Ultra-Weak Time Operators of Schrödinger Operators

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Abstract

In an abstract framework, a new concept on time operator, *ultra-weak time operator*, is introduced, which is a concept weaker than that of weak time operator. Theorems on the existence of an ultra-weak time operator are established. As an application of the theorems, it is shown that Schrödinger operators H_V with potentials V obeying suitable conditions, including the Hamiltonian of the hydrogen atom, have ultra-weak time operators. Moreover, a class of Borel measurable functions $f : \mathbb{R} \to \mathbb{R}$ such that $f(H_V)$ has an ultra-weak time operator is found.

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Contents

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1 Introduction

This paper is concerned with the mathematical theory of time operators developed in the papers [Miy01, Gal02, GCB04, Ara05, Ara07, Ara08a, Ara08b, Ara09, AM08a, AM08b , HKM09]. The main purposes are as follows: (1) to introduce a new concept on time operator, which we call *ultra-weak time operator* (see Subsection 1.2 below); (2) to establish theorems on the existence of ultra-weak time operators for a general class of self-adjoint operators with infinitely many discrete eigenvalues; (3) to apply the existence theorems to Schrödinger operators, including the Hamiltonian of the hydrogen atom. In this introduction, for the reader's convenience, we first describe some back grounds for the present work and then define the concept of ultra-weak time operator. At the end of this section, we outline the organization of the present paper.

1.1 Some backgrounds

Let A and B be linear operators on a complex Hilbert space $\mathscr{H}$, satisfying the canonical commutation relation (CCR)

$$[A, B] = -i\mathbb{1} \tag{1.1}$$

on a non-zero subspace $\mathscr{D} \subset \mathrm{D}(AB) \cap \mathrm{D}(BA)$, where, for a linear operator L on $\mathscr{H}$, $\mathrm{D}(L)$ denotes the domain of L, $[A, B] := AB - BA$ and $\mathbb{1}$ denotes identity (occasionally omitted). We call $\mathscr{D}$ a *CCR-domain* for the pair (A, B). It is well known [Pu67, p.2] that, if $\mathscr{D}$ is dense in $\mathscr{H}$, then (1.1) implies that $\mathscr{H}$ has to be infinite dimensional and at least one of A and B is unbounded. We call this property the *unbounded property* of CCR. It is easy to see that, if $\mathscr{D}$ is an invariant subspace of A and B, then $\mathscr{D}$ has to be infinite dimensional and hence at least one of A and B as linear operators on $\overline{\mathscr{D}}$ (the closure of $\mathscr{D}$) with domain $\mathscr{D}$ is unbounded. From representation theoretic point of view, $(\mathscr{H}, \mathscr{D}, \{A, B\})$ is called a *representation of the CCR with one degree of freedom* (usually $\mathscr{D}$ is assumed to be a dense invariant subspace of A and B, but, here, we do not require this property).

W denote by $(f, g)_{\mathscr{H}}$ $(f, g \in \mathscr{H})$ and $\|\cdot\|_{\mathscr{H}}$ the scalar (inner) product of $\mathscr{H}$, linear in g and antilinear in f, and the norm of $\mathscr{H}$ respectively. But we sometimes omit the subscript "$\mathscr{H}$" in $(f, g)_{\mathscr{H}}$ and $\|\cdot\|_{\mathscr{H}}$ if there is no danger of confusions.

The CCR (1.1) implies a physically important inequality: if A and B in (1.1) are symmetric operators on $\mathscr{H}$, (1.1) yields the *uncertainty relation* of Heisenberg type [vN32, Chapter III, §4]:

$$(\Delta A)_\psi (\Delta B)_\psi \geq \frac{1}{2} \tag{1.2}$$

for all $\psi \in \mathscr{D}$ with $\|\psi\| = 1$, where $(\Delta A)_\psi := \|(A - (\psi, A\psi)_{\mathscr{H}})\psi\|_{\mathscr{H}}$, $\psi \in \mathrm{D}(A)$, the *uncertainty* of A with respect to ψ.[1]

The concept of representation of the CCR with one degree of freedom can be extended to the case of finite degrees of freedom. Let A_j and B_j $(j, k = 1, \ldots, d, d \in \mathbb{N})$ be symmetric operators on $\mathscr{H}$ and $\mathscr{D}$ be a non-zero subspace of $\mathscr{H}$ such that $\mathscr{D} \subset \cap_{j,k=1}^{d} [\mathrm{D}(A_j B_k) \cap \mathrm{D}(B_k A_j) \cap \mathrm{D}(A_j A_k) \cap \mathrm{D}(B_j B_k)]$. Then the triple $(\mathscr{H}, \mathscr{D}, \{A_j, B_j | j = 1, \ldots, d\})$ is called a *representation of the CCR's with d degrees of freedom* if the CCR's with d degrees of freedom

$$[A_j, B_k] = -i\delta_{jk}\mathbb{1}, \quad [A_j, A_k] = 0, \quad [B_j, B_k] = 0, \quad j, k = 1, \ldots, d \tag{1.3}$$

hold on $\mathscr{D}$, where δ_{jk} is the Kronecker delta. The subspace $\mathscr{D}$ is called a *CCR-domain* for $\{A_j, B_j | j = 1, \ldots, d\}$.

There is a stronger version of representation of the CCR's with d degrees of freedom. A set $\{A_j, B_j | j = 1, \ldots, d\}$ of self-adjoint operators on $\mathscr{H}$ is called a *Weyl*

[1] Inequality (1.2) can be derived also from a weak version of (1.1): $(A\psi, B\phi) - (B\psi, A\phi) = -i(\psi, \phi)$, $\psi, \phi \in \mathscr{D}_{\mathrm{w}}$, where $\mathscr{D}_{\mathrm{w}}$ is a non-zero subspace of $\mathrm{D}(A) \cap \mathrm{D}(B)$.

representation of the CCR's with d degrees of freedom if the *Weyl relations*

$$e^{-isA_j}e^{-itB_k} = e^{ist\delta_{jk}}e^{-itB_k}e^{-isA_j}, \quad j,k = 1,\dots,d,\ s,t \in \mathbb{R} \tag{1.4}$$

hold.

The Weyl relations (1.4) imply that there exists a dense invariant domain $\mathscr{D}$ of A_j and B_j ($j = 1,\dots,d$) such that (1.3) holds on $\mathscr{D}$ [Pu67, Theorem 4.9.1]. Hence the Weyl representation $\{A_j, B_j | j = 1,\dots,d\}$ is a representation of the CCR's with d degrees of freedom. But *the converse is not true* (e.g., [Ara98, Fug67, Sch83b]).

A Weyl representation $\{A_j, B_k | j,k = 1,\dots,d\}$ of the CCR's with d degrees of freedom is said to be *irreducible* if any subspace $\mathscr{D}$ of $\mathscr{H}$ left invariant by e^{-itA_j} and e^{-itB_j} for all $t \in \mathbb{R}$ and $j = 1,\dots,d$ is $\{0\}$ or $\mathscr{H}$.

In quantum mechanics on the d-dimensional space $\mathbb{R}^d = \{x = (x_1,\dots,x_d) | x_j \in \mathbb{R}\}$, the momentum operator $P := (P_1,\dots,P_d)$ and the position operator $Q := (Q_1,\dots,Q_d)$ are defined by $P_j := -iD_j$ (D_j is the generalized partial differential operator in x_j)[2] and $Q_j := M_{x_j}$(the multiplication operator by x_j), $j = 1,\dots,d$. For all $j = 1,\dots,d$, P_j and Q_j are self-adjoint operators on the Hilbert space $L^2(\mathbb{R}^d)$, satisfying the CCR's with d degrees of freedom:

$$[P_j, Q_k] = -i\delta_{jk}\mathbb{1}, \quad [P_j, P_k] = 0, \quad [Q_j, Q_k] = 0 \tag{1.5}$$

on the domain $\cap_{j,k=1}^d [\mathrm{D}(P_jQ_k) \cap \mathrm{D}(Q_kP_j) \cap \mathrm{D}(Q_jQ_k) \cap \mathrm{D}(Q_kQ_j)]$. Hence $(L^2(\mathbb{R}^d), C_0^\infty(\mathbb{R}^d), \{P_j, Q_j | j = 1,\dots,d\})$ is a representation of the CCR's with d degrees of freedom, where $C_0^\infty(\mathbb{R}^d)$ is the space of infinitely differentiable functions on $\mathbb{R}^d$ with compact support. This representation of CCR's is called the *Schrödinger representation of the CCR* (or the *Schrödinger system* [Pu67]) *with d degrees of freedom*.

By an application of (1.2), one obtains the *position-momentum uncertainty relations*

$$(\Delta P_j)_\psi (\Delta Q_j)_\psi \geq \frac{1}{2}, \quad j = 1,\dots,d \tag{1.6}$$

for all $\psi \in \mathrm{D}(P_jQ_j) \cap \mathrm{D}(Q_jP_j)$ with $\|\psi\| = 1$, basic inequalities in quantum mechanics which show a big difference between quantum mechanics and classical mechanics.[3]

The Schrödinger representation $\{P_j, Q_k | j,k = 1,\dots,d\}$ is an irreducible Weyl representation ([Pu67, Theorem 4.5.1]; [Ara06, Theorem 3.12]). Conversely it is known as the von Neumann uniqueness theorem (e.g., [Pu67, Theorem 4.11.1]) that, if $\mathscr{H}$ is separable and $\{A_j, B_k | j,k = 1,\dots,d\}$ is an irreducible Weyl representation of the CCR's with d degrees of freedom, then

$$\mathscr{H} \cong L^2(\mathbb{R}^d), \quad A_j \cong P_j, \quad B_j \cong Q_j, \quad j = 1,...,d.$$

[2]In the present paper, we use the physical unit system where $\hbar = h/2\pi$ (h is the Planck constant) is equal to 1. In the original unit system (MKSA unit system), $P_j = -i\hbar D_j$.

[3]Inequality (1.6) holds also for all $\psi \in \mathrm{D}(P_j) \cap \mathrm{D}(Q_j)$ with $\|\psi\| = 1$.

Here $\cong$ denotes a unitary equivalence.

Usually models of quantum mechanics in $\mathbb{R}^d$ are constructed from the Schödinger representation of the CCR's with d degrees of freedom. In this case, physical quantities, which are required to be represented by self-adjoint operators on $L^2(\mathbb{R}^d)$, are made from P_j and Q_j, $j = 1, \ldots, d$. Among others, the Hamiltonian of a model, which describes the total energy of the quantum system under consideration, is important. The classical Hamiltonian of a non-relativistic particle of mass m in a potential $V : \mathbb{R}^d \to \mathbb{R}$ is given by $H_{\rm cl}(p, x) = p^2/2m + V(x)$, $(p, x) \in \mathbb{R}^d \times \mathbb{R}^d$. Then the corresponding quantum Hamiltonian is given by the Schrödinger operator (or the Schrödinger Hamiltonian)

$$H_V := H_{\rm cl}(P, Q) := \frac{1}{2m}\sum_{j=1}^{d} P_j^2 + V(Q) = -\frac{1}{2m}\Delta + V(Q)$$

on $L^2(\mathbb{R}^d)$, where $V(Q)$ is defined by the functional calculus using the joint spectral measure of $Q_1, \cdots, Q_d$ (note that $(Q_1, \ldots, Q_d)$ is a set of strongly commuting self-adjoint operators[4]) and $\Delta := \sum_{j=1}^{d} D_j^2$ is the d-dimensional generalized Laplacian. It is shown in fact that $V(Q)$ is the multiplication operator by the function V . Hence one simply denotes $V(Q)$ by V. Thus

$$H_V = H_0 + V, \tag{1.7}$$

where

$$H_0 := -\frac{1}{2m}\Delta. \tag{1.8}$$

In general, according to an axiom of quantum mechanics due to von Neumann, the time evolution of the quantum system whose Hamiltonian is given by a self-adjoint operator H on a Hilbert space $\mathscr{H}$ is described by the unitary operator e^{-itH} with time parameter $t \in \mathbb{R}$ in such a way that, if $\phi \in \mathscr{H}$ is a state vector at $t = 0$, then the state vector at time t is given by $\phi_t = e^{-itH}\phi$, provided that no measurement is made for the quantum system under consideration in the time interval $[0, t]$. If $\phi \in {\rm D}(H)$, then ϕ_t is strongly differentiable in t, $\phi_t \in D(H)$ for all $t \in \mathbb{R}$, and obeys the abstract Schrödinger equation

$$i\frac{d\phi_t}{dt} = H\phi_t.$$

Here time t is usually treated as a parameter, not as an operator. In relativistic classical mechanics, the energy variable is regarded as the variable canonically conjugate to the time variable as so is the momentum variable to the position variable and this may be extended to non-relativistic classical mechanics as a limit of relativistic one. From

[4]A set $\{A_1, \ldots, A_n\}$ of self-adjoint operators on a Hilbert space is said to be *strongly commuting* if the spectral measure E_{A_j} of A_j commutes with E_{A_k} for all $j, k = 1, \ldots, n, j \neq k$ (i.e., for all Borel sets $J, K \subset \mathbb{R}$, $E_{A_j}(J)E_{A_k}(K) = E_{A_k}(K)E_{A_j}(J)$).

this point of view (or in view of the time-energy uncertainty relation proposed by Heisenberg), one may infer that a quantum Hamiltonian H may have a symmetric operator T corresponding to time, satisfying CCR

$$[H,T] = -i\mathbb{1} \tag{1.9}$$

on a non-zero subspace $\mathscr{D}_{H,T}$ included in $\mathrm{D}(HT) \cap \mathrm{D}(TH)$. Such an operator T is called a *time operator* of H (some authors use the form $[H,T] = i\mathbb{1}$ instead of (1.9), but this is not essential, just a convention). From a purely mathematical point of view (apart from the context of quantum physics), this definition applies to any pair (H,T) of a self-adjoint operator H and a symmetric operator T obeying (1.9) on a non-zero subspace included in $\mathrm{D}(HT) \cap \mathrm{D}(TH)$.

Remark 1.1 It is obvious that, if T is a time operator of H, then, for all $\alpha \in \mathbb{R} \setminus \{0\}$, $\alpha^{-1}T$ is a time operator of αH.

The uncertainty relation

$$(\Delta H)_\psi (\Delta T)_\psi \geq \frac{1}{2}, \quad \psi \in \mathscr{D}_{T,H},\ \|\psi\| = 1 \tag{1.10}$$

implied by (1.9) is called the *time-energy uncertainty relation*. This gives a physical meaning of a time operator.

In the physics literature, formal (heuristic) constructions of “time operators” have been done for special classes of Schrödiner Hamiltonians (e.g., [AB61, Bau83, Fuj80, FWY80, GYS81]). But, since the theory of CCR’s with dense CCR-domains involves unbounded operators as remarked above, formal manipulations are questionable and results based on them remain vague and inconclusive. In fact, mathematically rigorous considerations lead one to distinguish some classes of time operators as recalled below. These classes correspond to different types of representations of CCR’s (see, e.g., [Dor84, Fug67, JM80, Sch83a, Sch83b]). It should be noted that there exist representations of CCR’s which are inequivalent to Schrödinger ones (e.g., [Fug67], [Sch83b], [Ara98]) and, interestingly enough, some of them are connected with characteristic physical phenomena such as the so-called Aharonov-Bohm effect (see [Ara98] and references therein).

