properties of diagonally dominant and off-diagonally dominant Hamiltonian operators of order 0.

2 Preliminaries

Throughout this paper, X and Y are always infinite dimensional complex Hilbert spaces unless otherwise stated. For a (linear) operator T on some Banach space, the domain, range and kernel of T are denoted by $\mathcal{D}(T)$, $\mathcal{R}(T)$ and $\mathcal{N}(T)$, respectively. If, in addition, T is an operator on a Hilbert space, we use T^* to denote its adjoint. The resolvent set of T is defined by

$$\rho(T) := \{\lambda \in \mathbb{C} : T - \lambda \text{ is a bijection with } (T-\lambda)^{-1} \text{ continuous}\},$$

and the set

$$\sigma(T) := \mathbb{C} \setminus \rho(T)$$

is called the spectrum of T.

In the following, we give some basic concepts which are used in our main theorems and their proofs.

Definition 2.1 (see [2]) *Let T be an operator on a Banach space X. The approximate point spectrum $\sigma_{ap}(T)$ of T is defined by*

$$\sigma_{ap}(T) := \{\lambda \in \mathbb{C} : \exists (x_n)_1^\infty \subset \mathcal{D}(T), \|x_n\| = 1 \textit{ such that } (T - \lambda I)x_n \to 0\}.$$

Set

$$\sigma_{r,1}(T) := \{\lambda \in \mathbb{C} : T - \lambda I \quad \textit{is injective}, \overline{\mathcal{R}(T-\lambda I)} \neq X, \mathcal{R}(T-\lambda I) \textit{ is closed}\},$$

and then, for a closed operator T, we have $\sigma(T) = \sigma_{ap}(T) \cup \sigma_{r,1}(T)$ by the closed graph theorem.

Definition 2.2 (see [4]) *For an operator T on X, the numerical range $W(T)$ of T is defined by*

$$W(T) := \{(Tx, x) : x \in \mathcal{D}(T), \|x\| = 1\}.$$

Definition 2.3 (see [9]) *For a block-operator matrix $\mathcal{A} = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)$ with $\mathcal{D}(\mathcal{A}) = (\mathcal{D}(A) \cap \mathcal{D}(C)) \oplus (\mathcal{D}(B) \cap \mathcal{D}(D)) = \mathcal{D}_1 \oplus \mathcal{D}_2$ in $X \oplus Y$, we define*

$$\mathcal{A}_{f,g} := \begin{pmatrix} (Af, f) & (Bg, f) \\ (Cf, g) & (Dg, g) \end{pmatrix}, \quad f \in \mathcal{D}_1, \; g \in \mathcal{D}_2,$$

which is clearly a 2×2 complex matrix. Then the set

$$W^2(\mathcal{A}) := \bigcup_{\substack{f \in \mathcal{D}_1, g \in \mathcal{D}_2 \\ \|f\| = \|g\| = 1}} \sigma_p(\mathcal{A}_{f,g})$$

is called the quadratic numerical range of $\mathcal{A}$.

Definition 2.4 (see [12]) *Let $T : \mathcal{D}(T) \subset X \to Y$ and $S : \mathcal{D}(S) \subset X \to Z$ be linear operators, where X, Y and Z are Banach spaces.*

(i) *S is called T-bounded (or relatively bounded with respect to T), if $\mathcal{D}(T) \subset \mathcal{D}(S)$ and there exist constants $a_s, b_s \geq 0$ such that*

$$\|Sx\| \leq a_s\|x\| + b_s\|Tx\|, \quad x \in \mathcal{D}(T). \tag{2.1}$$

The infimum δ_s of all b_s so that (2.1) *holds for some $a_s \geq 0$ is called the T-bound of S* (*or the relative bound of S with respect to T*).

(ii) *S is called T-compact* (*or relatively compact with respect to T*) *if $\mathcal{D}(T) \subset \mathcal{D}(S)$ and for every bounded sequence $(x_n)_1^\infty \subset \mathcal{D}(T)$ such that $(Tx_n)_1^\infty \subset F$ is bounded, the sequence $(Sx_n)_1^\infty \subset G$ contains a convergent subsequence.*

Note that if T is closed and S is closable, then $\mathcal{D}(T) \subset \mathcal{D}(S)$ already implies that S is T-bounded.

