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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.

1. Introduction

The present paper concerns a time operator in quantum theory which is defined, in a first stage of cognition, as a symmetric operator canonically conjugate to a Hamiltonian if it exists. The uncertainty relation which is derived from the canonical commutation relation of a time operator and a Hamiltonian may be interpreted as a mathematically rigorous form of *time–energy uncertainty relation*. Moreover, time operators may play important roles in quantum phenomena [1–6]. To explain motivations for studying time operators, we begin with a brief historical review on time and time operator in quantum theory (cf. also [5, Chapt. 1]).

1.1. Historical Backgrounds

In the old quantum theory, N. Bohr assumed that the interaction of the electrons in an atom with an electromagnetic field causes transitions among the allowed electron orbits in such a way that the transitions are accompanied by the absorption or the emission of electromagnetic radiations by the atom. In this hypothetical theory, however, no principle for the timing of occurrence of

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these transitions was shown. The new quantum theory presented by Heisenberg (1925), Born–Heisenberg–Jordan (1926) and Schrödinger (1926) provides a method of calculating the transition probabilities, but the question of the timing at which the events occur was not addressed explicitly.

Heisenberg introduced two kinds of uncertainty relations, i.e. the uncertainty relation for position and momentum, and that for time and energy. He argued ([7, p. 179, Eq. (2)]) that the imprecision within which the instant of transition is specifiable is given by Δt obeying the uncertainty relation

$$(\Delta t)(\Delta E) \sim \hbar = \frac{h}{2\pi} \tag{1.1}$$

with the change ΔE of energy in the quantum jump, where h is the Planck constant. Although many of the issues involved in the uncertainty principle for position and momentum have been clarified so far, similar clarity has not yet been achieved on the uncertainty principle for time and energy. For example, in [8,9], uncertainty relation (1.1) is derived, but Δt is not considered an imprecision of measurement on time; interpretations such as "a measurement act of the time gives an unexpected change to an energy level" or "it dishevels a clock to have been going to measure energy exactly" may be invalid unless any restrictions are imposed depending on measurement setups. In addition, the definition of Δt seems to vary from case to case.

1.2. Time in Quantum Theory and Time Operator

It is said that there exists a threefold role of time in quantum theory (see, e.g. [10] and [5, Chapt. 3]). Firstly, time is identified as the parameter entering the Schrödinger equation, which is a differential equation describing the causal continuous change of states of a quantum system, and measured by a laboratory clock. Time in this sense is called the external time. The external time measurement is carried out with clocks that are not dynamically connected with objects investigated in experiments.

By contrast, time as a dynamical one can be defined by the dynamical behaviour of quantum objects. A dynamical time is defined and measured in terms of a physical system undergoing changes. Examples include the linear uniform motion of a free particle and the oscillation of the atoms in an atomic clock.

Finally, time can be considered as a quantum object which forms a canonical pair with a Hamiltonian in a suitable sense. As already mentioned, time in this sense is called a time operator in its simplest form. There is in fact a hierarchy of time operators as is shown below. The main purpose of the present paper is to analyse this hierarchy mathematically and to establish abstract existence theorems on time operators in relation to the hierarchy with applications to Schrödinger Hamiltonians.

A simple example of time operator is given as follows. A non-relativistic quantum particle with mass $m > 0$ under the action of a constant force $F \in \mathbb{R}\backslash\{0\}$ in the one-dimensional space $\mathbb{R}$ is governed by the Hamiltonian

$$H_F = \frac{1}{2m}P^2 - FQ$$

acting in $L^2(\mathbb{R})$, the Hilbert space of square integrable Borel measurable functions on $\mathbb{R}$, with the momentum operator $P = -iD_x$ (D_x is the generalized differential operator in the variable $x \in \mathbb{R}$)[1] and Q being the multiplication operator by x. It is shown that H_F is essentially self-adjoint on $C_0^\infty(\mathbb{R})$, the space of infinitely differentiable functions on $\mathbb{R}$ with compact support, and hence, its closure $\overline{H}_F$ is self-adjoint (but, note that $\overline{H}_F$ is neither bounded from below nor from above). The self-adjoint operator $T_F = P/F$ satisfies the canonical commutation relation (CCR)

$$[H_F, T_F] = -i\mathbb{1}$$

on a dense domain $\mathcal{D}$ (e.g. $\mathcal{D} = C_0^\infty(\mathbb{R})$), where $\mathbb{1}$ denotes identity and $[A, B] := AB - BA$. This shows that T_F is a canonical conjugate operator to the Hamiltonian H_F and hence a time operator of H_F. From the CCR, one can derive the uncertainty relation of Heisenberg type

$$(\Delta H_F)_\psi (\Delta T_F)_\psi \geq \frac{1}{2}$$

for all unit vectors $\psi \in \mathcal{D}$, where $(\Delta A)_\psi$ denotes the uncertainty of A with respect to the state vector ψ (see (2.3) for its definition). This inequality may be interpreted as a form of time–energy uncertainty relation in the present model.