Mathematically rigorous studies on time operators, including general theories of time operators (not necessarily restricted to time operators of Schrödinger operators), have been made by some authors (e.g., [Miy01, Gal02, GCB04, Ara05, Ara07, Ara08a, Ara08b, AM08a, Ara09, AM08b , HKM09] and references therein; see also [Dor84, JM80, Sch83a, Sch83b] for earlier studies from purely mathematical points of view). The present paper is a continuation of those studies, in particular, concentrating on constructions of time operators *in a generalized sense* associated with a class of Schrödinger operators which contains the Hamiltonian of the hydrogen atom.

Let H be a self-adjoint operator on $\mathscr{H}$ and bounded from below. Then the von Neumann uniqueness theorem tells us that there exists no self-adjoint operator T such that pair (H, T) satisfies the Weyl relation (1.4) with $d = 1$, since $\sigma(P) = \mathbb{R}$ and then $H \not\cong P$, where, for a linear operator L, $\sigma(L)$ denotes the spectrum of L. Thus, to treat such a case, it is natural to introduce a weaker version of the Weyl representation with one degree of freedom to define a class of time operators.

Definition 1.2 (weak Weyl relation) A pair (A, B) consisting of a self-adjoint operator A and symmetric operator B on $\mathscr{H}$ is called a *weak Weyl representation* with one degree of freedom if $e^{-itA}\mathrm{D}(B) \subset \mathrm{D}(B)$ for all $t \in \mathbb{R}$ and the *weak Weyl relation*

$$Be^{-itA}\psi = e^{-itA}(B + t)\psi \tag{1.11}$$

holds for all $\psi \in \mathrm{D}(B)$ and all $t \in \mathbb{R}$.

Studies on this class of representations from purely mathematical points of view have been done in [Dor84, JM80, Sch83a, Sch83b]. It is easy to see that a Weyl representation $\{A, B\}$ is a weak Weyl representation and that the weak Weyl relation (1.11) implies the CCR (1.1) on $\mathrm{D}(AB) \cap \mathrm{D}(BA)$. But one should note that a weak Weyl representation (A, B) with both A and B being self-adjoint is not necessarily a Weyl representation.

Definition 1.3 (strong time operator) A symmetric operator T on $\mathscr{H}$ is called a *strong time operator* of a self-adjoint operator H on $\mathscr{H}$ if (H, T) is a weak Weyl representation.

Remark 1.4 (1) In relation to strong time operators, it may be convenient to give a name to a self-adjoint operator T on $\mathscr{H}$ such that (H, T) is a Weyl representation of the CCR with one degree of freedom. We call such an operator T an *ultra-strong time operator* of H. It follows that an ultra-strong time operator is a strong time operator. But the converse is not true. If $\mathscr{H}$ is separable, then, by the von Neumann uniqueness theorem, (H, T) is unitarily equivalent to the direct sum of the Schrödinger representation (P, Q) with $d = 1$.

(2) It is well known or easy to see that, if (H, T) is a Weyl representation of the CCR with one degree of freedom, then $\sigma(H) = \sigma(T) = \mathbb{R}$ (for this fact, separability of $\mathscr{H}$ is not assumed). Hence a semi-bounded self-adjoint operator (i.e. a self-adjoint operator which is bounded from below or above) has no ultra-strong time operators.

As far as we know, a firm mathematical investigation of a strong time operator was initiated by [Miy01], although the name "strong time operator" is not used in [Miy01] (it was introduced first in [Ara08b] to distinguish different classes of time operators). Further investigations and generalizations on strong time operators were done in [Ara05, Ara07]. See also [AM08a, AM08b , HKM09, RT09]. It is known that, if (H,T) satisfies the weak Weyl relation, then $\sigma(H)$ is purely absolutely continuous [Sch83a]. Hence, if H has an eigenvalue, then H has no strong time operator.

In the context of quantum physics, in addition to time-energy uncertainty relation (1.10), a strong time operator T of a Hamiltonian H may have properties richer than those of time operators of H. For example, it controls decay rates in time $t \in \mathbb{R}$ of transition probabilities $|(\phi, e^{-itH}\psi)|^2$ ($\phi, \psi \in \mathscr{H}$, $\|\phi\| = \|\psi\| = 1$) in the following form [Ara05, Theorem 8.5]: for each natural number $n \in \mathbb{N}$ and all unit vectors $\phi, \psi \in \mathrm{D}(T^n)$, there exists a constant $d_n^T(\phi,\psi) \geq 0$ such that, for all $t \in \mathbb{R} \setminus \{0\}$,

$$|(\phi, e^{-itH}\psi)|^2 \leq \frac{d_n^T(\phi,\psi)^2}{|t|^{2n}}.$$

This shows a very interesting correspondence between decay rates in time of transition probabilities and regularities of state vectors ϕ, ψ.[5]

In [Gal02, AM08b], a time operator of a self-adjoint operator whose spectrum is purely discrete with a growth condition is constructed. In [Ara09], necessary and sufficient conditions for a self-adjoint operator with purely discrete spectrum to have a time operator were given. From these investigations, it is suggested that the concept of time operator should be weakened for a self-adjoint operator (a Hamiltonian in the context of quantum mechanics) whose spectrum is not purely absolutely continuous and whose discrete spectrum does not satisfy conditions formulated in [Ara09]. One of weaker versions of time operator is defined as follows:

Definition 1.5 (weak time operator) A symmetric operator T on $\mathscr{H}$ is called a *weak time operator* of a self-adjoint operator H on $\mathscr{H}$ if there exists a non-zero subspace $\mathscr{D}_{\mathrm{w}} \subset \mathrm{D}(T) \cap \mathrm{D}(H)$ such that the *weak CCR* on $\mathscr{D}_{\mathrm{w}}$ holds:

$$(H\phi, T\psi) - (T\phi, H\psi) = -i(\phi,\psi), \quad \phi, \psi \in \mathscr{D}_{\mathrm{w}}. \tag{1.12}$$

We call $\mathscr{D}_{\mathrm{w}}$ a *weak-CCR domain* for the pair (H,T).

It is obvious that a time operator T of H is a weak time operator of H with $\mathscr{D}_{\mathrm{w}} = \mathscr{D}_{H,T}$. We remark that (1.12) implies the time-energy uncertainty relation (1.10) with $\psi \in \mathscr{D}_{\mathrm{w}}$ ($\|\psi\| = 1$).

One should keep in mind the following fact:

Proposition 1.6 *Let T be a weak time operator of a self-adjoint operator H and $\mathscr{D}_{\mathrm{w}}$ be a weak-CCR domain for (H,T). Then H has no eigenvectors in $\mathscr{D}_{\mathrm{w}}$.*

Proof: Let $H\psi = E\psi$ with $\psi \in \mathscr{D}_{\mathrm{w}}$ and $E \in \mathbb{R}$. Taking ϕ in (1.12) to be ψ, we see that the left hand side is equal to 0. Hence $\|\psi\|^2 = 0$, implying $\psi = 0$. □

Remark 1.7 Unfortunately we do not know whether or not there exists a weak time operator which cannot be a time operator. We leave this problem for future study.

[5] Here we mean by "regularity" of a vector ψ the number n such that $\psi \in \mathrm{D}(T^n)$.

1.2 Ultra-weak time operator

Proposition 1.6 implies that, if a self-adjoint operator H with an eigenvalue E has a weak time operator, then all the eigenvectors of H with eigenvalue E are out of any weak-CCR domain for (H, T). On the other hand, H may have a complete set of eigenvectors so that the subspace algebraically spanned by the eigenvectors of H is dense in $\mathscr{H}$. This suggests that such a self-adjoint operator may have tendency not to have a weak time operator. Taking into account this possibility and in the spirit of seeking ideas as general as possible, we generalize the concept of weak time operator:

Definition 1.8 (ultra-weak time operator) Let H be a self-adjoint operator on $\mathscr{H}$ and $\mathscr{D}_1$ and $\mathscr{D}_2$ be non-zero subspaces of $\mathscr{H}$. A sesquilinear form $\mathfrak{t} : \mathscr{D}_1 \times \mathscr{D}_2 \to \mathbb{C}$ ($\mathscr{D}_1 \times \mathscr{D}_2 \ni (\phi, \psi) \mapsto \mathfrak{t}[\phi, \psi] \in \mathbb{C}$) with domain $\mathrm{D}(\mathfrak{t}) = \mathscr{D}_1 \times \mathscr{D}_2$ ($\mathfrak{t}[\phi, \psi]$ is antilinear in ϕ and linear in ψ) is called *an ultra-weak time operator* of H if there exist non-zero subspaces $\mathscr{D}$ and $\mathscr{E}$ of $\mathscr{D}_1 \cap \mathscr{D}_2$ such that the following (i)–(iii) hold:

(i) $\mathscr{E} \subset D(H) \cap \mathscr{D}$.

(ii) (symmetry on $\mathscr{D}$) $\mathfrak{t}[\phi, \psi]^* = \mathfrak{t}[\psi, \phi]$, $\phi, \psi \in \mathscr{D}$, where, for a complex number $z \in \mathbb{C}$, z^* denotes the complex conjugate of z.

(iii) (ultra-weak CCR) $H\mathscr{E} \subset \mathscr{D}_1$ and, for all $\psi, \phi \in \mathscr{E}$,

$$\mathfrak{t}[H\phi, \psi] - \mathfrak{t}[H\psi, \phi]^* = -i(\phi, \psi) \tag{1.13}$$

We call $\mathscr{E}$ an *ultra-weak CCR-domain* for $(H, \mathfrak{t})$ and $\mathscr{D}$ a *symmetric domain* of $\mathfrak{t}$.

Remark 1.9 (1) As far as we know, the concept "ultra-weak time operator" introduced here is new.

(2) Although there may be no operators associated with the sesquilinear form $\mathfrak{t}$ in the above definition, we use, by abuse of word, "ultra-weak time operator" to indicate that it is a concept weaker than that of weak time operator as shown below.

Let T be a weak time operator of H with a weak CCR-domain $\mathscr{D}_{\mathrm{w}}$. Then one can define a sesquilinear form $\mathfrak{t}_T : \mathscr{H} \times \mathrm{D}(T) \to \mathbb{C}$ by

$$\mathfrak{t}_T[\phi, \psi] := (\phi, T\psi), \quad \phi \in \mathscr{H}, \psi \in \mathrm{D}(T).$$

Then it is easy to see that $\mathfrak{t}_T[\phi, \psi]^* = \mathfrak{t}_T[\psi, \phi]$, $\psi, \phi \in \mathrm{D}(T)$ and, for all $\phi, \psi \in \mathscr{D}_{\mathrm{w}}$, $\mathfrak{t}_T[H\phi, \psi] - \mathfrak{t}_T[H\psi, \phi]^* = -i(\psi, \phi)$. Hence $\mathfrak{t}_T$ is an ultra-weak time operator of H with $\mathscr{D}_{\mathrm{w}}$ being an ultra-weak CCR-domain and $\mathrm{D}(T)$ a symmetry domain. Therefore the concept of ultra-weak time operator is a generalization of weak time operator.

(3) If $H\psi \in \mathscr{D}$ in (1.13), then, by the symmetry of $\mathfrak{t}[\cdot, \cdot]$ on $\mathscr{D}$, (1.13) takes the following form:

$$\mathfrak{t}[H\phi, \psi] - \mathfrak{t}[\phi, H\psi] = -i(\phi, \psi)$$

For a sesquilinear form $\mathfrak{t} : \mathscr{D}_1 \times \mathscr{D}_2 \to \mathbb{C}$ and a constant $a \in \mathbb{R}$, we define a sesquilinear form $\mathfrak{t} - a : \mathscr{D}_1 \times \mathscr{D}_2 \to \mathbb{C}$ by

$$(\mathfrak{t} - a)[\phi, \psi] := \mathfrak{t}[\phi, \psi] - a(\phi, \psi), \quad \phi \in \mathscr{D}_1, \psi \in \mathscr{D}_2.$$

In the case of the pair $(H, \mathfrak{t})$ in Definition 1.8, the uncertainty relation (1.2) associated with CCR is generalized as follows:

Proposition 1.10 (uncertainty relation for $(H, \mathfrak{t})$**)** *Assume that H has an ultra-weak time operator $\mathfrak{t}$ as in Definition 1.8. Then, for all $a, b \in \mathbb{R}$ and a unit vector $\psi \in \mathscr{E}$,*

$$|(\mathfrak{t} - a)[(H - b)\psi, \psi]| \geq \frac{1}{2}. \tag{1.14}$$

Proof: Using (1.13), we have $\Im\{(\mathfrak{t} - a)[(H - b)\psi, \psi]\} = -\frac{1}{2}$. Since $|z| \geq |\Im z|$ for all $z \in \mathbb{C}$, (1.14) follows. □

In summary, we have seen that there exist five classes of time operators with the following inclusion relations:

$$\{\text{ultra-strong time operators}\} \subset \{\text{strong time operators}\} \subset \{\text{time operators}\}$$
$$\subset \{\text{weak time operators}\} \subset \{\text{ultra-weak time operators}\}.$$

1.3 Outline of the present paper

Having introduced the new concept "ultra-weak time operator, we now outline the contents of the present paper. In Section 2, we review an abstract theory of time operators and give new additional results. Among others, we prove an existence theorem on a strong time operator of an absolutely continuous self-adjoint operator (Theorem 2.16). Sections 3–5 are devoted to showing the existence of time operators of self-adjoint operators with purely discrete spectra. This includes an extension of existence theorems on time operators in [Gal02, AM08b]. In Section 6, we introduce a class $S_1(\mathscr{H})$ of self-adjoint operators on $\mathscr{H}$ (see Definition 6.3) such that each element of $S_1(\mathscr{H})$ has an ultra-weak time operator with a dense ultra-weak CCR-domain (Theorem 6.4). Moreover, for a class of Borel measurable functions $f : \mathbb{R} \to \mathbb{R}$, we formulate sufficient conditions for $f(H)$ to have an ultra-weak time operator (Corollary 6.6). In Section 7, we discuss applications of the abstract results to the Schrödinger operator H_V. We find classes of potentials V for which H_V has an ultra-weak time operator with a dense ultra-weak CCR-domain (Theorem 7.6) Also we show that the Hamiltonian of the hydrogen atom (i.e. the case where $V(x) = -\gamma/|x|$, $x \in \mathbb{R}^3 \setminus \{0\}$ with a constant $\gamma > 0$) has an ultra-weak time operator with a dense ultra-weak CCR-domain (Example 7.10). In the last section, for a class of f, an existence theorem on an ultra-weak time operator of $f(H_V)$ is proved (Theorem 8.2) and some examples are given.