Definition 2.5 (see [12]) *Let X and Y be Banach spaces. The block-operator matrix $\mathcal{A} = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)$ in $X \oplus Y$ is called*

(i) *diagonally dominant if C is A-bounded and B is D-bounded;*

(ii) *off-diagonally dominant if A is C-bounded and D is B-bounded.*

Definition 2.6 (see [12]) *Let X and Y be Banach spaces, and let $\delta \geq 0$. The block-operator matrix $\mathcal{A} = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)$ in $X \oplus Y$ is called*

(i) *diagonally dominant of order δ if C is A-bounded with A-bound δ_C, B is D-bounded with D-bound δ_B, and $\delta = \max\{\delta_B, \delta_C\}$;*

(ii) *off-diagonally dominant of order δ if A is C-bounded with C-bound δ_A, D is B-bounded with B-bound δ_D, and $\delta = \max\{\delta_A, \delta_D\}$.*

Definition 2.7 (see [12]) *For $\omega \in [0, \pi)$, we define the sector*

$$\Sigma_\omega := \{r\mathrm{e}^{\mathrm{i}\varphi} : r \geq 0, |\varphi| \leq \omega\} \subset \mathbb{C}.$$

A densely defined operator T in a Banach space X is called sectorial if there exists an $\omega \in [0, \pi)$ such that

(i) $\mathbb{C} \setminus \Sigma_\omega \subset \rho(T)$,

(ii) $\sup\limits_{\lambda \in \mathbb{C} \setminus \Sigma_\omega} \|(T - \lambda)^{-1}\| < \infty$.

3 Main Results

Lemma 3.1 (see [12]) *Let T be a closable operator in a Banach space X with closure $\overline{T}$. Then $\sigma_{ap}(T) = \sigma_{ap}(\overline{T})$.*

Lemma 3.2 (see [13]) *Let $\mathcal{A} = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)$ be diagonally dominant of order 0 in $X \oplus Y$. Then $\sigma_{ap}(\mathcal{A}) \subset \overline{W^2(\mathcal{A})}$.*

Lemma 3.3 (see [13]) *Let $\mathcal{A} = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)$ be off-diagonally dominant of order 0 in $X \oplus Y$, and let B, C be boundedly invertible. Then $\sigma_{ap}(\mathcal{A}) \subset \overline{W^2(\mathcal{A})}$.*

Remark 3.1 Lemma 3.3 does not hold without the assumption that B, C are boundedly invertible (see [13, Example 4.6]).

3.1 The off-diagonally Hamiltonian case

Theorem 3.1 *Let* $H = \left(\begin{smallmatrix} 0 & B \\ C & 0 \end{smallmatrix}\right)$ *be a Hamiltonian operator on* $X \oplus X$*. If* B *and* C *are surjective, then* $\sigma(H) \subset \overline{W^2(H)}$*.*

Proof Since B and C are self-adjoint operators, the surjectiveness of B and C implies that B and C are boundedly invertible. By Lemma 3.3, we obtain

$$\sigma_{ap}(H) \subset \overline{W^2(H)}.$$

For off-diagonally Hamiltonian operators, we can easily verify

$$\sigma_r(H) = \sigma_r(H^*), \quad \sigma_p(H) = \sigma_p(H^*).$$

So if $\lambda \in \sigma_r(H)$, we have $\overline{\lambda} \in \sigma_r(H)$ and

$$\lambda \in \sigma_p(H^*) = \sigma_p(H) \subset \sigma_{ap}(H).$$

Thus $\sigma(H) = \sigma_{ap}(H) \cup \sigma_{r,1}(H) \subset \overline{W^2(H)}$.

Corollary 3.1 *Let* H *be a bounded off-diagonally Hamiltonian operator in* $X \oplus X$*. Then* $\sigma(H) \subset \{\lambda \in \mathbb{C} : |\lambda^2| \leq \|B\|\|C\|\}$*.*

Proof For a bounded operator H, $\sigma(H) \subset \overline{W^2(H)}$ always holds. Thus,

$$\begin{aligned} W^2(H) &= \Big\{\lambda \in \mathbb{C} : \lambda = \pm\sqrt{\frac{(Bg, f)(Cf, g)}{\|f\|^2\|g\|^2}}, f \in \mathcal{D}(C), g \in \mathcal{D}(B)\Big\} \\ &\subset \{\lambda \in \mathbb{C} : |\lambda^2| \leq \|B\|\|C\|\} \end{aligned} \tag{3.1}$$

implies $\sigma(H) \subset \{\lambda \in \mathbb{C} : |\lambda^2| \leq \|B\|\|C\|\}$.