As for time operator, however, there is a long history of confusion and controversy.[2] The origin of this may come from the statement of Pauli made in 1933 ([11, p. 63, footnote 2]) that the introduction of a time observable T satisfying the CCR

$$[H, T] = -i\mathbb{1} \tag{1.2}$$

with a self-adjoint operator H having a discrete eigenvalue is basically forbidden. Although there are no explicit arguments for this statement in the cited literature (only reference to Dirac's textbook), a formal (false in fact) argument leading to the statement may be as follows: let ϕ be an eigenvector of H with a discrete eigenvalue E:$H\phi = E\phi$. Then, using (1.2) formally, one obtains $He^{i\varepsilon T}\phi = (E + \varepsilon)e^{i\varepsilon T}\phi \cdots (*)$ for all $\varepsilon \in \mathbb{R}$. Hence, $e^{i\varepsilon T}\phi$ is an eigenvector of H with eigenvalue $E + \varepsilon$. Since $\varepsilon \in \mathbb{R}$ is arbitrary, it follows that each point in $\mathbb{R}$ is an eigenvalue of H. But this obviously contradicts the discreteness of eigenvalues of H. It should be noted, however, that this argument is very formal and, in particular, no attention was paid to the domain of the operators involved. For example, if ϕ is not in the domain of T^n for some $n \in \mathbb{N}$, then the expansion $e^{i\varepsilon T}\phi = \sum_{n=0}^\infty (i\varepsilon)^n T^n \phi/n!$ is meaningless; even in the case where ϕ is in the domain of T^n for all $n \in \mathbb{N}$, $\sum_{n=0}^\infty (i\varepsilon)^n T^n \phi/n!$ is not necessarily convergent ; moreover, $e^{i\varepsilon T}\phi$ is not necessarily in the domain of H and, if $e^{i\varepsilon T}\phi$ is not in the domain of H, then $(*)$ is meaningless.

It is well known [12, p. 2] that at least one of T and H satisfying the CCR (1.2) on a dense domain is an unbounded operator and, for unbounded

[1] We use the physical unit system where $\hbar = 1$.

[2] A germ of the notion of time operator is found already in Heisenberg's paper [7, pp. 177–179] in 1927.

operators, their domain must be carefully considered. As a matter of fact, the above argument is incorrect and so is the Pauli's statement too. Indeed, one can construct a self-adjoint operator H which is bounded from below with purely discrete spectrum and a self-adjoint operator T such that (1.2) holds on a dense domain. This was pointed out in [10, p. 4], and mathematically rigorous constructions of such time operators T have been done in [3,13].

The history of studies on time operators as well as on representations of CCR suggests that there may be a hierarchy of time operators and this indeed is the case as is shown below in the present paper. It is important to distinguish each class from the others in the hierarchy. In our words, the time observable T such that the above formal argument may take a rigorous form is an *ultra-strong* time operator (see Remark 2.4 below), since the *operator equality* $e^{-i\varepsilon T}He^{i\varepsilon T} = H + \varepsilon$, $\varepsilon \in \mathbb{R} \cdots (\dagger)$ is tacitly assumed in the above argument in fact, which, however, is *not equivalent* to (1.2) in the mathematically rigorous sense [14], and, if H is self-adjoint, then $(\dagger)$ is equivalent to the Weyl relation $e^{i\varepsilon T}e^{itH} = e^{-it\varepsilon}e^{itH}e^{i\varepsilon T}$, $t, \varepsilon \in \mathbb{R} \cdots (\dagger\dagger)$, meaning that T is an ultra-strong time operator of H (but, if H is not essentially self-adjoint, then $(\dagger)$ does not imply $(\dagger\dagger)$ with H replaced by the closure $\overline{H}$ of H, because, in this case, "$e^{it\overline{H}}$" is meaningless as a unitary operator). If a self-adjoint operator H has an ultra-strong time operator T, then T is a strong time operator of H (see (1.3) below) and hence H is absolutely continuous (see Proposition 3.5 below) so that H has no eigenvalues. Therefore, in this case, the above argument becomes meaningless. Moreover, if H is semi-bounded, then no strong time operator T of H is essentially self-adjoint ([4], [1, Theorem 2.8]) and hence "$e^{i\varepsilon\overline{T}}$" makes no sense as a unitary operator. In this sense too, the above argument is meaningless.