2 Abstract Theory of Time Operators–Review with Additional Results

2.1 A general structure of time operators

We first note an elementary fact:

Proposition 2.1 *Let H be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and T be a time operator of H with a CCR-domain $\mathscr{D}$ for (H,T). Let H' be a self-adjoint operator on a Hilbert space $\mathscr{H}'$ such that $UHU^{-1} = H'$ for a unitary operator $U : \mathscr{H} \to \mathscr{H}'$. Then $T' := UTU^{-1}$ is a time operator of H' with a CCR-domain $U\mathscr{D}$ for (H',T').*

Proof: An easy exercise. □

In what follows, H denotes a self-adjoint operator on a complex Hilbert space $\mathscr{H}$. As is well known (e.g., [Ka76, §10.1], [RS72, Theorem VII.24]), $\mathscr{H}$ has the orthogonal decomposition

$$\mathscr{H} = \mathscr{H}_{\rm ac}(H) \oplus \mathscr{H}_{\rm sc}(H) \oplus \mathscr{H}_{\rm p}(H), \tag{2.1}$$

where $\mathscr{H}_{\rm ac}(H)$ (resp. $\mathscr{H}_{\rm sc}(H)$, $\mathscr{H}_{\rm p}(H)$) is the subspace of absolute continuity (resp. of singular continuity, of discontinuity) with respect to H, and H is reduced by each subspace $\mathscr{H}_\#(H)$ ($\#$ = ac, sc, p). We denote the reduced part of H to $\mathscr{H}_\#(H)$ by $H_\#$ and set

$$\sigma_{\rm ac}(H) := \sigma(H_{\rm ac}), \quad \sigma_{\rm sc}(H) := \sigma(H_{\rm sc}),$$

which are called the absolutely continuous spectrum and the singular continuous spectrum of H respectively. We denote by $\sigma_{\rm p}(H)$ the set of all eigenvalues of H. We remark that $\sigma(H_{\rm p}) = \overline{\sigma_{\rm p}(H)}$, the closure of $\sigma_{\rm p}(H)$. We have

$$H = H_{\rm ac} \oplus H_{\rm sc} \oplus H_{\rm p} \tag{2.2}$$

and

$$\sigma(H) = \sigma_{\rm ac}(H) \cup \sigma_{\rm sc}(H) \cup \overline{\sigma_{\rm p}(H)}.$$

An eigenvalue of H is called a discrete eigenvalue of H if it is an isolated eigenvalue of H with a finite multiplicity. The set $\sigma_{\rm disc}(H)$ of all the discrete eigenvalues of H is called the discrete spectrum of H.

The following proposition shows that the problem of constructing time operators of H is reduced to that of constructing time operators of each $H_\#$.

Proposition 2.2 *Suppose that each $H_\#$ has a time operator $T_\#$ with a CCR-domain $\mathscr{D}_\#$. Then the direct sum*

$$T := T_{\rm ac} \oplus T_{\rm sc}(H) \oplus T_{\rm p}$$

is a time operator of H with a CCR-domain $\mathscr{D}_{\rm ac} \oplus \mathscr{D}_{\rm sc} \oplus \mathscr{D}_{\rm p}$.

Proof: Since the direct sum of symmetric operators is again a symmetric operator in general, it follows that T is symmetric. By the assumption, we have for all $\psi_{\#} \in \mathscr{D}_{\#}$

$$[H_{\#}, T_{\#}]\psi_{\#} = -i\psi_{\#}.$$

Let $\psi = (\psi_{\rm ac}, \psi_{\rm sc}, \psi_{\rm p}) \in \mathscr{D}_{\rm ac} \oplus \mathscr{D}_{\rm sc} \oplus \mathscr{D}_{\rm p}$. Then, by (2.2), $\psi \in D(HT) \cap D(TH)$ and

$$[H, T]\psi = ([H_{\rm ac}, T_{\rm ac}]\psi_{\rm ac}, [H_{\rm sc}, T_{\rm sc}]\psi_{\rm sc}, [H_{\rm p}, T_{\rm p}]\psi_{\rm p}) = -i\psi.$$

Hence T is a time operator of H with a CCR-domain $\mathscr{D}_{\rm ac} \oplus \mathscr{D}_{\rm sc} \oplus \mathscr{D}_{\rm p}$. □

2.2 Strong time operators

2.2.1 A summary of known results and additional results

We summarize some basic facts on strong time operators of H.

Proposition 2.3 *A symmetric operator T is a strong time operator of H if and only if operator equality $e^{itH}Te^{-itH} = T + t$ holds for all $t \in \mathbb{R}$.*

Proof: See [Ara05, Proposition 2.1]. □

Note that the operator equality given in this proposition implies that, for all $t \in \mathbb{R}$, $e^{-itH}\mathrm{D}(T) = \mathrm{D}(T)$.

Proposition 2.4 *Let T be a strong time operator of H and H' be a self-adjoint operator on a Hilbert space $\mathscr{H}'$ such that, for a unitary operator $U : \mathscr{H} \to \mathscr{H}'$, $UHU^{-1} = H'$. Then $T' := UTU^{-1}$ is a strong time operator of H'.*

Proof: By the functional calculus, for all $t \in \mathbb{R}$, $e^{itH'} = Ue^{itH}U^{-1}$. By this fact and Proposition 2.3, we have

$$e^{itH'}T'e^{-itH'} = Ue^{itH}Te^{-itH}U^{-1} = U(T + t)U^{-1} = T' + t.$$

Hence T' is a strong time operator of H'. □

Proposition 2.5 ([Ara05]) *Suppose that H has a strong time operator T. Then:*

(1) The closure $\overline{T}$ of T is also a strong time operator of H.

(2) If H is semi-bounded, then T is not essentially self-adjoint.

(3) The operator H is absolutely continuous.

Proposition 2.6 *Let $T_1, \ldots, T_n$ $(n \geq 2)$ be strong time operators of H.*

(1) Let $S := \sum_{k=1}^{n} a_k T_k$ with $a_k \in \mathbb{R}$ $(k = 1, \ldots, n)$ satisfying $\sum_{k=1}^{n} a_k = 1$. Then, for all $t \in \mathbb{R}$, operator equality

$$e^{itH} S e^{-itH} = S + t \tag{2.3}$$

holds. In particular, if $\cap_{k=1}^{n} D(T_k)$ is dense, then S is a strong time operator of H.

(2) For any pair (k, ℓ) with $k \neq \ell$ $(k, \ell = 1, \ldots, n)$, $(T_k - T_\ell) e^{itH} \psi = e^{itH}(T_k - T_\ell)\psi$ for all $t \in \mathbb{R}$ and $\psi \in D(T_k) \cap D(T_\ell)$.

Proof: (1) By Proposition 2.3, we have operator equalities

$$e^{itH} T_k e^{-itH} = T_k + t, \quad t \in \mathbb{R}, k = 1, \ldots, n. \tag{2.4}$$

Since $e^{itH} S e^{-itH} = \sum_{k=1}^{n} e^{itH} a_k T_k e^{-itH}$ (operator equality), (2.4) implies (2.3). If $\cap_{k=1}^{d} \mathrm{D}(T_k)$ is dense, then S is a symmetric operator and hence it is a strong time operator of H.

(2) This easily follows from (2.4). □

Proposition 2.6-(1) shows that any real convex combination S of strong time operators of H such that $\mathrm{D}(S)$ is dense is a strong time operator of H.

Let $\{H_1, \ldots, H_n\}$ be a set of strongly commuting self-adjoint operators on $\mathscr{H}$. Then $\sum_{j=1}^{n} H_j$ is essentially self-adjoint and, for all $t \in \mathbb{R}$,

$$e^{it\overline{\sum_{j=1}^{n} H_j}} = \prod_{j=1}^{n} e^{itH_j}, \tag{2.5}$$

where the order of the product of $e^{itH_1}, \ldots, e^{itH_n}$ on the right hand side is arbitrary (this is due to the commutativity of e^{itH_j} and e^{itH_k} $(j, k = 1, \ldots, n)$ which follows the strong commutativity of $\{H_1, \ldots, H_n\}$).

Proposition 2.7 *Let $\{H_1, \ldots, H_n\}$ be as above and assume that, for some j, H_j has a strong time operator T_j such that $e^{itH_k} T_j e^{-itH_k} = T_j$ for all $k \neq j$. Then T_j is a strong time operator of $\overline{\sum_{j=1}^{n} H_j}$.*

Proof: By the present assumption and Proposition 2.3, we have operator equality $e^{itH_j} T_j e^{-itH_j} = T_j + t$ for all $t \in \mathbb{R}$. Hence, by (2.5) and the commutativity of the operators e^{itH_k}, $k = 1, \ldots, n$, we have

$$e^{it\overline{\sum_{j=1}^{n} H_j}} T_j e^{-it\overline{\sum_{j=1}^{n} H_j}} = \left(\prod_{k \neq j} e^{itH_k}\right) (T_j + t) \left(\prod_{k \neq j} e^{-itH_k}\right) = T_j + t.$$

Thus the desired result follows. □

Proposition 2.7 may be useful to find strong time operators of a self-adjoint operator which is given by the closure of the sum of strongly commuting self-adjoint operators.

A variant of Proposition 2.7 is formulated as follows. Let $\{A_1, \ldots, A_n\}$ be a set of strongly commuting self-adjoint operators on $\mathscr{H}$ such that each A_j is injective. Suppose that each A_j has a strong time operator B_j such that, for all $j = 1, \ldots, n$, $\mathrm{D}(B_j A_j^{-1}) \cap \mathrm{D}(A_j^{-1} B_j)$ is dense and, for all $t \in \mathbb{R}$, $e^{itA_k} B_j e^{itA_k} = B_j$, $k \neq j, k = 1, \ldots, n$. By the strong commutativity of $\{A_1, \ldots, A_n\}$, the operator

$$H_A := \sum_{j=1}^{n} A_j^2$$

is a non-negative self-adjoint operator. For each $j = 1, \ldots, n$, the operator

$$T_j := \frac{1}{4}\left(\overline{B}_j A_j^{-1} + A_j^{-1} \overline{B}_j\right)$$

is symmetric.

Proposition 2.8 ([Ara05]) *For each $j = 1, \ldots, n$, T_j is a strong time operator of H_A.*

A general scheme to construct strong time operators for a given pair (H, T) of a weak Weyl representation is described in [Ara05, §10]. A generalization of this scheme is given as follows. By the functional calculus, for any real-valued continuous function f on $\mathbb{R}$, $f(H)$ is a self-adjoint operator on $\mathscr{H}$. Then a natural question is: does $f(H)$ has a strong time operator ? A heuristic argument to answer the question is as follows. Let $f \in C^1(\mathbb{R})$ and denote the derivative of f by f'. We have $[T, H] = +i\mathbb{1}$, which intuitively implies that $T = +id/dH$. Hence we may formally see that $[T, f(H)] = if'(H)$(in [Ara05, Theorem 6.2], this is justified for all $f \in C^1(\mathbb{R})$ such that f and f' are bounded), and then $Te^{-itf(H)} = e^{-itf(H)}(T + tf'(H))$ holds. Multiplying $f'(H)^{-1}$ on the both sides, we may have $Tf'(H)^{-1}e^{-itf(H)} = e^{-itf(H)}(Tf'(H)^{-1} + t)$, and, by symmetrizing $Tf'(H)^{-1}$, we expect that $\frac{1}{2}(Tf'(H)^{-1} + f'(H)^{-1}T)$ is a strong time operator of $f(H)$. Actually this result is justified under some conditions:

Proposition 2.9 ([HKM09, Theorem 1.9]) *Let K be a closed null subset of $\mathbb{R}$ with respect to the Lebesgue measure. Assume that $f \in C^2(\mathbb{R} \setminus K)$ and $L := \{\lambda \in \mathbb{R} \setminus K | f'(\lambda) = 0\}$ is a null set with respect to the Lebesgue measure. Suppose that H has a strong time operator T_H which is closed and let*

$$D := \{g(H)\mathrm{D}(T_H) | g \in C_0^\infty(\mathbb{R} \setminus L \cup K)\}.$$

Then

$$T_{f(H)} := \frac{1}{2}\overline{(T_H f'(H)^{-1} + f'(H)^{-1} T_H)\lceil D}$$

is a strong time operator of $f(H)$*, where, for a linear operator* L *and a subspace* $\mathscr{D} \subset \mathrm{D}(L)$*,* $L\lceil\mathscr{D}$ *denotes the restriction of* L *to* $\mathscr{D}$*.*

Example 2.10 (Aharonov-Bohm time operator) Let $m > 0$ be a constant. Then it is obvious that $\sqrt{2m}Q_j$ is a strong time operator of $P_j/\sqrt{2m}$ in the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^d)$. Consider the function $f(\lambda) = \lambda^2$, $\lambda \in \mathbb{R}$. Then $f'(\lambda) = 2\lambda$. Hence $\{\lambda \in \mathbb{R} | f'(\lambda) = 0\} = \{0\}$. Therefore the subspace D in Proposition 2.9 takes the form $D_{\mathrm{AB},j} := \mathrm{L.H.}\{g(P_j)\mathrm{D}(Q_j) | g \in C_0^\infty(\mathbb{R} \setminus \{0\})\}$. Hence, letting

$$T_{\mathrm{AB},j} := \frac{m}{2}\left(Q_j P_j^{-1} + P_j^{-1} Q_j\right),$$

the operator

$$\widetilde{T}_{\mathrm{AB},j} := \overline{T_{\mathrm{AB},j}\lceil D_{\mathrm{AB},j}}$$

is a strong time operator of $P_j^2/2m$. Since $(P_1, \ldots, P_d)$ is a set of strongly commuting self-adjoint operators, it follows from Proposition 2.8 that $\widetilde{T}_{\mathrm{AB},j}$ is a strong time operator of H_0.

There is another domain on which $T_{\mathrm{AB},j}$ becomes a strong time operator of H_0 [Ara07]. Let $\Omega_j := \{k \in \mathbb{R}^d | k_j \neq 0\}$ and $D'_{\mathrm{AB},j} := \{f \in L^2(\mathbb{R}^d) | \hat{f} \in C_0^\infty(\Omega_j)\}$, where $\hat{f}$ is the L^2-Fourier transform of f. Then $D'_{\mathrm{AB},j}$ is dense. Moreover, by using the Fourier analysis, it is shown that the operators $Q_j, P_j^{-1}, e^{itP_j^2/2m}$ and e^{itH_0} ($\forall t \in \mathbb{R}$) leave $D'_{\mathrm{AB},j}$ invariant and, for all $t \in \mathbb{R}$, $e^{itH_0} T_{\mathrm{AB},j} e^{-itH_0} = T_{\mathrm{AB},j} + t$ on $D'_{\mathrm{AB},j}$. Hence

$$T'_{\mathrm{AB},j} := T_{\mathrm{AB},j}\lceil D'_{\mathrm{AB},j}$$

is a strong time operator of H_0. We note that $\mathrm{D}(Q_j) \supset D'_{\mathrm{AB},j}$. Hence, for each $g \in C_0^\infty(\mathbb{R} \setminus \{0\})$, $g(P_j)\mathrm{D}(Q_j) \supset g(P_j)D'_{\mathrm{AB},j}$. For any $g \in C_0^\infty(\mathbb{R} \setminus \{0\})$ such that $\hat{g}(k_j) > 0, \forall k_j \in \mathbb{R}$, $g(P_j)D'_{\mathrm{AB},j} = D'_{\mathrm{AB},j}$. It is not so difficult to show that such a function g exists. Therefore $D_{\mathrm{AB},j} \supset D'_{\mathrm{AB},j}$ in fact. A time operator of H_0 obtained as a restriction of $T_{\mathrm{AB},j}$ to a subspace or its closure is called an *Aharonov-Bohm time operator* [AB61, Miy01].