3.2 The upper triangular Hamiltonian case

First, we consider the relation $\sigma_{ap}(H) \subset \overline{W^2(H)}$.

Theorem 3.2 *Let* $H = \left(\begin{smallmatrix} A & B \\ 0 & -A^* \end{smallmatrix}\right)$ *be a Hamiltonian operator in* $X \oplus X$*. If* $-A^*_{\mathcal{D}(B)\cap\mathcal{D}(-A^*)}$ *is closable, then* $\sigma_{ap}(H) \subset \overline{W^2(H)}$*.*

Proof Clearly, $\mathcal{D}(H) = \mathcal{D}(A) \oplus (\mathcal{D}(B) \cap \mathcal{D}(-A^*))$. For convenience, set

$$-A_1^* := -A^*_{\mathcal{D}(B)\cap\mathcal{D}(-A^*)}.$$

For the closable operator $-A_1^*$, we have $\sigma_{ap}(-A_1^*) = \sigma_{ap}(-\overline{A_1^*})$ by Lemma 3.1 and $\overline{W(-\overline{A_1^*})} = \overline{W(-A_1^*)}$. In fact, the inclusion $\overline{W(-A_1^*)} \subset \overline{W(-\overline{A_1^*})}$ is obvious. Conversely, if $\lambda \in \overline{W(-\overline{A_1^*})}$, then there exists a $g \in \mathcal{D}(-\overline{A_1^*})$, $\|g\| = 1$ such that $\lambda = (-\overline{A_1^*}g, g)$. Thus, there is a sequence $(g_n)_1^\infty \subset \mathcal{D}(-A_1^*)$ with $g_n \to g$ such that

$$(-\overline{A_1^*}g, g) = \Big(\lim_{n\to\infty} -A_1^*g_n, \lim_{n\to\infty} g_n\Big) = \lim_{n\to\infty}(-A_1^*g_n, g_n).$$

So $\lambda \in \overline{W(A_1^*)}$, i.e., $\overline{W(-\overline{A_1^*})} \subset \overline{W(-A_1^*)}$. Thus,

$$\begin{aligned}\sigma_{ap}(H) &\subset \sigma_{ap}(A) \cup \sigma_{ap}(-A_1^*) \subset \overline{W(A)} \cup \overline{W(-\overline{A_1^*})} \\ &\subset \overline{W(A)} \cup \overline{W(-A_1^*)} = \overline{W(A) \cup W(-A_1^*)} \\ &= \overline{W^2(H)}. \end{aligned} \tag{3.2}$$

Corollary 3.2 *Let $H = \begin{pmatrix} A & B \\ 0 & -A^* \end{pmatrix}$ be a Hamiltonian operator in $X \oplus X$. If $\mathcal{D}(B) \cap \mathcal{D}(-A^*)$ is a core of $-A^*$, then $\sigma_{ap}(H) \subset \overline{W^2(H)}$.*

Recall that if the numerical range of a densely defined operator T is not the whole complex plane, then T is closable (see [4, Theorem V.3.4]). So we can obtain the next corollary immediately.

Corollary 3.3 *Let $H = \begin{pmatrix} A & B \\ 0 & -A^* \end{pmatrix}$ be a Hamiltonian operator in $X \oplus X$. If*

$$W(-A^*_{\mathcal{D}(B)\cap\mathcal{D}(-A^*)}) \neq \mathbb{C},$$

then $\sigma_{ap}(H) \subset \overline{W^2(H)}$.

Theorem 3.3 *Let $H = \begin{pmatrix} A & B \\ 0 & -A^* \end{pmatrix}$ be a Hamiltonian operator with diagonally dominant of order $\delta < 1$ on $X \oplus X$. If $\mathcal{D}(A) = \mathcal{D}(A^*)$, then $\sigma(H) \subset \overline{W^2(H)}$.*