It has been absurd that studies on time observables have been ruled out for so many years due to the Pauli's statement without any questions. If one could have carefully examined the Pauli's statement with mathematically rigorous thinking, then one could have found incorrectness of it.

1.3. Rough Description of Main Results

As already mentioned, a time operator T of a self-adjoint operator H is defined to be a symmetric operator satisfying CCR (1.2) on a suitable dense domain (we give a more detailed description of time operators in Sect. 2). Another approach to consider time operators as observables is an application of positive operator-valued measures (POVM) [5, Chapt. 10]. In this paper, however, we take an operator-theoretical approach to classify time operators and to construct a time operator for a given self-adjoint operator without invoking POVM. Consequently, we are led to extend the conventional notion of time operator. Indeed, commutation relation (1.2) can be weakened in at least two manners and we find a time operator T for each weakened form. As we have learned from the formal argument on the Pauli's statement, taking care of domains of T and H is crucial not to be led to incorrect conclusions. Thus, the domain of time operators is one key ingredient to study them.

We now outline main results obtained in the present paper in (1)–(5) below (rigorous statements of assumptions and results are given in Sect. 2). Let H be a self-adjoint operator acting in a complex Hilbert space $\mathcal{H}$.

(1) Ultra-weak time operators and a hierarchy of time operators. It has so far been known that there are at least three classes of time operators [2,15], i.e. time operators as canonical conjugates of a Hamiltonian in the conventional sense, which may be called *ordinary time operators* to distinguish them from other classes of time operators, *strong time operators* and *weak time operators*. In the present paper, in addition to these classes of time operators, we introduce a new concept on time operator, which we call *ultra-weak time operator*, and study it. An ultra-weak time operator, however, is not an operator in general, but defined to be a sesquilinear form $\mathfrak{t} : \mathcal{D}_1 \times \mathcal{D}_2 \to \mathbb{C}$ with nonzero subspaces $\mathcal{D}_1$ and $\mathcal{D}_2$ of $\mathcal{H}$ such that

$$\mathfrak{t}[H\phi, \psi] - \mathfrak{t}[H\psi, \phi]^* = -i(\phi, \psi), \quad \psi, \phi \in \mathcal{E},$$

where, for $z \in \mathbb{C}$, z^* denotes the complex conjugate of z, $(\ , \ )$ is the inner product of $\mathcal{H}$ (linear in the second variable), and $\mathcal{E}$ is a nonzero subspace of $\mathcal{H}$ (for the rigorous definition of $\mathfrak{t}$, see Definition 2.8). The class of ultra-weak time operators may be compared to the space of distributions in the context of theory of functions (as there exists a distribution which is not a function, there may exist an ultra-weak time operator which is not an operator).

For convenience, we also introduce the concept of ultra-strong time operator which has been already mentioned above. These five classes of time operators form a hierarchy in the following sense:

$$\{\text{ultra-strong t.o.}\} \subset \{\text{strong t.o.}\} \subset \{\text{t.o.}\} \subset \{\text{weak t.o.}\} \subset \{\text{ultra-weak t.o.}\}, \quad (1.3)$$

where t.o. is abbreviation of "time operators". See Sect. 2 for more details. Generally speaking, it is expected that each class in the hierarchy of time operators has proper roles in connection with quantum phenomena. In this paper, we particularly concentrate our attention on strong time operators, time operators and ultra-weak time operators. As a possible physical aspect of ultra-weak time operators, a weak form of uncertainty relation is given (see Proposition 2.10).

(2) Existence of strong time operators in an abstract framework. A strong time operator T of a self-adjoint operator H is defined through the weak Weyl relation (see Definitions 2.2, 2.3). It is known that (1.2) is satisfied on a dense domain and the spectrum $\sigma(H)$ of H must be purely absolutely continuous. Hence, if H has an eigenvalue, no strong time operator of H exists. Then a natural question is to ask the existence of a strong time operator for an absolutely continuous self-adjoint operator. We introduce a class $S_0(\mathcal{H})$ of self-adjoint operators on $\mathcal{H}$ in Definition 3.13 and prove the following theorem (Theorem 3.16):

Theorem 1.1. *Assume that $\mathcal{H}$ is separable and that $H \in S_0(\mathcal{H})$. Then H has a strong time operator.*

It may be interesting to consider extensions of this theorem to a more general class of absolutely continuous self-adjoint operators. But this will be done elsewhere. In this paper, we next proceed to construction of a time operator for a self-adjoint operator which has point spectra (eigenvalues).