Example 2.11 As a generalization of Aharonov-Bohm time operators, one can construct strong time operators of a self-adjoint operator H of the form $H = F(P)$ with $F \in C^1(\mathbb{R}^d)$, which includes the free relativistic Schrödinger Hamiltonian $(-\Delta + m^2)^{1/2}$ $(m > 0)$ and its fractional version $(-\Delta + m^2)^\alpha$ $(\alpha > 0)$. This approach can be applied also to constructions of strong time operators of Dirac type operators [Th92]. See [Ara05, §11]) for the details.

2.2.2 Existence of a strong time operator for a class of absolutely continuous self-adjoint operators

As already mentioned, a self-adjoint operator which has a strong time operator is absolutely continuous. Then a natural question is: does an absolutely continuous self-adjoint operator have a strong time operator ? To our best knowledge, this question has not been answered in an abstract framework. In what follows, we give a partial affirmative answer to the question.

We recall an important concept. For a linear operator A on a Hilnbert space $\mathscr{H}$, a vector $\phi \in \cap_{n=1}^{\infty} \mathrm{D}(A^n)$ is called a *cyclic vector* for A if $\mathrm{L.H.}\{A^n\phi | n \in \{0\} \cup \mathbb{N}\}$ is dense in $\mathscr{H}$, where, for a subset $\mathscr{D}$ of $\mathscr{H}$, $\mathrm{L.H.}\mathscr{D}$ denotes the algebraic linear hull of vectors in $\mathscr{D}$. It is obvious that, if $\mathscr{H} \neq \{0\}$, then $\phi \neq 0$.

For a non-zero vector $\psi \in \mathscr{H}$, a measure μ_ψ on $\mathbb{R}$ is defined by

$$\mu_\psi(B) := \|E_H(B)\psi\|^2, \quad B \in \boldsymbol{B},$$

where $\boldsymbol{B}$ is the family of Borel sets of $\mathbb{R}$. We define a function X on $\mathbb{R}$ by

$$X(\lambda) := \lambda, \quad \lambda \in \mathbb{R}.$$

We note the following fact:

Lemma 2.12 *Assume that $\mathscr{H}$ is separable. Suppose that H has a cyclic vector ϕ. Then there exists a unitary operator U from $\mathscr{H}$ to $L^2(\mathbb{R}, d\mu_\phi)$ such that $U\phi = 1$ and $UHU^{-1} = M_X$, the multiplication operator by the function X acting in $L^2(\mathbb{R}, d\mu_\phi)$. Moreover, the subspace* $\mathrm{L.H.}\{e^{itX} | t \in \mathbb{R}\}$ *is dense in* $L^2(\mathbb{R}, d\mu_\phi)$.

Proof: The first half of the lemma follows from an easy extension of Lemma 1 in [RS72, §VII.2] to the case of unbounded self-adjoint operators [Ara06, Theorem 1.8]. To prove the second half of the lemma, we note that, by the cyclicity of ϕ for H, $\mathrm{L.H.}\{H^n\phi | n \in \{0\} \cup \mathbb{N}\}$ is dense in $\mathscr{H}$. By the functional calculus, we have

$$\lim_{t \to 0} (-i)^n \left(\frac{e^{itH} - 1}{t} \right)^n \phi = H^n \phi.$$

Hence it follows that $\mathrm{L.H.}\{e^{itH}\phi | t \in \mathbb{R}\}$ is dense in $\mathscr{H}$. By the first half of the lemma, we have $Ue^{itH}\phi = e^{itX}$. Hence $\mathrm{L.H.}\{e^{itX} | t \in \mathbb{R}\}$ is dense in $L^2(\mathbb{R}, d\mu_\phi)$.

□

Let $\psi \in \mathscr{H}$. If μ_ψ is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}$, then we denote by ρ_ψ the Radon-Nykodým derivative of μ_ψ: $\rho_\psi \geq 0$ and $\mu_\psi(B) = \int_B \rho_\psi(\lambda) d\lambda$, $B \in \boldsymbol{B}$.

We introduce a class of self-adjoint operators on $\mathscr{H}$.

Definition 2.13 We say that a self-adjoint operator H on $\mathscr{H}$ is in the class $S_0(\mathscr{H})$ if it satisfies the following (i) and (ii):

(i) H is absolutely continuous.

(ii) H has a cyclic vector ϕ such that ρ_ϕ is differentiable on $\mathbb{R}$ and

$$\lim_{x\to\pm\infty}\rho_\phi(\lambda)=0,\quad \int_{\rho(\lambda)>0}\frac{\rho'_\phi(\lambda)^2}{\rho_\phi(\lambda)}d\lambda<\infty.$$

Let $\mathscr{H}$ be separable and $H\in S_0(\mathscr{H})$ with a cyclic vector ϕ satisfying the above (ii) and

$$W_\phi(\lambda):=\begin{cases}\dfrac{\rho'_\phi(\lambda)}{\rho_\phi(\lambda)} & \text{for } \rho_\phi(\lambda)>0\\ 0 & \text{for } \rho_\phi(\lambda)=0\end{cases}.$$

Then we define an operator Y on $L^2(\mathbb{R},d\mu_\phi)$ as follows:

$$D(Y):=\text{L.H.}\{e^{itX}|t\in\mathbb{R}\},\quad Y:=i\frac{d}{d\lambda}+\frac{i}{2}W_\phi.$$

Lemma 2.14 *The operator Y is a symmetric operator.*

Proof: By Lemma 2.12, $D(Y)$ is dense in $L^2(\mathbb{R},d\mu_\phi)$. Using (ii) and integration by parts, we see that, for all $f,g\in D(Y)$, $(f,Yg)_{L^2(\mathbb{R},d\mu_\phi)}=(Yf,g)_{L^2(\mathbb{R},d\mu_\phi)}$. Hence Y is a symmetric operator. □

Lemma 2.15 *The operator Y is a strong time operator of M_X.*

Proof: It is obvious that, for all $t\in\mathbb{R}$, $e^{itM_X}D(Y)\subset D(Y)$. Let $f(\lambda)=e^{is\lambda}$, $s\in\mathbb{R},\lambda\in\mathbb{R}$. Then, using the fact that $if'(\lambda)=-sf(\lambda)$, we see that

$$(e^{itM_X}Ye^{-itM_X}f)(\lambda)=e^{it\lambda}\left(i\frac{d}{d\lambda}+\frac{i}{2}W_\phi\right)e^{-i(t-s)\lambda}=tf(\lambda)+(Yf)(\lambda).$$

Thus Y is a strong time operator of M_X. □

Theorem 2.16 *Assume that $\mathscr{H}$ is separable and that $H\in S_0(\mathscr{H})$. Then H has a strong time operator.*

Proof: We have $U^{-1}M_XU=H$. By Lemma 2.15, Y is a strong time operator of M_X. Hence, by an application of Proposition 2.4, $U^{-1}YU$ is a strong time operator of H.□

Thus we have found a class $S_0(\mathscr{H})$ of self-adjoint operators on a separable Hilbert space $\mathscr{H}$ which each have a strong time operator.

2.3 Construction of strong time operators of a self-adjoint operator from those of another self-adjoint operator

We consider two self-adjoint operators H and H' acting in Hilbert spaces $\mathscr{H}$ and $\mathscr{H}'$ respectively. If $\mathscr{H} = \mathscr{H}'$, then $H' = H + (H' - H)$ on $\mathrm{D}(H) \cap \mathrm{D}(H')$ and hence H' can be regarded as a perturbation of H.

We denote by $P_{\mathrm{ac}}(H)$ the orthogonal projection onto the absolutely continuous subspace $\mathscr{H}_{\mathrm{ac}}(H)$ of H. For a linear operator A, we denote by $\mathrm{Ran}(A)$ the range of A.

Lemma 2.17 *Assume the following (A.1)–(A.3):*

(A.1) The wave operators

$$W_\pm := \text{s-}\lim_{t\to\pm\infty} e^{itH'} J e^{-itH} P_{\mathrm{ac}}(H)$$

exist, where s- lim *means strong limit and* $J : \mathscr{H} \to \mathscr{H}'$ *is a bounded linear operator.*

(A.2) $\lim_{t\to\pm\infty} \|Je^{-itH} P_{\mathrm{ac}}(H)\psi\| = \|P_{\mathrm{ac}}(H)\psi\|, \quad \psi \in \mathscr{H}$.

(A.3)(completeness) $\mathrm{Ran}(W_\pm) = \mathscr{H}_{\mathrm{ac}}(H')$.

Let $U_\pm := W_\pm \lceil \mathscr{H}_{\mathrm{ac}}(H)$. *Then* $U_\pm$ *are unitary operators from* $\mathscr{H}_{\mathrm{ac}}(H)$ *to* $\mathscr{H}_{\mathrm{ac}}(H')$ *such that*

$$H'_{\mathrm{ac}} = U_\pm H_{\mathrm{ac}} U_\pm^{-1}.$$

Proof: See textbooks of quantum scattering theory (e.g., [Ku79, RS79]). □

Theorem 2.18 *Assume (A.1)–(A.3) in Lemma 2.17. Suppose that* H_{ac} *has a strong time operator* T. *Then* $T'_\pm := U_\pm T U_\pm^{-1}$ *are strong time operators of* H'_{ac}.

Proof: This follows from Lemma 2.17 and an application of Proposition 2.4. □

Theorem 2.18 can be used to construct strong time operators of H' from those of H.

3 Time Operators in the Case where H has a Pure Discrete Spectrum (I)

If $\sigma_{\mathrm{disc}}(H) \neq \emptyset$, then no strong time operator of H exists by Proposition 2.5-(3). But, even in that case, H may have time operators or weak time operators. We first recall basic results on this aspect.

Proposition 3.1 ([Ara09, Gal02]) *Suppose that $\sigma(H) = \sigma_{\rm disc}(H) = \{E_n\}_{n=1}^\infty$ ($E_n \neq E_m$ for $n \neq m$), each eigenvalue E_n is simple, and, for some $N \geq 1$, $E_n \neq 0$, $n \geq N$, $\sum_{n=N}^\infty 1/E_n^2 < \infty$. Let e_n be a normalized eigenvector of H with eigenvalue E_n: $He_n = E_n e_n$ and define*

$$T\phi = i\sum_{n=1}^\infty \left(\sum_{m\neq n} \frac{(e_m,\phi)}{E_n - E_m}\right) e_n, \quad \phi \in \mathrm{D}(T) \tag{3.1}$$

with domain

$$\mathrm{D}(T) := \mathscr{F} := \mathrm{L.H.}\{e_n | n \in \mathbb{N}\}, \tag{3.2}$$

Then T is a symmetric operator and $[H, T] = -i\mathbb{1}$ holds on $\mathscr{E} := \mathrm{L.H.}\{e_n - e_m | n, m \in \mathbb{N}\}$. Furthermore $\mathscr{E}$ is dense.

This proposition shows that T is a time operator of H with a dense CCR-domain $\mathscr{E}$ and hence T is a weak time operator of H too with a weak-CCR domain $\mathscr{E}$. But $\mathrm{D}(T) = \mathrm{D}(T) \cap \mathrm{D}(H)$ cannot be a weak-CCR domain for (H, T), since $\mathrm{D}(T)$ contains an eigenvector of H (see Proposition 1.6) (note that $\mathscr{E}$ contains no eigenvectors of H).

Example 3.2 (1-dimensional quantum harmonic oscillator) The Hamiltonian of a 1-dimensional quantum harmonic oscillator is given by

$$H_{\rm osc} := -\frac{1}{2}\Delta + \frac{1}{2}\omega^2 x^2$$

acting in $L^2(\mathbb{R})$, where Δ is the 1-dimensional generalized Laplacian and $\omega > 0$ is a constant. It is shown that $H_{\rm osc}$ is self-adjoint, $\sigma(H_{\rm osc}) = \sigma_{\rm disc}(H_{\rm osc}) = \{\omega(n + \frac{1}{2})\}_{n=0}^\infty$ and each eigenvalue $\omega(n + \frac{1}{2})$ is simple. Since $\sum_{n=1}^\infty 1/(n + \frac{1}{2})^2 < \infty$, the assumption in Proposition 3.1 holds. Hence $H_{\rm osc}$ has a time operator $T_{\rm osc}$ given by

$$T_{\rm osc} f := \frac{i}{\omega}\sum_{n=1}^\infty \left(\sum_{m\neq n} \frac{(e_m, f)}{n - m}\right) e_m, \quad f \in \mathrm{D}(T_{\rm osc}).$$

One can show that T is bounded and $\sigma(\overline{T}) = [-\pi/\omega, \pi/\omega]$ (see [AM08a, Example 4.2]).

Corollary 3.3 *Suppose that $\sigma(H) \setminus \{0\} = \sigma_{\rm disc}(H) = \{E_n\}_{n=1}^\infty$, each E_n is simple, $E_1 < E_2 < \cdots < 0$, $0 \notin \sigma_{\rm p}(H)$, and $\sum_{n=1}^\infty E_n^2 < \infty$. Then the operator $T_{\rm d}$ defined by*

$$T_{\rm d}\phi := i\sum_{n=1}^\infty \left(\sum_{m\neq n} \frac{(e_m,\phi)}{\frac{1}{E_n} - \frac{1}{E_m}}\right) e_n, \quad \phi \in \mathrm{D}(T_{\rm d}) := \mathscr{F} \tag{3.3}$$

is a time operator of H^{-1}, where $\mathscr{F}$ is given by (3.2), i.e., $[H^{-1}, T_{\rm d}] = -i\mathbb{1}$ on $\mathscr{E}$.

Proof: We see that $\sigma(H^{-1}) = \sigma_{\rm disc}(H^{-1}) = \{1/E_n\}_{n=1}^\infty$ and $\sum_{n=1}^\infty 1/(1/E_n)^2 < \infty$. Hence the corollary follows from Proposition 3.1. □

4 Time Operators in the Case where H has a Pure Discrete Spectrum (II)

In Corollary 3.3, condition $\sum_{n=1}^{\infty} E_n^2 < \infty$ is imposed to construct a time operator of H^{-1}, which is needed to apply Proposition 3.1 with H replaced by H^{-1}. In this section, we show that the condition $\sum_{n=1}^{\infty} E_n^2 < \infty$ can be removed. The idea is to decompose $\mathscr{H}$ into the direct sum of appropriate mutually orthogonal closed subspaces [SW14].