Proof Since H is diagonally dominant of order $\delta < 1$, H^* can be written as

$$H^* = \begin{pmatrix} A^* & 0 \\ B & -A \end{pmatrix}.$$

Then, for $f \in \mathcal{D}(A)$, $g \in \mathcal{D}(A^*)$, $\|f\| = \|g\| = 1$, we see that

$$\begin{aligned}(H^*)_{f,g} &= \begin{pmatrix} (A^*f, f) & 0 \\ (Bf, g) & (-Ag, g) \end{pmatrix} \\ &= \begin{pmatrix} (Af, f) & (Bg, f) \\ 0 & (-A^*g, g) \end{pmatrix}^* \\ &= (H_{f,g})^* \end{aligned} \tag{3.3}$$

by $\mathcal{D}(A) = \mathcal{D}(A^*)$, and hence $W^2(H^*) = W^2(H)^*$. From Theorem 3.2, $\sigma_{ap}(H) \subset \overline{W^2(H)}$ follows immediately, so we only need to prove $\sigma_r(H) \subset \overline{W^2(H)}$. If $\lambda \in \sigma_r(H)$, then $\overline{\lambda} \in \sigma_p(H^*) \subset W^2(H^*) = W^2(H)^*$, i.e., $\lambda \in W^2(H)$. Thus, $\sigma(H) \subset \overline{W^2(H)}$.

Theorem 3.4 *Let $H = \begin{pmatrix} A & B \\ 0 & -A^* \end{pmatrix}$ be a Hamiltonian operator with diagonally dominant of order $\delta < 1$ in $X \oplus X$. Then, $\sigma(H) \subset \overline{W^2(H)}$, if one of the following statements is fulfilled:*

(i) $\sigma_r(H) = \emptyset$;

(ii) $\sigma_p(H)$ *is symmetric with respect to the imaginary axis;*

(iii) $\sigma_r(A) = \emptyset$ *and* $\sigma_p(A)$ *is symmetric with respect to the imaginary axis.*

Proof Since H is diagonally dominant of order $\delta < 1$, H is a symplectic self-adjoint operator, i.e., $JH = (JH)^*$, where $J = \left(\begin{smallmatrix} 0 & I \\ -I & 0 \end{smallmatrix}\right)$.

(i) If $\sigma_r(H) = \emptyset$, then $\sigma(H) = \sigma_{ap}(H) \subset \overline{W^2(H)}$ by Theorem 3.2.

(ii) For a symplectic self-adjoint operator H, $\sigma_p(H) \cup \sigma_r(H)$ is symmetric with respect to the imaginary axis, and $\sigma_r(H)$ contains no point symmetric with respect to the imaginary axis. Then, we further have that $\sigma_r(H) = \emptyset$ if and only if $\sigma_p(H)$ is symmetric with respect to the imaginary axis. Thus, the relation $\sigma(H) \subset \overline{W^2(H)}$ follows from (i) immediately.

(iii) From $\sigma_r(A) = \emptyset$, we have

$$\sigma_p(H) \cup \sigma_r(H) = \{\lambda \in \mathbb{C} : \lambda \in \sigma_p(A) \text{ or } -\overline{\lambda} \in \sigma_p(A)\}.$$

If $\sigma_p(A)$ is symmetric with respect to the imaginary axis, we get $\sigma_p(H) \cup \sigma_r(H) = \sigma_p(A)$. Note that $\sigma_p(A) \subseteq \sigma_p(H)$, and therefore $\sigma_r(H) = \emptyset$, from which the claim follows.

Theorem 3.5 *Let $H = \left(\begin{smallmatrix} A & B \\ 0 & -A^* \end{smallmatrix}\right) : \mathcal{D}(A) \oplus \mathcal{D}(-A^*) \subset X \oplus X \to X \oplus X$ be a Hamiltonian operator. If every component of $\mathbb{C} \setminus \overline{W(A)}$ contains a point $\lambda \in \rho(A)$ and every component of $\mathbb{C} \setminus \overline{W(-A^*)}$ contains a point $\mu \in \rho(-A^*)$, then $\sigma(H) \subset \overline{W^2(H)}$.*

Proof If every component of $\mathbb{C} \setminus \overline{W(A)}$ contains a point $\lambda \in \rho(A)$ and every component of $\mathbb{C} \setminus \overline{W(-A^*)}$ contains a point $\mu \in \rho(-A^*)$, we obtain $\sigma(A) \subset \overline{W(A)}$ and $\sigma(-A^*) \subset \overline{W(-A^*)}$ by [4, Theorem V.3.2]. Thus, $\sigma(H) \subset \sigma(A) \cup \sigma(-A^*) \subset \overline{W(A)} \cup \overline{W(-A^*)} = \overline{W^2(H)}$.