(3) Existence of time operators of a self-adjoint operator with point spectra. As for general existence of time operators of a self-adjoint operator H with point spectra, only limited classes of H have been found [3,13,16,17]. In this paper we extend these results (Theorem 4.8):

Theorem 1.2. *Let* $\sigma(H) = \{E_n\}_{n=1}^{\infty}$*,* $E_1 < E_2 < \cdots$ *and* $\lim_{n\to\infty} E_n = \infty$*. Then there exists a time operator* T *of* H*.*

In [3,13,17], time operators of H having purely discrete spectrum are constructed, but the growth condition $\sum_{n=1}^{\infty} 1/E_n^2 < \infty$ for $\{E_n\}_n$ is imposed. This condition seems to be artificial. An important point in Theorem 1.2 is that this condition is not required. We show in Sect. 4.3 that the non-commutative harmonic oscillator Hamiltonian [18] and the Rabi Hamiltonian [19–22] are included in this class of Hamiltonians as concrete examples.

Remark 1.3. After submitting the first version of the present paper, we have learned that Teranishi [23] has proved a theorem essentially same as Theorem 1.2 by a method different from ours.

(4) Ultra-weak time operators. We also establish a theorem on the existence of ultra-weak time operators for a general class of self-adjoint operators with infinitely many discrete eigenvalues but the accumulation point is not ∞ (Theorem 5.2).

Theorem 1.4. *Suppose that* $\sigma(H)\setminus\{0\} = \{E_j\}_{j=1}^{\infty}$*,* $E_1 < E_2 < \cdots < 0$*,* $\lim_{j\to\infty} E_j = 0$*, and* 0 *is not an eigenvalue of* H*. Then there exists an ultra-weak time operator* $\mathfrak{t}$ *of* H*.*

It is shown in Sect. 3.2.2 that $\mathfrak{t}[\phi,\psi] = (\phi, A\psi)$ formally with some operator A. The crucial point is that A is of the form

$$A = -\frac{1}{2}(T_{-1}H^{-2} + H^{-2}T_{-1}),$$

where T_{-1} denotes a time operator of H^{-1}. It is difficult to show, however, that $\mathrm{D}(A) \neq \{0\}$ and $\mathrm{D}(HA) \cap \mathrm{D}(AH) \neq \{0\}$. This is the reason why the introduction of an ultra-weak time operator $\mathfrak{t}$ as a sesquilinear form is needed and may be even natural.

(5) Ultra-weak time operators for Schrödinger operators. Finally, by applying the results described in (1)–(4) above, we construct an ultra-weak time operator for a class of Schrödinger operators, including the Hamiltonian of the hydrogen atom. It is shown in Theorem 6.6 that, for a class of potentials $V : \mathbb{R}^d \to \mathbb{R}$, the d-dimensional Schrödinger operator

$$H_V := -\frac{1}{2m}\Delta + V$$

acting in $L^2(\mathbb{R}^d)$ has an ultra-weak time operator, where Δ is the d-dimensional generalized Laplacian. Below are some examples of H_V having an ultra-weak time operator (see Sect. 6.1 for more details).

(i) Let $U \in L^\infty(\mathbb{R}^3)$ and

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

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 $2\varepsilon + \alpha < 1$. Then H_V has an ultra-weak time operator. See Example 6.9.

(ii) Let

$$H_{\mathrm{hyd}} := -\frac{1}{2m}\Delta - \frac{\gamma}{|x|}$$

be the 3-dimensional hydrogen Schrödinger operator with a constant $\gamma > 0$. Then H_{hyd} has an ultra-weak time operator. See Example 6.8.

(iii) Suppose that H_V has an ultra-weak time operator. Then, under some conditions, we can show that the following operators $f(H_V)$ also have an ultra-weak time operator (see Theorem 6.12):

(a) $f(H_V) = e^{-\beta H_V}$ for $\beta \in \mathbb{R}\backslash\{0\}$;
(b) $f(H_V) = \sum_{j=0}^N a_j H_V^j$ $(a_j \in \mathbb{R}, N \in \mathbb{N})$;
(c) $f(H_V) = \sin(2\pi\beta H_V)$ for $\beta \in \mathbb{R}\backslash\{k/2E_j | k \in \mathbb{Z}, j \in \mathbb{N}\}$, where $\{E_j\}_{j\in\mathbb{N}}$ denotes the discrete spectrum of H_V.