Lemma 4.1 *Let $p > 1$ and $\{a_n\}_{n=1}^{\infty}$ be a complex sequence such that $\lim_{n\to\infty} a_n = 0$ and $a_n \neq a_m$ for $n \neq m$, $n, m \in \mathbb{N}$. Let $A := \{a_n | n \in \mathbb{N}\}$ be the set corresponding to the sequence $\{a_n\}_{n=1}^{\infty}$. Then there exist an $N \in \mathbb{N} \cup \{\infty\}$ and subsequences $\{a_{kn}\}_{n=1}^{\infty}$ of $\{a_n\}_{n=1}^{\infty}$ $(k = 1, \ldots, N)$ such that the sets $A_k := \{a_{kn} | n \in \mathbb{N}\}$, $k = 1, \ldots, N$, have the following properties: $A_k \cap A_l = \emptyset$ for $k \neq l$, $k, l = 1, \ldots, N$; $A = \cup_{k=1}^{N} A_k$; $\sum_{n=1}^{\infty} |a_{kn}|^p < \infty$, $k = 1, \ldots, N$.*

Proof: For each $k \in \mathbb{N}$, let $J_k := \{a_n | 1/(k+1) < |a_n| \leq 1/k\} \subset A$ and $\{k | J_k \neq \emptyset\} = \{k_1, k_2, \ldots\}$ with $k_1 < k_2 < \ldots$, which is an infinite set by the condition $\lim_{n\to\infty} a_n = 0$. It is obvious that $A = \cup_{n=1}^{\infty} J_{k_n}$ and $J_{k_n} \cap J_{k_m} = \emptyset$ for all (n, m) with $n \neq m$. Let $a_{1n} \in J_{k_n}$. Then $\sum_{n=1}^{\infty} |a_{1n}|^p \leq \sum_{n=1}^{\infty} 1/k_n^p < \infty$. Let $A_1 := \{a_{1n} | n \in \mathbb{N}\}$ and $A' := A \setminus A_1$. Write $A' = \{b_n | n \in \mathbb{N}\}$ with $b_n \neq b_m$ $(n \neq m)$. Then we can apply the preceding procedure on $\{a_n\}_{n=1}^{\infty}$ to $\{b_n\}_{n=1}^{\infty}$ to conclude that there exists a subsequence $\{a_{2n}\}_{n=1}^{\infty}$ of $\{b_n\}_{n=1}^{\infty}$ such that $\sum_{n=1}^{\infty} |a_{2n}|^p < \infty$. Hence we obtain a subset $A_2 := \{a_{2n} | n \in \mathbb{N}\}$. Obviously $A_1 \cap A_2 = \emptyset$. Then we give a similar consideration to $A'' := A' \setminus A_2 = A \setminus (A_1 \cup A_2)$. In this way, by induction, we can show that, for each $k \in \mathbb{N}$, there exists a subset A_k which is empty or $A_k = \{a_{kn} | n \in \mathbb{N}\} \subset A$ such that $\sum_{n=1}^{\infty} |a_{kn}|^p < \infty$, $A_k \cap A_j = \emptyset, k \neq j$ and $A = \cup_{k=1}^{\infty} A_k$ (if, for some $N \in \mathbb{N}$, $A = \cup_{k=1}^{N} A_k$, then $A_k = \emptyset, k \geq N+1$). □

If a self-adjoint operator S on a Hilbert space $\mathscr{K}$ is reduced by a closed subspace $\mathscr{D}$ of $\mathscr{K}$, then we denote by $S_{\mathscr{D}}$ the reduced part of S to $\mathscr{D}$, unless otherwise stated.

Lemma 4.2 *Let $\sigma(H) = \sigma_{\mathrm{disc}}(H) = \{E_n\}_{n=1}^{\infty}$, $E_1 < E_2 < \cdots < 0$, $\lim_{n\to\infty} E_n = 0$ and $0 \notin \sigma_{\mathrm{p}}(H)$. Then there exist mutually orthogonal closed subspaces $\mathscr{H}_j$ of $\mathscr{H}$ $(j = 1, \ldots, N, N \leq \infty)$ such that $\mathscr{H}$ is decomposed as $\mathscr{H} = \oplus_{j=1}^{N} \mathscr{H}_j$ $(N \leq \infty)$ and (1)–(3) below are satisfied.*

(1) Each $\mathscr{H}_j$ reduces H and $\sigma(H_j) \setminus \{0\} = \sigma_{\mathrm{disc}}(H_j)) = \{F_{jk}\}_{k=1}^{\infty}$, where $H_j := H_{\mathscr{H}_j}$.

(2) Each eigenvalue F_{jk} $(1 \leq j \leq N, 1 \leq k \leq \infty)$ is simple.

(3) $\sum_{k=1}^{\infty} F_{jk}^2 < \infty$ for each $1 \leq j \leq N$.

Proof: Note that 0 is the unique accumulation point of the set $\{E_n | n \in \mathbb{N}\}$. Let M_n be the multiplicity of E_n (which is finite, since $E_n \in \sigma_{\rm disc}(H)$). Let $\{e_n^i | i = 1, \cdots, M_n\}$ be a complete orthonormal system (CONS) of $\ker(H - E_n)$: $He_n^i = E_n e_n^i$, $i = 1, \ldots, M_n$. We set

$$\sup_{n \geq 1} M_n = M \quad \text{and} \quad \limsup_{n \to \infty} M_n = m.$$

We consider two cases: (I) $m = \infty$ and (II) $m < \infty$.

Case (I) Suppose that $m = \infty$. In this case, $M = \infty$ and, for each $k \geq 1$ and each n, there exists an $N \geq n$ such that $M_N \geq k$. Using this fact, we see that, for each $k \geq 1$, the subspace

$$\mathscr{G}_k = \text{L.H.}\{e_j^k |\ M_j \geq k\}$$

is infinite dimensional and $\mathscr{G}_k$ is orthogonal to $\mathscr{G}_l$ for all k, l with $k \neq l$. Since $\{e_n^i | n \geq 1, i = 1, \ldots, M_n\}$ is a CONS of $\mathscr{H}$, we have the orthogonal decomposition

$$\mathscr{H} = \oplus_{k=1}^{\infty} \overline{\mathscr{G}_k}. \tag{4.1}$$

Fix k and consider $\mathscr{G}_k$. Let $\mathscr{A} := \sigma_{\rm disc}(H_{\mathscr{G}_k}) = \{a_j | j \in \mathbb{N}\}$ $(= \{E_n | M_n \geq k\})$. Then each eigenvalue a_j is simple and $a_j \neq a_k$ for $j \neq k$, $\lim_{j \to \infty} a_j = 0$. Hence, we can apply Lemma 4.1 with $p = 2$ to conclude that there exist an $N_k \leq \infty$ and subsets $\mathscr{A}_l := \{a_j^l \in \mathscr{A} | j \in \mathbb{N}, \sum_{j=1}^{\infty} |a_j^l|^2 < \infty\}$ of $\mathscr{A}$ such that $\mathscr{A} = \cup_{l=1}^{N_k} \mathscr{A}_l$ (a disjoint union). Hence we can decompose $\overline{\mathscr{G}_k}$ as

$$\overline{\mathscr{G}_k} = \oplus_{l=1}^{N_k} \overline{\mathscr{G}_k^l}, \tag{4.2}$$

where $\mathscr{G}_k^l := \text{L.H}\{g_j \in \mathscr{G}_k | Hg_j = a_j^l g_j, j \in \mathbb{N}\}$ (hence $\sigma_{\rm disc}(H_{\mathscr{G}_k^l}) = \mathscr{A}_l$). Thus

$$\mathscr{H} = \oplus_{k=1}^{\infty} \oplus_{l=1}^{N_k} \overline{\mathscr{G}_k^l} \tag{4.3}$$

and the lemma follows.

Case (II) Suppose that $m < \infty$. Then we have $m \leq M < \infty$. Hence we need only to consider four cases $(a) - (d)$ below.

(a) $M = m = 1$. In this case, $\mathscr{H} = \overline{\mathscr{G}_1}$ and $\overline{\mathscr{G}_1}$ can be decomposed as (4.2). Then the lemma follows.

(b) $M \geq 2$ **and** $M = m$. In this case, for all $k = 1, \ldots, M$, $\mathscr{G}_k$ is infinite dimensional. Hence, in the same way as in the case $m = \infty$ we can see that $\mathscr{H} = \oplus_{k=1}^{M} \overline{\mathscr{G}_k}$ and $\overline{\mathscr{G}_k}$ can be decomposed as (4.2). Thus the lemma follows.

(c) $M \geq 2$ **and** $m = 1$. In this case, there exists a $j_0 \in \mathbb{N}$ such that for all $j \geq j_0$, $M_j = 1$. Let $\mathscr{B}_k = \text{L.H.}\{e_j^k | j < j_0, k \leq M_j\}$, $k = 1, \cdots, M$ and $\mathscr{C} := \text{L.H.}\{e_j^1 | j \geq j_0\}$. Then we can decompose $\mathscr{C}$ as $\overline{\mathscr{C}} = \oplus_{k=1}^{M} \overline{\mathscr{C}_k}$, where $\mathscr{C}_k = \text{L.H.}\{e_{j_k}^1 | j_k \geq j_0, j_k = j_0 + k - 1 + Mr, r \in \{0\} \cup \mathbb{N}\}$ $(k = 1, \ldots, M)$. Define $\mathscr{D}_k = \mathscr{B}_k \oplus \overline{\mathscr{C}_k}$, $k = 1, \cdots, M$. Then we have $\mathscr{H} = \oplus_{k=1}^{M} \mathscr{D}_k$. In the same way as in the case (I), we can decompose $\mathscr{D}_k$ like (4.2). Thus the lemma follows.

(d) $M \geq 2$**,** $M > m$ **and** $m \geq 2$. In this case, $\{j | M_j = m\}$ is a countable infinite set. Hence, for $j = 1, \ldots, m$, $\mathscr{G}_j$ is infinite dimensional. We have the orthogonal decomposition

$$\mathscr{H} = \left(\oplus_{j=1}^{m-1} \overline{\mathscr{G}_j}\right) \oplus \mathscr{K}, \tag{4.4}$$

where $\mathscr{K} = \left(\oplus_{j=1}^{m-1} \overline{\mathscr{G}_j}\right)^{\perp}$. The closed subspace $\mathscr{K}$ reduces H. Since $\mathscr{G}_m \subset \mathscr{K}$, it follows that $\sigma(H_{\mathscr{K}}) \setminus \{0\} = \sigma_{\rm disc}(H_{\mathscr{K}})$ is an infinite set. Let $\sigma_{\rm disc}(H_{\mathscr{K}}) = \{b_j\}_{j=1}^{\infty}$ and β_j be the multiplicity of eigenvalue b_j. Then $\sup_j \beta_j = M - m + 1$ and $\sup_j \beta_j \geq \limsup_j \beta_j = 1$. Hence by (a) and (c), we can decompose $\mathscr{K}$ as $\mathscr{K} = \oplus_{j=1}^{M-m+1} \mathscr{K}_j$, where $\mathscr{K}_j$ is an infinite dimensional closed subspace of $\mathscr{K}$. Hence

$$\mathscr{H} = \left(\oplus_{j=1}^{m-1} \overline{\mathscr{G}_j}\right) \oplus \left(\oplus_{j=1}^{M-m+1} \mathscr{K}_j\right). \tag{4.5}$$

In the same way as in the case (I), we can decompose $\overline{\mathscr{G}_j}$ and $\mathscr{K}_j$ like (4.2). Thus the lemma follows. □

Combining Corollary 3.3 and Lemma 4.2, we can prove the following lemma.

Theorem 4.3 (time operator of H^{-1}) *Suppose that* $\sigma(H) \setminus \{0\} = \sigma_{\rm disc}(H) = \{E_j\}_{j=1}^{\infty}$*,* $E_1 < E_2 < \cdots < 0$*,* $\lim_{j \to \infty} E_j = 0$*, and* $0 \notin \sigma_{\rm p}(H)$*. Then there exists a time operator* T_{-1} *of* H^{-1} *with a dense CCR-domain for* (H^{-1}, T_{-1})*.*

Proof: By Lemma 4.2, $\mathscr{H}$ can be decomposed as $\mathscr{H} = \oplus_{j=1}^{N} \mathscr{H}_j$ with $N \leq \infty$. By Proposition 3.1, a time operator S_j of H_j^{-1} exists:

$$[H_j^{-1}, S_j] = -i\mathbb{1}$$

on $\mathscr{E}_j :=$ L.H.$\{e_n^j - e_m^j, n, m \in \mathbb{N}\}$, where $\{e_n^j\}_{n=1}^{\infty}$ denotes the eigenvectors of H_j such that $H_j e_n^j = F_{jn} e_n^j$ and $\mathrm{D}(S_j) =$ L.H.$\{e_n^j | n \in \mathbb{N}\}$. Define T_{-1} by $T_{-1} := \oplus_{j=1}^{N} S_j$ with $\mathrm{D}(T_{-1}) := \oplus_{j=1}^{N} \mathrm{D}(S_j)$ (algebraic direct sum). Then T_{-1} is a time operator of H^{-1} with a CCR-domain given by $\oplus_{j=1}^{N} \mathscr{E}_j$ (algebraic direct sum), which is dense in $\mathscr{H}$. □

5 Time Operators in the Case where H has a Pure Discrete Spectrum (III)

We next consider an extension of Proposition 3.1 to the case where no restriction is imposed on the growth order of the discrete eigenvalues $\{E_n\}_{n=1}^{\infty}$ of H.

Lemma 5.1 *Suppose that* $\sigma(H) = \sigma_{\rm disc}(H) = \{E_n\}_{n=1}^{\infty}$ *with* $0 < E_1 < E_2 < \cdots < E_n < E_{n+1} < \cdots$ *and* $\lim_{n \to \infty} E_n = \infty$*. Then there exist mutually orthogonal closed subspaces* $\mathscr{H}_j$ *of* $\mathscr{H}$ $(j = 1, \ldots, N, N \leq \infty)$ *such that* $\mathscr{H} = \oplus_{j=1}^{N} \mathscr{H}_j$ *and (1)–(3) below are satisfied:*

(1) Each $\mathscr{H}_j$ *reduces* H *and* $\sigma(H_{\mathscr{H}_j}) = \sigma_{\rm disc}(H_{\mathscr{H}_j}) = \{F_{jk}\}_{k=1}^{\infty}$.

(2) Each F_{jk} $(1 \le j \le N, k \in \mathbb{N})$ *is simple.*

(3) $\displaystyle\sum_{k=1}^{\infty} \frac{1}{F_{jk}^2} < \infty$ *for each* $1 \le j \le N$.