3.3 The general 2 × 2 Hamiltonian case

Theorem 3.6 *Let H given by* (1.1) *be a Hamiltonian operator with diagonally dominant of order* 0*. If $\mathcal{D}(A) = \mathcal{D}(A^*)$, then $\sigma(H) \subset \overline{W^2(H)}$.*

Proof From Lemma 3.2, $\sigma_{ap}(H) \subset \overline{W^2(H)}$. Similar to the proof of Theorem 3.3, we can obtain $\sigma_r(H) \subset \overline{W^2(H)}$, and therefore $\sigma(H) \subset \overline{W^2(H)}$.

The next corollary is a direct consequence of Theorem 3.6. In fact, the boundedness and relative compactness both imply relative boundedness with relative bound 0 (see [3, Corollary III.7.7]).

Corollary 3.4 *Let H given by* (1.1) *be a Hamiltonian operator with $\mathcal{D}(A) = \mathcal{D}(A^*)$. If B is bounded or $-A^*$-compact, and if C is bounded or A-compact, then $\sigma(H) \subset \overline{W^2(H)}$.*

For a sectorial operator T, the fractional powers T^γ, $\gamma \in (0, 1)$, are defined (see [10, Section 2.6], [5, Chapter 1.5.8]).

Corollary 3.5 *Let H given by* (1.1) *be a Hamiltonian operator with $\mathcal{D}(A) = \mathcal{D}(A^*)$. Then,*

(i) *if A and A^* are sectorial operators, and if there are $\gamma, \eta \in (0, 1)$ with $\mathcal{D}(A^\gamma) \subset \mathcal{D}(C)$ and $\mathcal{D}((A^*)^\eta) \subset \mathcal{D}(B)$, then $\sigma(H) \subset \overline{W^2(H)}$;*

(ii) *if there are* $\gamma, \eta \in (0,1)$ *with* $\mathcal{D}(|A|^\gamma) \subset \mathcal{D}(C)$ *and* $\mathcal{D}(|A^*|^\eta) \subset \mathcal{D}(B)$*, then* $\sigma(H) \subset \overline{W^2(H)}$.

Proof (i) Since A^γ and C are closed operators, the inclusion $\mathcal{D}(A^\gamma) \subset \mathcal{D}(C)$ implies C is A^γ-bounded. By [10, Corollary 2.6.11], there is a $K > 0$ such that

$$\|A^\gamma x\| \leq K(\varepsilon^{-\gamma}\|x\| + \varepsilon^{1-\gamma}\|Ax\|), \quad x \in \mathcal{D}(A) \subset \mathcal{D}(A^\gamma)$$

for every $\varepsilon > 0$. This and $\gamma < 1$ imply that A^γ is A-bounded with A-bound 0. Since C is A^γ-bounded, we see that C is A-bounded with C-bound 0. Similarly, we can prove that B is A^*-bounded with A^*-bound 0. Thus, applying Theorem 3.6 yields $\sigma(H) \subset \overline{W^2(H)}$.

(ii) For non-sectorial operators A and A^* in the Hilbert space, $|A|$ and $|A^*|$ are sectorial operators. By [12, Corollary 2.1.20], we have that H is diagonally dominant of order 0, and hence $\sigma(H) \subset \overline{W^2(H)}$.

Theorem 3.7 *Let H given by* (1.1) *be a Hamiltonian operator with off-diagonally dominant of order* 0*. If* $\mathcal{D}(B) = \mathcal{D}(C)$ *and* $0 \notin \sigma_p(B) \cap \sigma_p(C)$*, then* $\sigma(H) \subset \overline{W^2(H)}$.

Proof By Lemma 3.3, $\sigma_{ap}(H) \subset \overline{W^2(H)}$. Since H is off-diagonally dominant of order 0, H^* can also be written as

$$H^* = \begin{pmatrix} A^* & C \\ B & -A \end{pmatrix} : \mathcal{D}(B) \oplus \mathcal{D}(C) \subset X \oplus X \to X \oplus X.$$

From $\mathcal{D}(B) = \mathcal{D}(C)$, for $f \in \mathcal{D}(B),\ g \in \mathcal{D}(C),\ \|f\| = \|g\| = 1$, we have

$$\begin{aligned} (H^*)_{f,g} &= \begin{pmatrix} (A^*f, f) & (Cg, f) \\ (Bf, g) & (-Ag, g) \end{pmatrix} \\ &= \begin{pmatrix} (Af, f) & (Bg, f) \\ (Cf, g) & (-A^*g, g) \end{pmatrix}^* \\ &= (H_{f,g})^*, \end{aligned} \tag{3.4}$$

which implies $W^2(H^*) = W^2(H)^*$. If $\lambda \in \sigma_r(H)$, then $\overline{\lambda} \in \sigma_p(H^*) \subset W^2(H)^*$. Thus, $\sigma(H) \subset \overline{W^2(H)}$.