See Examples 6.13, 6.14 and 6.15.

In the next section we give definitions of terminology used in this paper and remarks from mathematical point of view.

2. Mathematical Backgrounds of Time Operators

2.1. A Review on Mathematical Analysis on Time Operators

Mathematical analysis on time operators has been developed in the papers [1–4,13,15–17,24–27]. Let A and B be linear operators on a complex Hilbert space $\mathcal{H}$, satisfying the canonical commutation relation

$$[A, B] = -i\mathbb{1} \tag{2.1}$$

on a nonzero subspace $\mathcal{D} \subset \mathrm{D}(AB) \cap \mathrm{D}(BA)$, where, for a linear operator L on $\mathcal{H}$, $\mathrm{D}(L)$ denotes the domain of L. We call $\mathcal{D}$ a *CCR domain* for the pair (A, B). It is well known [12, p. 2] that, if $\mathcal{D}$ is dense in $\mathcal{H}$, then (2.1) implies that $\mathcal{H}$ 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 $\mathcal{D}$ is an invariant subspace of A and B, then $\mathcal{D}$ has to be infinite dimensional and hence at least one of A and B as linear operators on $\overline{\mathcal{D}}$ (the closure of $\mathcal{D}$) with domain $\mathcal{D}$ is unbounded. From representation theoretical point of view, $(\mathcal{H}, \mathcal{D}, \{A, B\})$ is called a *representation of the CCR with one* *degree of freedom* (usually $\mathcal{D}$ is assumed to be a dense invariant subspace of A and B, but, here, we do not require this property).

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

The CCR (2.1) implies an physically important inequality: if A and B in (2.1) are symmetric operators on $\mathcal{H}$, then (2.1) yields the *uncertainty relation* of Heisenberg type [28, Chapt. III, Sect. 4]:

$$(\Delta A)_\psi (\Delta B)_\psi \geq \frac{1}{2} \tag{2.2}$$

for all $\psi \in \mathcal{D}$ with $\|\psi\| = 1$, where

$$(\Delta A)_\psi := \|(A - (\psi, A\psi)_{\mathcal{H}})\psi\|_{\mathcal{H}},\ \psi \in \mathrm{D}(A),\ \|\psi\| = 1, \tag{2.3}$$

the *uncertainty* of A with respect to ψ.[3]

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 $\mathcal{H}$ and $\mathcal{D}$ be a nonzero subspace of $\mathcal{H}$ such that $\mathcal{D} \subset \cap_{j,k=1}^d [\mathrm{D}(A_jB_k) \cap \mathrm{D}(B_kA_j) \cap \mathrm{D}(A_jA_k) \cap \mathrm{D}(B_jB_k)]$. Then the triple $(\mathcal{H}, \mathcal{D}, \{A_j, B_j | j = 1,\ldots,d\})$ is called a *representation of the CCRs with* d *degrees of freedom* if the CCRs with d degrees of freedom

$$[A_j, B_k] = -i\delta_{jk}\mathbb{1}, \quad [A_j, A_k] = 0, \quad [B_j, B_k] = 0, \quad j,k = 1,\ldots,d \tag{2.4}$$

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

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

$$e^{-isA_j} e^{-itB_k} = e^{ist\delta_{jk}} e^{-itB_k} e^{-isA_j}, \quad j,k = 1,\ldots,d,\ s,t \in \mathbb{R} \tag{2.5}$$

hold.

The Weyl relations (2.5) imply that there exists a dense invariant domain $\mathcal{D}$ of A_j and B_j $(j = 1,\ldots,d)$ such that (2.4) holds on $\mathcal{D}$ [12, Theorem 4.9.1]. Hence, the Weyl representation $\{A_j, B_j | j = 1,\ldots,d\}$ is a representation of the CCRs with d degrees of freedom. But *the converse is not true* (e.g. [14,29,30]).

A Weyl representation $\{A_j, B_k | j,k = 1,\ldots,d\}$ of the CCRs with d degrees of freedom is said to be *irreducible* if any subspace $\mathcal{D}$ of $\mathcal{H}$ left invariant by e^{-itA_j} and e^{-itB_j} for all $t \in \mathbb{R}$ and $j = 1,\ldots,d$ is $\{0\}$ or $\mathcal{H}$.