Proof: Let $K = H^{-1}$. Then K is self-adjoint and $\sigma(K) \setminus \{0\} = \sigma_{\rm disc}(K) = \{1/E_n\}_{n=1}^{\infty}$, $1/E_1 > 1/E_2 > \cdots > 0$, $\lim_{j\to\infty} 1/E_j = 0$ and $0 \notin \sigma_{\rm p}(K)$. Hence, by applying Lemma 4.2 to the case where H and E_n there are replaced by $-K$ and $-1/E_n$ respectively, we see that $\mathscr{H}$ has an orthogonal decomposition $\mathscr{H} = \oplus_{j=1}^{N} \mathscr{H}_j$ $(N \le \infty)$ with closed subspaces $\mathscr{H}_j$ of $\mathscr{H}$ such that (1)–(3) above are satisfied. □

Theorem 5.2 (time operator of H**)** *Suppose that* $\sigma(H) = \sigma_{\rm disc}(H) = \{E_n\}_{n=1}^{\infty}$, $E_1 < E_2 < \cdots$ *and* $\lim_{n\to\infty} E_n = \infty$. *Then there exists a time operator* T *of* H *with a dense CCR-domain for* (H, T).

Proof: The method of proof is similar to that of Theorem 4.3. By Lemma 5.1, $\mathscr{H}$ can be decomposed as $\mathscr{H} = \oplus_{j=1}^{N} \mathscr{H}_j$ with $N \le \infty$. By Proposition 3.1 a time operator T_j of $H_{\mathscr{H}_j}$ exists: $[H_{\mathscr{H}_j}, T_j] = -i\mathbb{1}$ on $\mathscr{E}_j = \mathrm{L.H.}\{e_n^j - e_m^j, n, m \in \mathbb{N}\}$, where $\{e_n^j\}_{n=1}^{\infty}$ denotes the eigenvectors of $H_{\mathscr{H}_j}$ such that $He_n^j = F_{jn} e_n^j$, and the domain of T_j is given by $\mathrm{D}(T_j) = \mathrm{L.H.}\{e_n^j | n \in \mathbb{N}\}$. Define T by $T := \oplus_{j=1}^{N} T_j$ with $\mathrm{D}(T) = \oplus_j^N \mathrm{D}(T_j)$ (algebraic direct sum). Then T is a time operator of H with a CCR-domain $\oplus_{j=1}^{N} \mathscr{E}_j$ (algebraic direct sum), which is dense in $\mathscr{H}$. □

Example 5.3 (d**-dimensional quantum harmonic oscillator)** Let $\omega_j > 0$ $(j = 1, \ldots, d)$ be a constant and

$$H_{{\rm osc},\, j} := -\frac{1}{2} D_j^2 + \frac{1}{2} \omega_j^2 x_j^2$$

acting in $L^2(\mathbb{R}^d)$ (see Example 3.2). Then the Hamiltonian of a d-dimensional quantum harmonic oscillator is given by

$$H_{\rm osc}^{(d)} := \sum_{j=1}^{d} H_{{\rm osc},\, j}$$

acting in $L^2(\mathbb{R}^d)$. It follows that $H_{\rm osc}^{(d)}$ is self-adjoint and

$$\sigma(H_{\rm osc}^{(d)}) = \sigma_{\rm disc}(H_{\rm osc}^{(d)}) = \left\{ \sum_{j=1}^{d} \omega_j \left(n_j + \frac{1}{2} \right) | n_j \in \{0\} \cup \mathbb{N},\ j = 1, \ldots, d \right\}.$$

Hence, by Theorem 5.2, $H_{\rm osc}^{(d)}$ has a time operator with a dense CCR-domain.

Example 5.4 (non-commutative harmonic oscillator) Let A and J be 2×2 matrices defined by

$$A = \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix}, \quad \alpha, \beta \geq 0, \quad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Let $\alpha\beta > 1$. The Hamiltonian $H(\alpha, \beta)$ of the non-commutative harmonic oscillator [Par10] is defined by the self-adjoint operator

$$H(\alpha, \beta) = A \otimes (-\frac{1}{2}\Delta + \frac{1}{2}x^2) + J \otimes (xD + \frac{1}{2}) \tag{5.1}$$

on the Hilbert space $\mathbb{C}^2 \otimes L^2(\mathbb{R})$, where D is the generalized differential operator in x. It is shown in [IW07] that $\sigma(H(\alpha, \beta)) = \sigma_{\rm disc}(H(\alpha, \beta)) = \{\lambda_n\}_{n=1}^\infty$ and the multiplicity of each λ_n is not greater than 2 with $\lambda_n \to \infty$ $(n \to \infty)$. Hence, by Theorem 5.2, $H(\alpha, \beta)$ has a time operator with a dense CCR-domain.

Example 5.5 (Rabi model) Let $\mathbb{Z}_+ := \{0\} \cup \mathbb{N}$ be the set of nonnegative integers and

$$\ell^2(\mathbb{Z}_+) := \left\{ \psi = \{\psi_n\}_{n=0}^\infty \middle| \psi_n \in \mathbb{C}, n \geq 0, \sum_{n=0}^\infty |\psi_n|^2 < \infty \right\}$$

be the Hilbert space of absolutely square summable complex sequences indexed by $\mathbb{Z}_+$. The Hilbert space $\ell^2(\mathbb{Z}_+)$ is in fact the boson Fock space $\mathscr{F}_{\rm b}(\mathbb{C})$ over $\mathbb{C}$ (e.g. [RS72, p.53, Example 2] and [RS75, §X.7]): $\ell^2(\mathbb{Z}_+) = \mathscr{F}_{\rm b}(\mathbb{C})$. We denote by a the annihilation operator on $\mathscr{F}_{\rm b}(\mathbb{C})$:

$$(a\psi)_n := \sqrt{n+1}\psi_{n+1}, \quad n \geq 0, \psi \in {\rm D}(a) := \left\{ \psi \in \ell^2(\mathbb{Z}_+) \middle| \sum_{n=0}^\infty n|\psi_n|^2 < \infty \right\}.$$

We have $(a^*\psi)_0 = 0$, $(a^*\psi)_n = \sqrt{n}\psi_{n-1}$, $n \geq 1$ for all $\psi \in {\rm D}(a^*)$. The commutation relation $[a, a^*] = \mathbb{1}$ holds on the dense subspace $\ell_0(\mathbb{Z}_+) := \{\psi \in \ell^2(\mathbb{Z}_+) | \exists n_0 \in \mathbb{N}$ such that $\psi_n = 0, \forall n \geq n_0\}$.

Let $\sigma_x, \sigma_y, \sigma_z$ be the Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and

$$H_{\rm Rabi} := \mu\sigma_z \otimes \mathbb{1} + \omega\mathbb{1} \otimes a^*a + g\sigma_x \otimes (a + a^*) \tag{5.2}$$

on $\mathbb{C}^2 \otimes \mathscr{F}_{\rm b}(\mathbb{C})$, where $\mu > 0$, $\omega > 0$ and $g \in \mathbb{R}$ are constants. The model whose Hamiltonian is given by $H_{\rm Rabi}$ is called the Rabi model [Rab36, Rab37, Bra11]. The matrix

$$U := \frac{1}{\sqrt{2}}(\sigma_x + \sigma_z)$$

is unitary and self-adjoint. By direct computations using the properties that $\sigma_j\sigma_k + \sigma_k\sigma_j = 2\delta_{jk}, j, k = x, y, z$, we see that

$$\widetilde{H}_{\rm Rabi} := UH_{\rm Rabi}U^{-1} = \mu\sigma_x + H, \quad H := \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix},$$

where $H_\pm := \omega a^*a \pm g(a+a^*)$ and we have used the natural identification $\mathbb{C}^2 \otimes \mathscr{F}_{\rm b}(\mathbb{C}) = \mathscr{F}_{\rm b}(\mathbb{C}) \oplus \mathscr{F}_{\rm b}(\mathbb{C})$. It is well known that the operator $\pi_g := (g/\omega)\overline{i(a-a^*)}$ is self-adjoint and

$$e^{\pm i\pi_g} a e^{\mp i\pi_g} = a \mp \frac{g}{\omega}.$$

Hence

$$e^{\pm i\pi_g} H_\pm e^{\mp i\pi_g} = \omega a^* a - \frac{g^2}{\omega},$$

implying that $\sigma(H_\pm) = \sigma_{\rm disc}(H_\pm) = \sigma(\omega a^*a - \frac{g^2}{\omega}) = \{\nu_n | n \in \mathbb{Z}_+\}$ with $\nu_n := \omega n - \frac{g^2}{\omega}$. Hence $\sigma(H) = \sigma_{\rm disc}(H) = \{\nu_n | n \in \mathbb{Z}_+\}$ with the multiplicity of each eigenvalue ν_n being two. Since $\mu\sigma_x$ is bounded, it follows from the min-max principle that $\widetilde{H}_{\rm Rabi}$ (and hence $H_{\rm Rabi}$) has purely discrete spectrum with $\sigma(H_{\rm Rabi}) = \sigma_{\rm disc}(H_{\rm Rabi}) = \sigma_{\rm disc}(\widetilde{H}_{\rm Rabi}) = \{\nu'_n | n \in \mathbb{Z}_+\}$ satisfying $\nu_n - \mu \le \nu'_{2n} \le \nu_n + \mu$, $n \ge 0$, where $\nu'_0 \le \nu'_1 \le \cdots \le \nu'_n \le \nu'_{n+1} \le \cdots$ counting multiplicities (see also [Bra11, MPS14] for studies on spectral properties of $H_{\rm Rabi}$). Hence we can apply Theorem 5.2 to conclude that $H_{\rm Rabi}$ has a time operator with a dense CCR-domain.

6 Existence Theorems on Ultra-Weak Time Operators in an Abstract Framework

In this section, we consider the case where H obeys the assumption of Theorem 4.3 and ask if H has a time operator. We first give a formal heuristic argument. By Theorem 4.3, we know that H^{-1} has a time operator T_{-1} with a dense CCR-domain for (H^{-1}, T_{-1}). Since the unique accumulation point of $\sigma(H)$ is 0, but not ∞, it is not straightforward to apply Proposition 3.1 to construct a time operator of H. The key idea we use is to regard H as $H = (H^{-1})^{-1}$. Let $f(x) = x^{-1}$. Then $H = f(H^{-1})$. Since $f'(x) = -x^{-2}$, a formal application of Proposition 2.9 suggests that $A = -\frac{1}{2}(T_{-1}H^{-2} + H^{-2}T_{-1})$ may be a time operator of H. But, we note that no eigenvectors of H are in $\mathrm{D}(H^{-2}T_{-1})$. Hence it seems to be difficult to show that $\mathrm{D}(A) \ne \{0\}$ and $\mathrm{D}(HA) \cap \mathrm{D}(AH) \ne \{0\}$. Thus we are led to consider a form version of A.

We use the notation in the proof of Theorem 4.3. It is obvious that, for all $k \in \mathbb{Z}$, $\mathrm{D}(S_j) \subset \mathrm{D}(H_j^k)$. Hence we define a sesquilinear form $\mathfrak{t}_j : \mathrm{D}(S_j) \times \mathrm{D}(S_j) \to \mathbb{C}$ by

$$\mathfrak{t}_j[\phi, \psi] := -\frac{1}{2}\left\{(S_j\phi, H_j^{-2}\psi) + (H_j^{-2}\phi, S_j\psi)\right\}, \quad \phi, \psi \in \mathrm{D}(S_j). \tag{6.1}$$

Lemma 6.1 *Let*

$$H_j^{-1}\mathscr{E}_j := \{H_j^{-1}\psi | \psi \in \mathscr{E}_j\} = \text{L.H.}\left\{\frac{1}{E_n}e_n^j - \frac{1}{E_m}e_m^j)\big| n, m \in \mathbb{N}\right\}.$$

Then, for all $\psi, \phi \in H_j^{-1}\mathscr{E}$, $H_j\phi$ *and* $H_j\psi$ *are in* $\mathrm{D}(S_j)$ *and*

$$\mathfrak{t}_j[H_j\phi, \psi] - \mathfrak{t}_j[\phi, H_j\psi] = -i(\phi, \psi). \tag{6.2}$$

Proof: Since $H_j(H_j^{-1}\mathscr{E}_j) = \mathscr{E}_j \subset \mathrm{D}(S_j)$, $H_j\phi \in \mathrm{D}(S_j)$ for all $\phi \in H_j^{-1}\mathscr{E}_j$. By direct computations, we have

$$\begin{aligned}\mathfrak{t}[H_j\phi, \psi] - \mathfrak{t}[\phi, H_j\psi] = -\frac{1}{2}\Big\{&(S_jH_j\phi, H_j^{-2}\psi) - (S_j\phi, H_j^{-1}\psi)\\ &+ (H_j^{-1}\phi, S_j\psi) - (H_j^{-2}\phi, S_jH_j\psi)\Big\}.\end{aligned}$$

We can write $\phi = H_j^{-1}\eta$ and $\psi = H_j^{-1}\chi$ with $\eta, \chi \in \mathscr{E}_j$. Then we have

$$\begin{aligned}(S_jH_j\phi, H_j^{-2}\psi) - (S_j\phi, H_j^{-1}\psi) &= (H_j^{-1}S_j\eta, H_j^{-1}\psi) - (S_jH_j^{-1}\eta, H_j^{-1}\psi)\\ &= (-i\eta, H_j^{-1}\psi) = i(\phi, \psi),\end{aligned}$$

where we have used that S_j is a time operator of H_j^{-1} with a CCR-domain $\mathscr{E}_j$. Similarly we have

$$(H_j^{-1}\phi, S_j\psi) - (H_j^{-2}\phi, S_jH_j\psi) = (H_j^{-1}\phi, S_jH_j^{-1}\chi) - (H_j^{-1}\phi, H_j^{-1}S_j\chi) = i(\phi, \psi).$$

Thus (6.2) follows. □

Lemma 6.1 shows that $\mathfrak{t}_j$ is an ultra-weak time operator of H_j with $H_j^{-1}\mathscr{E}_j$ being an ultra-weak CCR-domain.

We introduce

$$\widetilde{\mathscr{E}} := \oplus_{j=1}^N H_j^{-1}\mathscr{E}_j \quad \text{(algebraic direct sum)}.$$

Since $H_j^{-1}\mathscr{E}_j$ is dense in $\mathscr{H}_j$, $\widetilde{\mathscr{E}}$ is dense in $\mathscr{H}$ and $\widetilde{\mathscr{E}} \subset \mathrm{D}(H)$.

Theorem 6.2 *Under the same assumption as in Theorem 4.3, there exists an ultra-weak time operator* $\mathfrak{t}_\mathrm{p}$ *of* H *with* $\widetilde{\mathscr{E}}$ *being an ultra-weak CCR-domain.*

Proof: Let T_{-1} be as in Theorem 4.3 and define a sesquilinear form $\mathfrak{t}_\mathrm{p} : \mathrm{D}(T_{-1}) \times \mathrm{D}(T_{-1}) \to \mathbb{C}$ by

$$\mathfrak{t}_\mathrm{p}[\psi, \phi] := \sum_{j=1}^N \mathfrak{t}[\psi_j, \phi_j], \quad \psi = (\psi_j)_{j=1}^N, \phi = (\phi_j)_{j=1}^N \in \mathrm{D}(T_{-1}).$$

We remark that, in the case $N = \infty$, $\psi_j = 0$ for all sufficiently large j and hence the sum $\sum_{j=1}^N$ on the right hand side is over only finite terms, being well defined. It follows from Lemma 6.1 that, for all $\psi, \phi \in \widetilde{\mathscr{E}}$, $H\psi, H\phi \in \mathscr{E} \subset \mathrm{D}(T_{-1})$ and

$$\mathfrak{t}_{\mathrm{p}}[H\phi, \psi] - \mathfrak{t}_{\mathrm{p}}[\phi, H\psi] = -i(\phi, \psi).$$

This means that $\mathfrak{t}_{\mathrm{p}}$ is an ultra-weak time operator of H with $\widetilde{\mathscr{E}}$ being an ultra-weak CCR domain. □

We now proceed to showing existence of an ultra-weak time operator of a self-adjoint operator in a general class.