Remark 3.2 For a Hamiltonian operator, if it is diagonally dominant of order $\delta < 1$ and $\mathcal{D}(A) = \mathcal{D}(A^*)$, or if it is off-diagonally dominant of order $\delta < 1$ and $\mathcal{D}(B) = \mathcal{D}(C)$, the quadratic numerical range $W^2(H)$ is symmetric with respect to the imaginary axis. In the following, we take a Hamiltonian matrix

$$H := \left(\begin{array}{cc|cc} \mathrm{i} & 1 & 1 & \mathrm{i} \\ 2 & 2\mathrm{i} & -\mathrm{i} & 0 \\ \hline 2 & 1-\mathrm{i} & \mathrm{i} & -2 \\ 1+\mathrm{i} & 2 & -1 & 2\mathrm{i} \end{array}\right) \tag{3.5}$$

as an example to illustrate this property. Figure 1 is the quadratic numerical range of H, which is figured by the Monte-Carlo method. The random vectors f and g are sampled from two independent uniform distributions on the unit sphere of $\mathbb{C}^2$, the red dot is the eigenvalue of H, and the different colors between blue and yellow show the density of the eigenvalues of the $H_{f,g}$. Here we call it the density of the quadratic numerical range of H. From the figure, the quadratic numerical range and the eigenvalues of H are both obviously symmetric with respect to the imaginary axis. In addition, it is interesting that the density of $W^2(H)$ is also symmetric with respect to the imaginary axis.

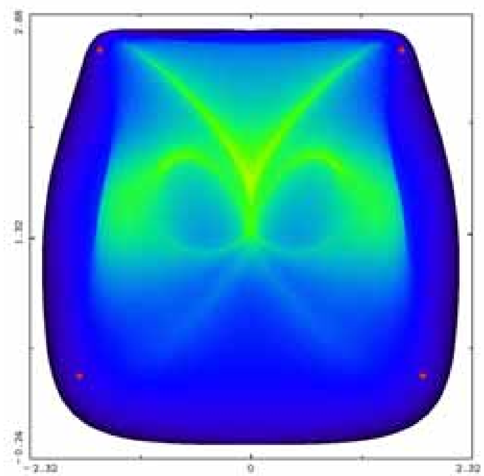

Figure 1 The quadratic numerical range of H defined in (3.5)

Corollary 3.6 *Let H given by* (1.1) *be a Hamiltonian operator, and let B and C be injective with $\mathcal{D}(B) = \mathcal{D}(C)$. If A is bounded, or if A is C-compact and $-A^*$ is B-compact, then $\sigma(H) \subset \overline{W^2(H)}$.*

Corollary 3.7 *Let H given by* (1.1) *be a Hamiltonian operator, and let B and C be injective with $\mathcal{D}(B) = \mathcal{D}(C)$. Then,*

(i) *if B and C are sectorial operators with $\mathcal{D}(C^\gamma) \subset \mathcal{D}(A)$ and $\mathcal{D}(B^\eta) \subset \mathcal{D}(A^*)$ for some $\gamma, \eta \in (0,1)$, then $\sigma(H) \subset \overline{W^2(H)}$;*

(ii) *if $\mathcal{D}(|C|^\gamma) \subset \mathcal{D}(A)$ and $\mathcal{D}(|B|^\eta) \subset \mathcal{D}(A^*)$ for some $\gamma, \eta \in (0,1)$, then $\sigma(H) \subset \overline{W^2(H)}$.*

Corollary 3.8 *Let H given by* (1.1) *be a Hamiltonian operator with $\mathcal{D}(A) = \mathcal{D}(A^*)$ and B, C be bounded. If $\inf\{|\operatorname{Re}\lambda| : \lambda \in W(A)\} > \|B\|\|C\|$, then H is boundedly invertible.*