In quantum mechanics on the d-dimensional space

$$\mathbb{R}^d = \{x = (x_1,\ldots,x_d) | x_j \in \mathbb{R}\},$$

the momentum operator $P := (P_1,\ldots,P_d)$ and the position operator $Q := (Q_1,\ldots,Q_d)$ are defined by $P_j := -iD_j$ (D_j is the generalized partial differential operator in x_j) and $Q_j := M_{x_j}$(the multiplication operator by x_j),

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[3] Inequality (2.2) can be derived also from a weak version of (2.1): $(A\psi, B\phi) - (B\psi, A\phi) = -i(\psi, \phi)$, $\psi, \phi \in \mathcal{D}_{\mathrm{w}}$, where $\mathcal{D}_{\mathrm{w}}$ is a nonzero subspace of $\mathrm{D}(A) \cap \mathrm{D}(B)$.

$j = 1, \ldots, d$. For all $j = 1, \ldots, d$, P_j and Q_j are self-adjoint operators on the Hilbert space $L^2(\mathbb{R}^d)$, satisfying the CCRs with d degrees of freedom:

$$[P_j, Q_k] = -i\delta_{jk}\mathbb{1}, \quad [P_j, P_k] = 0, \quad [Q_j, Q_k] = 0 \tag{2.6}$$

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, $(L^2(\mathbb{R}^d), C_0^\infty(\mathbb{R}^d), \{P_j, Q_j | j = 1, \ldots, d\})$ are a representation of the CCRs 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 CCRs is called the *Schrödinger representation of the CCR* (or the *Schrödinger system* [12]) *with d degrees of freedom*.

By an application of (2.2), one obtains the *position–momentum uncertainty relations*

$$(\Delta P_j)_\psi (\Delta Q_j)_\psi \geq \frac{1}{2}, \quad j = 1, \ldots, d \tag{2.7}$$

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.[4]

The Schrödinger representation $\{P_j, Q_k | j, k = 1, \ldots, d\}$ is an irreducible Weyl representation ([12, Theorem 4.5.1]; [31, Theorem 3.12]). Conversely, it is known as the von Neumann uniqueness theorem (e.g. [12, Theorem 4.11.1]) that, if $\mathcal{H}$ is separable and $\{A_j, B_k | j, k = 1, \ldots, d\}$ is an irreducible Weyl representation of the CCRs with d degrees of freedom, then

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

Here $\cong$ denotes a unitary equivalence.

Usually models of quantum mechanics in $\mathbb{R}^d$ are constructed from the Schödinger representation of the CCRs 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 $H_{\mathrm{cl}}(p, x) = p^2/2m + V(x)$, $(p, x) \in \mathbb{R}^d \times \mathbb{R}^d$. Then the corresponding quantum Hamiltonian is given by the Schrödinger operator (or the Schrödinger Hamiltonian)

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

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[5]) and $\Delta := \sum_{j=1}^{d} D_j^2$ is the d-dimensional

[4] Inequality (2.7) holds also for all $\psi \in \mathrm{D}(P_j) \cap \mathrm{D}(Q_j)$ with $\|\psi\| = 1$.

[5] 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 $J, K \subset \mathbb{R}$, $E_{A_j}(J)E_{A_k}(K) = E_{A_k}(K)E_{A_j}(J)$).

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,

$$H_V = H_0 + V, \tag{2.8}$$

where

$$H_0 := -\frac{1}{2m}\Delta. \tag{2.9}$$

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 $\mathcal{H}$ is described by the unitary operator e^{-itH} with time parameter $t \in \mathbb{R}$ in such a way that, if $\phi \in \mathcal{H}$ 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 $\phi \in \mathrm{D}(H)$, 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. It is the external time mentioned in Sect. 1.2. 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 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

$$[H, T] = -i\mathbb{1} \tag{2.10}$$

on a nonzero subspace $\mathcal{D}_{H,T}$ 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 (2.10), 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 (2.10) on a nonzero subspace included in $\mathrm{D}(HT) \cap \mathrm{D}(TH)$.

Remark 2.1. 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

$$(\Delta H)_\psi(\Delta T)_\psi \geq \frac{1}{2}, \quad \psi \in \mathcal{D}_{T,H}, \ \|\psi\| = 1 \tag{2.11}$$

implied by (2.10) may be interpreted as a form of *time–energy uncertainty relation*. The time operator T is physical in the sense that it gives a lower bound for the uncertainty $(\Delta H)_\psi$ of H with respect to the state $\psi \in \mathcal{D}_{T,H}$.

In the physics literature, formal (heuristic) constructions of "time operators" have been done for special classes of Schrödiner Hamiltonians (e.g.