Definition 6.3 (class $S_1(\mathscr{H})$) A self-adjoint operator H on $\mathscr{H}$ is said to be in the class $S_1(\mathscr{H})$ if it has the following properties (H.1)–(H.4):

(H.1) $\sigma_{\mathrm{sc}}(H) = \emptyset$.

(H.2) $\sigma_{\mathrm{ac}}(H) = [0, \infty)$.

(H.3) $\sigma_{\mathrm{disc}}(H) = \sigma_{\mathrm{p}}(H) = \{E_n\}_{n=1}^\infty$, $E_1 < E_2 < \cdots < 0$, $\lim_{n\to\infty} E_n = 0$ (hence $0 \notin \sigma_{\mathrm{p}}(H)$).

(H.4) There exists a strong time operator T_{ac} of H_{ac} in $\mathscr{H}_{\mathrm{ac}}(H)$.

Let $H \in S_1(\mathscr{H})$. Then we have the orthogonal decomposition

$$\mathscr{H} = \mathscr{H}_{\mathrm{ac}}(H) \oplus \mathscr{H}_{\mathrm{p}}(H).$$

By (H.3), we can apply Theorem 6.2 to the case where H is replaced by H_{p} to conclude that H_{p} has an ultra-weak time operator $\mathfrak{t}_{\mathrm{p}}$ with a dense ultra-weak CCR domain $\mathscr{E}_{\mathrm{p}}$ such that

$$\mathfrak{t}_{\mathrm{p}}[H_{\mathrm{p}}\phi, \psi] - \mathfrak{t}_{\mathrm{p}}[\phi, H_{\mathrm{p}}\psi] = -i(\phi, \psi), \quad \phi, \psi \in \mathscr{E}_{\mathrm{p}}.$$

We denote by $\mathscr{D}_{\mathrm{p}}$ the subspace $\mathrm{D}(T_{-1})$ in the proof of Theorem 6.2. Hence $\mathfrak{t}_{\mathrm{p}} : \mathscr{D}_{\mathrm{p}} \times \mathscr{D}_{\mathrm{p}} \to \mathbb{C}$ with $\mathscr{E}_{\mathrm{p}} \subset \mathrm{D}(H_{\mathrm{p}}) \cap \mathscr{D}_{\mathrm{p}}$ and $H_{\mathrm{p}}\mathscr{E}_{\mathrm{p}} \subset \mathscr{D}_{\mathrm{p}}$. By (H.4), there exists a dense CCR-domain $\mathscr{D}_{\mathrm{ac}}$ for $(H_{\mathrm{ac}}, T_{\mathrm{ac}})$. Let $\widetilde{\mathscr{E}}_{\mathrm{p}} := H_{\mathrm{p}}^{-1}\mathscr{E}_{\mathrm{p}}$ and

$$\mathscr{D}_H := \mathscr{D}_{\mathrm{ac}} \oplus \widetilde{\mathscr{E}}_{\mathrm{p}}, \tag{6.3}$$

which is dense in $\mathscr{H}$.

We define a sesquilinear form $\mathfrak{t}_H : (\mathscr{H}_{\mathrm{ac}}(H) \oplus \mathscr{D}_{\mathrm{p}}) \times (\mathrm{D}(T_{\mathrm{ac}}) \oplus \mathscr{D}_{\mathrm{p}}) \to \mathbb{C}$ by

$$\begin{aligned} \mathfrak{t}_H[\phi_1 \oplus \phi_2, \psi_1 \oplus \psi_2] =& (\phi_1, T_{\mathrm{ac}}\psi_1) + \mathfrak{t}_{\mathrm{p}}[\phi_2, \psi_2], \\ & \phi_1 \in \mathscr{H}_{\mathrm{ac}}(H), \psi_1 \in \mathrm{D}(T_{\mathrm{ac}}), \phi_2, \psi_2 \in \mathscr{D}_{\mathrm{p}}. \end{aligned} \tag{6.4}$$

Now we are in the position to state and prove the main result in this section.

Theorem 6.4 (abstract ultra-weak time operator 1) *Let $H \in S_1(\mathscr{H})$. Then the sesquilinear form $\mathfrak{t}_H$ defined by (6.4) is an ultra-weak time operator of H with $\mathscr{D}_H$ being an ultra-weak CCR-domain.*

Proof: Let $\mathfrak{t}_{\rm ac} : \mathscr{H}_{\rm ac}(H) \times {\rm D}(T_{\rm ac}) \to \mathbb{C}$ by $\mathfrak{t}_{\rm ac}[\phi, \psi] := (\phi, T_{\rm ac}\psi)$, $\phi \in \mathscr{H}_{\rm ac}(H), \psi \in {\rm D}(T_{\rm ac})$. Then, by Remark 1.9-(2), $\mathfrak{t}_{\rm ac}$ is an ultra-weak time operator of $H_{\rm ac}$ with $\mathscr{D}_{\rm ac}$ being an ultra-weak CCR-domain. Then, in the same way as in the proof of Theorem 6.2, one can show that $\mathfrak{t}_H$ is an ultra-weak time operator of H with $\mathscr{D}_H$ being an ultra-weak CCR-domain. □

We can also construct an ultra-weak time operator of $f(H)$ for some function $f : \mathbb{R} \to \mathbb{R}$. A strong time operator of $f(H_{\rm ac})$ is already constructed in Proposition 2.9. Hence we need only to construct an ultra-weak time operator of $f(H_{\rm p})$. A set of conditions for that is as follows.

Assumption 6.5 Let $H \in S_1(\mathscr{H})$.

(1) The function $f : \mathbb{R} \to \mathbb{R}$ satisfies the same assumption as in Proposition 2.9.

(2) The function f is continuous at $x = 0$.

(3) $f(\sigma_{\rm disc}(H))$ is an infinite set such that the multiplicity of each point in $f(\sigma_{\rm disc}(H))$ as an eigenvalue of $f(H)$ is finite.

(4) $f(0) \notin \sigma_{\rm p}(f(H))$.

Suppose that Assumption 6.5 holds. Then $f(H)$ is self-adjoint and reduced by $\mathscr{H}_{\rm ac}(H)$ and $\mathscr{H}_{\rm p}(H)$ (these properties follow from only the fact that $f : \mathbb{R} \to \mathbb{R}$, Borel measurable, and the general theory of functional calculus). We denote the reduced part of $f(H)$ to $\mathscr{H}_{\rm ac}(H)$ and $\mathscr{H}_{\rm p}(H)$ by $f(H)_{\rm ac}$ and $f(H)_{\rm p}$ respectively. By the functional calculus, we have $f(H)_{\rm ac} = f(H_{\rm ac})$, $f(H)_{\rm p} = f(H_{\rm p})$ and $f(H) = f(H_{\rm ac}) \oplus f(H_{\rm p})$. This implies that

$$\sigma(f(H)) = \sigma(f(H_{\rm ac})) \cup \sigma(f(H_{\rm p})) = \overline{f([0,\infty))} \cup \overline{\{f(E_j)\}_{j=1}^{\infty}}. \tag{6.5}$$

Corollary 6.6 (abstract ultra-weak time operator 2) *Under Assumption 6.5, there exists an ultra-weak time operator $\mathfrak{t}_H^f$ of $f(H)$ with a dense ultra-weak CCR-domain.*

Proof: Let $T_{\rm ac}$ be a strong time operator of $H_{\rm ac}$. Then the strong time operator of $f(H_{\rm ac})$ is given by

$$T_{\rm ac}^f = \frac{1}{2}\overline{(T_{\rm ac}f'(H_{\rm ac})^{-1} + f'(H_{\rm ac})^{-1}T_{\rm ac})\lceil D}$$

by Proposition 2.9, where $D := \{g(H_{\rm ac})\mathrm{D}(T_{\rm ac})|g \in C_0^\infty(\mathbb{R}\setminus L\cup K)\}$. Let

$$\tilde{f}(x) = f(x) - f(0).$$

Then $\lim_{x\to 0}\tilde{f}(x) = 0$. We can write $\sigma(\tilde{f}(H_{\rm p})) = \{F_j\}_{j=1}^\infty$, where $F_j \neq F_k$, $j \neq k$ and the multiplicity of each F_j is finite. It follows that $\lim_{j\to\infty} F_j = 0$ and $0 \notin \sigma_{\rm p}(\tilde{f}(H_{\rm p}))$. Hence, by a minor modification of the proof of Lemma 6.1, we can show that there is an ultra-weak time operator $\mathfrak{t}_{\rm p}^{\tilde{f}} : \mathscr{D}_{\rm p}^f \times \mathscr{D}_{\rm p}^f \to \mathbb{C}$ of $\tilde{f}(H_{\rm p})$, where $\mathscr{D}_{\rm p}^f$ is a dense subspace in $\mathscr{H}_{\rm p}(H)$. We define a sesquilinear form $\mathfrak{t}_H^f : (\mathscr{H}_{\rm ac}(H)\oplus\mathscr{D}_{\rm p}^f)\times(\mathrm{D}(T_{\rm ac}^f)\oplus\mathscr{D}_{\rm p}^f) \to \mathbb{C}$ by

$$\mathfrak{t}_H^f[\phi_1\oplus\phi_2, \psi_1\oplus\psi_2] = (\phi_1, T_{\rm ac}^f\psi_1) + \mathfrak{t}_{\rm p}^{\tilde{f}}[\phi_2,\psi_2] \tag{6.6}$$

for $\phi_1 \in \mathscr{H}_{\rm ac}(H), \psi_1 \in \mathrm{D}(T_{\rm ac}^f)$ and $\phi_2, \psi_2 \in \mathscr{D}_{\rm p}^f$. Note that $f(0)$ is a scalar. Then one can show that $\mathfrak{t}_H^f$ is an ultra-weak time operator with $\mathscr{D}_{\rm ac}\oplus\widetilde{\mathscr{E}}_{\rm p}^{\tilde{f}}$ being a ultra-weak CCR-domain, where $\mathscr{D}_{\rm ac}$ is a dense CCR-domain for $(f(H_{\rm ac}), T_{\rm ac}^f)$. and $\widetilde{\mathscr{E}}_{\rm p}^{\tilde{f}}$ is an ultra-weak CCR-domain for $(\tilde{f}(H_{\rm p}), \mathfrak{t}_{\rm p}^{\tilde{f}})$. □

7 Applications to Schrödinger Operators

In this section, we apply Theorem 6.4 to the Schrödinger operator H_V given by (1.7) to show that, for a general class of potentials V, H_V has an ultra-weak time operator with a *dense* ultra-weak CCR-domain. This is done by collecting known results on spectral properties of Schrödinger operators.

Suppose that V is of the form

$$V(x) = \frac{W(x)}{(|x|^2+1)^{\frac{1}{2}+\varepsilon}}, \tag{7.1}$$

where $\varepsilon > 0$ and $W : \mathbb{R}^d \to \mathbb{R}$ is a Borel measurable function such that $W(-\Delta + i)^{-1}$ is a compact operator on $L^2(\mathbb{R}^d)$. Such a potential V is called an *Agmon potential* ([RS79, p.439] or [RS78, p.169]). It is easily shown that V is relatively compact with respect to the free Hamiltonian H_0 given by (1.8). Hence, by a general fact [RS78, p.113, Corollary 2], H_V is self-adjoint with $\mathrm{D}(H_V) = \mathrm{D}(H_0)$ and

$$\sigma_{\rm ess}(H_V) = \sigma_{\rm ess}(H_0) = [0,\infty), \tag{7.2}$$

where, for a self-adjoint operator S, $\sigma_{\rm ess}(S)$ denotes the essential spectrum of S.

Following facts are known as Agmon-Kato-Kuroda theorem:

Proposition 7.1 (absence of $\sigma_{\rm sc}(H)$, existence and completeness of wave operators) *Let V be an Agmon potential. Then:*

(1) $\sigma_{\mathrm{sc}}(H_V) = \emptyset$.

(2) The set of positive eigenvalues of H_V *is a discrete subset of* $(0, \infty)$.

(3) The wave operators $\Omega_\pm := \text{s-}\lim_{t\to\pm\infty} e^{itH_V} e^{-itH_0}$ *exist and complete:* $\mathrm{Ran}(\Omega_\pm) = \mathscr{H}_{\mathrm{ac}}(H_V)$. *In particular* $\sigma_{\mathrm{ac}}(H_V) = [0, \infty)$.

Proof: See [RS78, Theorem XIII. 33]. □

In order to construct an ultra-weak time operator of $(H_V)_{\mathrm{p}}$, we need the condition $\#\sigma_{\mathrm{disc}}(H_V) = \infty$. For this purpose, we introduce an assumption.

Assumption 7.2 There are constants $R_0, a > 0$ and $\delta > 0$ such that

$$V(x) \le -\frac{a}{|x|^{2-\delta}} \quad \text{for } |x| > R_0. \tag{7.3}$$

Lemma 7.3 (infinite number of negative eigenvalues) *Let* V *be an Agmon potential. Then, under Assumption 7.2,* $\sigma_{\mathrm{disc}}(H_V) \subset (-\infty, 0)$ *and* $\sigma_{\mathrm{disc}}(H_V)$ *is an infinite set. In particular, the point* $0 \in \mathbb{R}$ *is the unique accumulation point of* $\sigma_{\mathrm{disc}}(H_V)$.

Proof: Let $\mu_1 := \inf_{\psi\in \mathrm{D}(H_V);\|\psi\|=1}(\psi, H_V\psi)$ and

$$\mu_n := \sup_{\phi_1,\ldots,\phi_{n-1}\in L^2(\mathbb{R}^d)} \inf_{\substack{\psi\in D(H_V);\|\psi\|=1\\ \psi\in\{\phi_1,\ldots,\phi_{n-1}\}^\perp}} (\psi, H_V\psi), \quad n \ge 2.$$

In the case $d = 3$, it is already known that $\mu_n < 0$ for all $n \in \mathbb{N}$ [RS78, Theorem XIII.6(a)]. It is easy to see that the method of the proof of this fact is valid also in the case of arbitrary d. Hence we have $\mu_n < 0$ for all $n \in \mathbb{N}$. Then (7.2) and the min-max principle imply the desired results. □

Assumption 7.4 The potential V is spherically symmetric, $V = V(|x|)$, and

$$\int_a^\infty |V(r)|dr < \infty \tag{7.4}$$

for some $a > 0$.