Proof By the assumption $\inf\{|\operatorname{Re}\lambda| : \lambda \in W(A)\} > \|B\|\|C\|$, we obtain $\overline{W(A)} \cap \overline{W(-A^*)} = \emptyset$ and $\operatorname{dist}(W(A), W(-A^*)) > 2\sqrt{\|B\|\|C\|}$. Set $\beta := \operatorname{dist}(W(A), W(-A^*))$ and assume that λ belongs to the line that separates the convex sets $W(A)$ and $W(-A^*)$, and has the distance $\frac{\beta}{2}$ to both of them. Then, for all $f \in \mathcal{D}(A)$ and $g \in \mathcal{D}(-A^*)$,

$$|\det(H_{f,g} - \lambda I)| = |(\lambda - (Af, f))(\lambda - (-A^* g, g)) - (Bg, f)(Cf, g)|$$

$$
\begin{aligned}
&\geq |\lambda - (Af, f)||\lambda - (-A^*g, g)| - \|B\|\|C\| \\
&\geq \frac{\beta^2}{4} - \|B\|\|C\| > 0,
\end{aligned} \tag{3.6}
$$

which shows that $\lambda \notin \overline{W^2(H)}$. By Theorem 3.6, $0 \notin \sigma(H)$, i.e., H is boundedly invertible.

The norm of the resolvent $(T-\lambda I)^{-1}$ of a bounded linear operator T can be estimated in terms of the numerical range as

$$
\|(T-\lambda I)^{-1}\| \leq \frac{1}{\operatorname{dist}(\lambda, W(T))}, \quad \lambda \notin \overline{W(T)}. \tag{3.7}
$$

For an unbounded operator T, the above resolvent estimation is invalid in general. But for the Hamiltonian operators in Theorems 3.1, 3.3, 3.6–3.7, we claim that (3.7) holds true.

Corollary 3.9 *Let H be Hamiltonian operators defined as in Theorem* 3.1, 3.3, 3.6–3.7*. Then* $\|(H-\lambda I)^{-1}\| \leq \frac{1}{\operatorname{dist}(\lambda, W(H))}$, $\lambda \notin \overline{W(H)}$.

Proof By Theorems 3.1, 3.3, 3.6–3.7, we have $\sigma(H) \subset \overline{W^2(H)} \subset \overline{W(H)}$. Then every component of $\mathbb{C} \backslash \overline{W(H)}$ contains a point $\lambda \in \rho(H)$. So, the resolvent satisfies the norm estimate (see [4, Theorem V.3.2])

$$
\|(H-\lambda I)^{-1}\| \leq \frac{1}{\operatorname{dist}(\lambda, W(H))}, \quad \lambda \notin \overline{W(H)}.
$$

Finally, we conclude with an example, which is inspired by [4, Example V.3.34]. In what follows, $\mathrm{L}^2([a,b],\mathbb{C})$ is the Hilbert space of square Lebesgue integrable complex-valued functions on $[a,b]$, and $\mathrm{AC}([a,b],\mathbb{C})$ denotes the space of complex-valued functions on $[a,b]$ that are absolutely continuous on every compact subinterval of $[a,b]$.

Example 3.1 Let $X = \mathrm{L}^2([a,b],\mathbb{C})$ and $K = \mathrm{AC}([a,b],\mathbb{C})$. Consider the Hamiltonian operator $H = \left(\begin{smallmatrix} A & B \\ 0 & -A^* \end{smallmatrix}\right)$ with $Au = p_0(x)u'' + p_1(x)u' + p_2(x)u$, $-A^*u = -p_0(x)u'' + p_1(x)u' - p_2(x)u$ and $Bu = \mathrm{i}u'$, where $p_k(x)$, $k = 1,2,3$ are real-valued, $p_0(x) < 0$, p_0'', p_1', p_2 are continuous on $[a,b]$, and

$$
\begin{aligned}
&\mathcal{D}(A) = \mathcal{D}(-A^*) = \{x \in X:\ x, x' \in K,\ x'' \in X,\ x(a) = x(b) = 0\}, \\
&\mathcal{D}(B) = \{x \in X:\ x \in K,\ x' \in X,\ x(a) = x(b)\}.
\end{aligned}
$$