[32–37]). But, since the theory of CCRs 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 CCRs (see, e.g. [14,30,38–40]). It should be noted that there exist representations of CCRs which are inequivalent to Schrödinger ones (e.g. [14,29,30]) and, interestingly enough, some of them are connected with characteristic physical phenomena such as the so-called Aharonov–Bohm effect (see [29] 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. [1–4,13,16,17,24–27] and references therein; see also [30,38–40] 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 $\mathcal{H}$ 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 (2.5) with $d = 1$, since $\sigma(P) = \mathbb{R}$ and then $H \ncong P$, 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 2.2 *(weak Weyl relation).* A pair (A, B) consisting of a self-adjoint operator A and symmetric operator B on $\mathcal{H}$ 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*

$$Be^{-itA}\psi = e^{-itA}(B + t)\psi \tag{2.12}$$

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 [30,38–40]. It is easy to see that a Weyl representation $\{A, B\}$ is a weak Weyl representation and that the weak Weyl relation (2.12) implies the CCR (2.1) 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 2.3 *(Strong time operator).* A symmetric operator T on $\mathcal{H}$ is called a *strong time operator* of a self-adjoint operator H on $\mathcal{H}$ if (H, T) is a weak Weyl representation.

Remark 2.4. (1) In relation to strong time operators, it may be convenient to give a name to a self-adjoint operator T on $\mathcal{H}$ 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 $\mathcal{H}$ 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 $\mathcal{H}$ 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 [4], although the name "strong time operator" is not used in [4] (it was introduced first in [2] to distinguish different classes of time operators). Further investigations and generalizations on strong time operators were done in [1,24]. See also [3,17,27,41]. It is known that, if (H, T) satisfies the weak Weyl relation, then $\sigma(H)$ is purely absolutely continuous [40]. 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 (2.11), 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 $|(\phi, e^{-itH}\psi)|^2$ $(\phi, \psi \in \mathcal{H}, \|\phi\| = \|\psi\| = 1)$ in the following form [1, 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 $t \in \mathbb{R}\backslash\{0\}$,

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

This shows a very interesting correspondence between decay rates in time of transition probabilities and regularities of state vectors ϕ, ψ.[6] It tells us also the importance of domains of time operators.

In [3,13], a time operator of a self-adjoint operator whose spectrum is purely discrete with a growth condition is constructed. In [16], 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 [16]. One of the weaker versions of time operator is defined as follows:

Definition 2.5 *(Weak time operator).* A symmetric operator T on $\mathcal{H}$ is called a *weak time operator* of a self-adjoint operator H on $\mathcal{H}$ if there exists a nonzero subspace $\mathcal{D}_{\mathrm{w}} \subset \mathrm{D}(T) \cap \mathrm{D}(H)$ such that the *weak CCR* on $\mathcal{D}_{\mathrm{w}}$ holds:

$$(H\phi, T\psi) - (T\phi, H\psi) = -i(\phi, \psi), \quad \phi, \psi \in \mathcal{D}_{\mathrm{w}}. \tag{2.13}$$

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

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

It is obvious that a time operator T of H is a weak time operator of H with $\mathcal{D}_{\rm w} = \mathcal{D}_{H,T}$. We remark that (2.13) implies the time–energy uncertainty relation (2.11) with $\psi \in \mathcal{D}_{\rm w}$ ($\|\psi\| = 1$).

One should keep in mind the following fact:

Proposition 2.6. *Let T be a weak time operator of a self-adjoint operator H and $\mathcal{D}_{\rm w}$ be a weak-CCR domain for (H, T). Then H has no eigenvectors in $\mathcal{D}_{\rm w}$.*

Proof. Let $H\psi = E\psi$ with $\psi \in \mathcal{D}_{\rm w}$ and $E \in \mathbb{R}$. Taking ϕ in (2.13) to be ψ, we see that the left-hand side is equal to 0. Hence, $\|\psi\|^2 = 0$, implying $\psi = 0$. □

Remark 2.7. 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.