Lemma 7.5 (absence of strictly positive eigenvalues) *Let* V *be an Agmon potential. Then, under Assumption 7.4,* H_V *has no strictly positive eigenvalues.*

Proof: Since $\mathrm{D}(V) \supset \mathrm{D}(H_0) \supset C_0^\infty(\mathbb{R}^d)$, it follows that $V \in L^2_{\mathrm{loc}}(\mathbb{R}^d \setminus \{0\})$. Hence we can apply [RS78, Theorem XIII.56] to derive the desired result. □

Theorem 7.6 *Let V be an Agmon potential such that $0 \notin \sigma_{\mathrm{p}}(H_V)$. Suppose that Assumptions 7.2 and 7.4 hold. Then H_V has an ultra-weak time operator with a dense ultra-weak CCR-domain.*

Proof: By Proposition 7.1, $\sigma_{\mathrm{sc}}(H_V) = \emptyset$ and the wave operators $\Omega_\pm$ exist and are complete. Hence, by Theorem 2.18,

$$T_{\mathrm{ac},j\pm} := \Omega_\pm \tau_j \Omega_\pm^{-1} P_{\mathrm{ac}}(H_V) \quad (j = 1, \ldots, d)$$

are strong time operators of $(H_V)_{\mathrm{ac}}$, where $\tau_j := \widetilde{T}_{\mathrm{AB},j}$ or $T'_{\mathrm{AB},j}$, the Aharonov-Bohm time operators in Example 2.10. Under Assumptions 7.2 and 7.4, we can see that $\sigma(H_V) = \{E_j\}_{j=1}^\infty \cup [0, \infty)$, $E_1 < E_2 < \cdots < 0$, $\lim_{n\to\infty} E_n = 0$, $\sigma_{\mathrm{disc}}(H_V) = \{E_n\}_{n=1}^\infty$ and $\sigma_{\mathrm{ac}}(H_V) = [0, \infty)$. Hence $H_V \in S_1(L^2(\mathbb{R}^d))$. Thus, by Theorem 6.4, we obtain the desired result. □

Finally we consider conditions for the absence of zero eigenvalue of H_V.

Proposition 7.7 (absence of zero eigenvalue) *Assume the following (1) and (2):*

(1) $d \geq 3$, $V \in L^{d/2}_{\mathrm{loc}}(\mathbb{R}^d)$.

(2) V can be written as $V = V_1 + V_2$, where V_1 and V_2 are real-valued Borel measurable functions on $\mathbb{R}^d$ satisfying the following conditions:

- *(i) There exists a constant $R > 0$ such that V_1 and V_2 are locally bounded on $S_R = \{x \in \mathbb{R}^d \| x| > R\}$ and V_1 is strictly negative on S_R,*
- *(ii) Let $S^{d-1} := \{w \in \mathbb{R}^d \mid |w| = 1\}$, the $(d-1)$-dimensional unit sphere. Then $V_1(rw)$ $(r = |x|)$ is differentiable in $r > R$ and there exist a constant $s \in (0, 1)$ and a positive differentiable function h on $[R, \infty)$ such that*

$$\sup_{w \in S^{d-1}} \frac{d}{dr}(r^{s+1} V_1(rw)) \leq -r^s h(r)^2, \quad r > R.$$

- *(iii)* $\displaystyle\lim_{r\to\infty} \frac{r^{-1} + r \sup_{w\in S^{d-1}} |V_2(rw)|}{h(r)} = 0.$
- *(iv) There exists a constant $C > 0$ such that $\frac{d}{dr} h(r) \leq C h^2(r)$ on S_R.*
- *(v) For all all $f \in D(H_V)$,*

$$\int_{S_R} h^2(|x|)|f(x)|^2 dx < \infty, \quad \int_{S_R} |V_1(x)||f(x)|^2 dx < \infty.$$

Then $0 \notin \sigma_{\mathrm{p}}(H_V)$.

Proof: This is due to [FS04, Theorem 2.4] and [JK85]. Also see [Uch87]. □

A key fact to prove Proposition 7.7 is as follows. Condition $d \geq 3$ and $V \in L^{d/2}_{\mathrm{loc}}(\mathbb{R}^d)$ imply that, if a solution f of partial differential equation $-\Delta f + Vf = 0$ satisfies that $f(x) = 0$ for all $x \in S_R$ with some $R > 0$, then $f(x) = 0$ for all $x \in \mathbb{R}^d$ by the unique continuation proven in [JK85].

Example 7.8 Let $d \geq 3$ and $V(x) = -1/|x|^{2-\varepsilon}$ with $0 < \varepsilon < 2$. Then it is easy to check that the potential V satisfies conditions (1) and (2) in Proposition 7.7 (take $V_1 = V$, $V_2 = 0$ and $h(r) = \sqrt{s-1+\varepsilon}\, r^{(\varepsilon-2)/2}$, $r > 0$ with $1-\varepsilon < s < 1$). Hence, by Proposition 7.7, H_V has no zero eigenvalue. In particular, the hydrogen Schrödinger operator

$$H_{\mathrm{hyd}} := H_0 - \frac{\gamma}{|x|} \tag{7.5}$$

for $d = 3$ with a constant $\gamma > 0$ has no zero eigenvalue.

Example 7.9 Let $d \geq 3$. Suppose that $U \in L^\infty(\mathbb{R}^3)$. Then

$$V(x) = \frac{U(x)}{(1+|x|^2)^{\frac{1}{2}+\varepsilon}}$$

is an Agmon potential for all $\varepsilon > 0$. Suppose that U is negative, continuous, spherically symmetric and satisfies that $U(x) = -1/|x|^\alpha$ for $|x| > R$ with $0 < \alpha < 1$ and $R > 0$. For each α, we can choose $\varepsilon > 0$ such that $2\varepsilon + \alpha < 1$. Hence V satisfies (7.3) and (7.4). Moreover it is easy to see that V satisfies (1) and (2) in Proposition 7.7 with

$$V_1(x) := -\frac{\chi_{[R,\infty)}(|x|)}{|x|^{1+2\varepsilon+\alpha}}, \quad V_2(x) := \frac{U(x)}{(1+|x|^2)^{\frac{1}{2}+\varepsilon}} + \frac{\chi_{[R,\infty)}(|x|)}{|x|^{1+2\varepsilon+\alpha}},$$

where $\chi_{[R,\infty)}$ is the characteristic function of the interval $[R, \infty)$. Hence, by Proposition 7.7, $0 \notin \sigma_{\mathrm{p}}(H_V)$. Thus, by Theorem 7.6, H_V has an ultra-weak time operator with a dense ultra-weak CCR-domain.

Example 7.10 (hydrogen atom) It is well known that the hydrogen Schrödinger operator H_{hyd} given by (7.5) is self-adjoint with $\mathrm{D}(H_{\mathrm{hyd}}) = D(H_0)$. It is easy to see that the Coulomb potential $-\gamma/|x|$ with $d = 3$ is not an Agmon potential. Hence we can not apply Theorem 7.6 to the case $H_V = H_{\mathrm{hyd}}$. But we can show that H_{hyd} has an ultra-weak time operator in the following way. The spectral properties of H_{hyd} are also well known:

$$\sigma(H_{\mathrm{hyd}}) = \sigma_{\mathrm{p}}(H_{\mathrm{hyd}}) \cup \sigma_{\mathrm{ac}}(H_{\mathrm{hyd}}), \quad \sigma_{\mathrm{sc}}(H_{\mathrm{hyd}}) = \emptyset$$

with

$$\sigma_{\rm p}(H_{\rm hyd}) = \sigma_{\rm disc}(H_{\rm hyd}) = \left\{ -\frac{m\gamma^2}{2n^2} | n \in \mathbb{N} \right\}, \quad \sigma_{\rm ac}(H_{\rm hyd}) = [0, \infty).$$

The fact that $0 \notin \sigma_{\rm p}(H_{\rm hyd})$ follows from Example 7.8 and Proposition 7.7. It is shown that the modified wave operators $\text{s-}\lim_{t\to\pm\infty} e^{itH_{\rm hyd}} J e^{-itH_0}$ with some unitary operator J exist and are complete [RS79, Theorems XI. 71 and XI.72]. These facts imply that $H_{\rm hyd} \in S_1(L^2(\mathbb{R}^3))$. Thus, by Theorem 6.4, $H_{\rm hyd}$ has an ultra-weak time operator with a dense ultra-weak CCR-domain.

8 Ultra-Weak Time Operators of $f(H_V)$

In this section, we assume that $H_V \in S_1(L^2(\mathbb{R}^d))$ (see Definition 6.3) and give some examples of functions $f : \mathbb{R} \to \mathbb{R}$ such that $f(H_V)$ has a ultra-weak-time operator with a dense ultra-weak CCR-domain. We first give a sufficient condition for (4) in Assumption 6.5 to hold.

Lemma 8.1 *Let $H_V \in S_1(L^2(\mathbb{R}^d))$ and $f : \mathbb{R} \to \mathbb{R}$, Borel measurable. Suppose that, for all $n \in \mathbb{N}$, $f(E_n) \neq f(0)$ and $f(x) \neq f(0)$, a.e.$x \geq 0$. Then $f(0) \notin \sigma_{\rm p}(H_V)$.*

Proof: Let $\psi \in D(f(H_V))$ such that $f(H_V)\psi = f(0)\psi$. Then $\|(f(H_V) - f(0))\psi\|^2 = 0$ which is equivalent to $\int_{\mathbb{R}} |f(\lambda) - f(0)|^2 d\|E(\lambda)\psi\|^2 = 0$, where $E(\cdot)$ is the spectral measure of H_V. We can decompose ψ as $\psi = (\psi_{\rm ac}, \psi_{\rm p}) \in \mathscr{H}_{\rm ac}(H_V) \oplus \mathscr{H}_{\rm p}(H_V)$. We denote by ρ the Radon-Nykodým derivative of the absolutely continuous measure $\|E(\cdot)\psi_{\rm ac}\|^2$ with respect to the Lebesgue measure on $\mathbb{R}$. Then we have

$$\int_{\mathbb{R}} |f(\lambda) - f(0)|^2 d\|E(\lambda)\psi\|^2 = \sum_{n=1}^{\infty} |f(E_n) - f(0)|^2 \|E(\{E_n\})\psi_{\rm p}\|^2 + \int_{[0,\infty)} |f(\lambda) - f(0)|^2 \rho(\lambda) d\lambda.$$

Hence, by the present assumption, $\|E(\{E_n\})\psi_{\rm p}\|^2 = 0 \cdots (*)$ for all $n \in \mathbb{N}$ and $\int_{[0,\infty)} |f(\lambda) - f(0)|^2 \rho(\lambda) d\lambda = 0 \cdots (**)$. Equation $(*)$ implies that $E(\{E_n\})\psi_{\rm p} = 0$, $\forall n \geq 1$. Since H_V is $S_1(L^2(\mathbb{R}^d))$, it follows that $\psi_{\rm p} \in \mathscr{H}_{\rm p}(H_V)^\perp$. Hence $\psi_{\rm p} = 0$. On the other hand, $(**)$ implies that $\rho(\lambda) = 0$ a.e.$\lambda \in [0, \infty)$, from which it follows that $\psi_{\rm ac} = 0$. Thus $\psi = 0$. □

Theorem 8.2 *Let $H_V \in S_1(L^2(\mathbb{R}^d))$ and $f : \mathbb{R} \to \mathbb{R}$, Borel measurable. Assume the following (1)–(4):*

(1) The function $f : \mathbb{R} \to \mathbb{R}$ satisfies the same assumption as in Proposition 2.9.

(2) The function f is continuous at $x = 0$.

(3) $f(\sigma_{\rm disc}(H_V))$ is an infinite set such that the multiplicity of each point in $f(\sigma_{\rm disc}(H_V))$ as an eigenvalue of $f(H_V)$ is finite.

(4) For all $n \in \mathbb{N}$, $f(E_n) \neq f(0)$ and $f(x) \neq f(0)$, a.e.$x \geq 0$.

Then $f(H_V)$ has an ultra-weak time operator with a dense ultra-weak CCR-domain.

Proof: By Lemma 8.1, property (4) in Assumption 6.5 is satisfied. Hence, by Corollary 6.6, the desired result is derived. □

In Examples below, we assume that $H_V \in S_1(L^2(\mathbb{R}^d))$.

Example 8.3 ($f(H_V) = e^{-\beta H_V}$) Let $f(x) = e^{-\beta x}$, $\beta \in \mathbb{R} \setminus \{0\}$. Then it is easy to see that the function f satisfies the assumption in Theorem 8.2. Hence $e^{-\beta H_V}$ has an ultra-weak time operator with a dense ultra-weak CCR-domain. Note that, if $\beta > 0$ (resp. $\beta < 0$), $e^{-\beta H_V}$ is bounded (resp. unbounded). In particular, $e^{-\beta H_{\rm hyd}}$ has an ultra-weak time operator with a dense ultra-weak CCR-domain.

Example 8.4 ($f(H_V) = \sum_{j=0}^N a_j H_V^j$) Let $f(x) = \sum_{j=0}^N a_j x^j$ be a real polynomial ($a_j \in \mathbb{R}, N \in \mathbb{N}$, $a_N \neq 0$). We have $f(0) = a_0$. Suppose that, for all $n \in \mathbb{N}$, $\sum_{j=1}^N a_j E_n^j \neq 0$ and $\sum_{j=1}^N a_j x^{j-1} \neq 0$, $x \geq 0$. Then one can show that f satisfies the assumption in Theorem 8.2. Hence $\sum_{j=0}^N a_j {H_V}^j$ has an ultra-weak time operator with a dense ultra-weak CCR-domain. In particular, $\sum_{j=0}^N a_j H_{\rm hyd}^j$ has an ultra-weak time operator with a dense ultra-weak CCR-domain.

Example 8.5 ($f(H_V) = \sin(2\pi\beta H_V)$) Let $f(x) = \sin(2\pi\beta x)$, $\beta \in \mathbb{R} \setminus \{0\}$. Then $f(0) = 0$. Let $\beta \notin \{k/2E_n | k \in \mathbb{Z}, n \in \mathbb{N}\}$. Then $\sin(2\pi\beta E_n) \neq 0$ for all $n \in \mathbb{N}$ and hence $f(E_n) \neq f(0)$. It is obvious that $f(x) \neq f(0)$ for a.e.$x \geq 0$. Moreover $\Lambda := \{\sin(2\pi\beta E_n) | n \in \mathbb{N}\}$ is an infinite set and each point in Λ as an eigenvalue of $\sin(2\pi\beta H_V)$ is in $\sigma_{\rm disc}(\sin(2\pi\beta H_V))$ (note that, for $-1/4\beta \leq x < 0$, $\sin(2\pi\beta x)$ is strictly monotone increasing). In this way we can show that, in the present case, the assumption in Theorem 8.2 holds. Thus $\sin(2\pi\beta H_V)$ has an ultra-weak time operator with a dense ultra-weak CCR-domain. In particular, $\sin(2\pi\beta H_{\rm hyd})$ has an ultra-weak time operator with a dense ultra-weak CCR-domain.

In the same manner as above, one can find many concrete functions f such that $f(H_V)$ has an ultra-weak time operator with a dense ultra-weak CCR-domain.

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