We claim that

$$
\begin{aligned}
\sigma(H) \subset &\left\{\lambda \in \mathbb{C} : \operatorname{Re}\lambda \geq \gamma_1,\ |\arg(\lambda - \gamma_1)| \leq \arctan\left(\frac{1}{k_1}\right)\right\} \\
&\cup \left\{\lambda \in \mathbb{C} : \operatorname{Re}\lambda \leq \gamma_2,\ |\arg(\lambda - \gamma_2)| \geq \pi - \arctan\left(\frac{1}{k_2}\right)\right\}.
\end{aligned} \tag{3.8}
$$

Indeed, for $u \in \mathcal{D}(A)$, we have

$$
(Au, u) = \int_a^b (p_0(x)\, u'' + p_1(x)\, u' + p_2(x)\, u)\, \overline{u}\, \mathrm{d}x
$$

$$= -\int_a^b p_0\,|u'|^2\,\mathrm{d}x + \int_a^b [(p_1 - p_0')\,u' + p_2\,u]\,\overline{u}\mathrm{d}x. \tag{3.9}$$

Since $-p_0(x) \geq m_0 > 0$, $|p_1(x) - p_0'(x)| \leq M_1$, $|p_2(x)| \leq M_2$ for some positive constants m_0, M_1, M_2, we know for any $k_1 > 0$ that

$$\begin{aligned}
&\mathrm{Re}(Au,u) - k_1|\mathrm{Im}(Au,u)| \\
&\geq m_0 \int_a^b |u'|^2\,\mathrm{d}x - (1+k_1)M_1 \int_a^b |u'||u|\,\mathrm{d}x - M_2 \int_a^b |u|^2\,\mathrm{d}x \\
&\geq [m_0 - \varepsilon(1+k_1)M_1] \int_a^b |u'|^2\,\mathrm{d}x - \Big(\frac{(1+k_1)M_1}{4\varepsilon} + M_2\Big) \int_a^b |u|^2\,\mathrm{d}x,
\end{aligned} \tag{3.10}$$

where $\varepsilon > 0$ is arbitrary. If ε is chosen in such a way that $m_0 - \varepsilon(1+k_1)M_1 \geq 0$, then $\mathrm{Re}(Au,u) - k_1|\mathrm{Im}(Au,u)| \geq \gamma_1(u,u)$ for some negative number γ_1. In other words,

$$|\mathrm{Im}(Au,u)| \leq \frac{1}{k_1}\mathrm{Re}((A-\gamma_1)u,u).$$

This means

$$W(A) \subset \Big\{\lambda \in \mathbb{C} : \mathrm{Re}\,\lambda \geq \gamma_1,\ |\arg(\lambda - \gamma_1)| \leq \arctan\Big(\frac{1}{k_1}\Big)\Big\}.$$

Similarly, we deduce that

$$W(-A^*) \subset \Big\{\lambda \in \mathbb{C} : \mathrm{Re}\,\lambda \leq \gamma_2,\ |\arg(\lambda - \gamma_2)| \geq \pi - \arctan\Big(\frac{1}{k_2}\Big)\Big\}$$

for a given $k_2 > 0$ and some positive number γ_2. For a sufficiently large $\lambda \in \mathbb{R} \cap (\mathbb{C} \setminus \overline{W(A)})$, we easily verify $-\lambda \notin \sigma_p(A^*)$, i.e., $d(A+\lambda) = 0$, which together with $n(A+\lambda) = 0$ and the closedness of $\mathcal{R}(A+\lambda)$ implies $\lambda \in \rho(A)$. This means $\rho(A) \cap (\mathbb{C} \setminus \overline{W(A)}) \neq \emptyset$. Analogously, we also have $\rho(-A^*) \cap (\mathbb{C} \setminus \overline{W(-A^*)}) \neq \emptyset$. By Theorem 3.5, we obtain the following estimates:

$$\begin{aligned}
\sigma(H) \subset &\Big\{\lambda \in \mathbb{C} : \mathrm{Re}\,\lambda \geq \gamma_1,\ |\arg(\lambda - \gamma_1)| \leq \arctan\Big(\frac{1}{k_1}\Big)\Big\} \\
&\cup \Big\{\lambda \in \mathbb{C} : \mathrm{Re}\,\lambda \leq \gamma_2,\ |\arg(\lambda - \gamma_2)| \geq \pi - \arctan\Big(\frac{1}{k_2}\Big)\Big\}.
\end{aligned} \tag{3.11}$$

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