2.2. Ultra-Weak Time Operator

Proposition 2.6 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 $\mathcal{H}$. 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 2.8 (*Ultra-weak time operator*). Let H be a self-adjoint operator on $\mathcal{H}$ and $\mathcal{D}_1$ and $\mathcal{D}_2$ be nonzero subspaces of $\mathcal{H}$. A sesquilinear form $\mathfrak{t} : \mathcal{D}_1 \times \mathcal{D}_2 \to \mathbb{C}$ ($\mathcal{D}_1 \times \mathcal{D}_2 \ni (\phi, \psi) \mapsto \mathfrak{t}[\phi, \psi] \in \mathbb{C}$) with domain $\mathrm{D}(\mathfrak{t}) = \mathcal{D}_1 \times \mathcal{D}_2$ ($\mathfrak{t}[\phi, \psi]$ is antilinear in ϕ and linear in ψ) is called *an ultra-weak time operator* of H if there exist nonzero subspaces $\mathcal{D}$ and $\mathcal{E}$ of $\mathcal{D}_1 \cap \mathcal{D}_2$ such that the following (i)–(iii) hold:

- (i) $\mathcal{E} \subset D(H) \cap \mathcal{D}$.
- (ii) (symmetry on $\mathcal{D}$) $\mathfrak{t}[\phi, \psi]^* = \mathfrak{t}[\psi, \phi]$, $\phi, \psi \in \mathcal{D}$.
- (iii) (ultra-weak CCR) $H\mathcal{E} \subset \mathcal{D}_1$ and, for all $\psi, \phi \in \mathcal{E}$,

$$\mathfrak{t}[H\phi, \psi] - \mathfrak{t}[H\psi, \phi]^* = -i(\phi, \psi) \tag{2.14}$$

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

Remark 2.9. (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 $\mathcal{D}_{\mathrm{w}}$. Then one can define a sesquilinear form $\mathfrak{t}_T : \mathcal{H} \times \mathrm{D}(T) \to \mathbb{C}$ by

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

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 $\phi, \psi \in \mathcal{D}_{\mathrm{w}}$, $\mathfrak{t}_T[H\phi, \psi] - \mathfrak{t}_T[H\psi, \phi]^* = -i(\psi, \phi)$. Hence, $\mathfrak{t}_T$ is an ultra-weak time operator of H with $\mathcal{D}_{\mathrm{w}}$ 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 $H\psi \in \mathcal{D}$ in (2.14), then, by the symmetry of $\mathfrak{t}[\cdot, \cdot]$ on $\mathcal{D}$, (2.14) takes the following form:

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

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

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

In the case of the pair $(H, \mathfrak{t})$ in Definition 2.8, the uncertainty relation (2.2) associated with CCR is generalized as follows:

Proposition 2.10 (Uncertainty relation for $(H, \mathfrak{t})$). *Assume that H has an ultra-weak time operator $\mathfrak{t}$ as in Definition 2.8. Then, for all $a, b \in \mathbb{R}$ and a unit vector $\psi \in \mathcal{E}$,*

$$|(\mathfrak{t} - a)[(H - b)\psi, \psi]| \geq \frac{1}{2}. \tag{2.15}$$

Proof. Using (2.14), we have $\Im\{(\mathfrak{t} - a)[(H - b)\psi, \psi]\} = -\frac{1}{2}$. Since $|z| \geq |\Im z|$ for all $z \in \mathbb{C}$, (2.15) follows. □

In summary, we have seen that there exist five classes of time operators with inclusion relation (1.3).

2.3. Outline of the Present Paper

Having introduced the new concept "ultra-weak time operator", we now outline the contents of the present paper. In Sect. 3, 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 3.16). Section 4 is 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 [3,13]. In Sect. 5, we introduce a class $S_1(\mathcal{H})$ of self-adjoint operators on $\mathcal{H}$ (see Definition 5.3) such that each element of $S_1(\mathcal{H})$ has an ultra-weak time operator with a dense ultra-weak CCR domain (Theorem 5.4). 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 5.6). In Sect. 6, 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 6.6). Also we show that the Hamiltonian of the hydrogen atom (i.e. the case where $V(x) = -\gamma/|x|$, $x \in \mathbb{R}^3\backslash\{0\}$

with a constant $\gamma > 0$) has an ultra-weak time operator with a dense ultra-weak CCR domain (Example 6.10). Moreover, for a class of f, an existence theorem on an ultra-weak time operator of $f(H_V)$ is proved (Theorem 6.12) and some examples are given.

3. Abstract Theory of Time Operators—Review with Additional Results

3.1. A General Structure of Time Operators

We first note an elementary fact:

Proposition 3.1. *Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and T be a time operator of H with a CCR domain $\mathcal{D}$ for (H, T). Let H' be a self-adjoint operator on a Hilbert space $\mathcal{H}'$ such that $UHU^{-1} = H'$ for a unitary operator $U : \mathcal{H} \to \mathcal{H}'$. Then $T' := UTU^{-1}$ is a time operator of H' with a CCR domain $U\mathcal{D}$ for (H', T').*

Proof. An easy exercise. □

In what follows, H denotes a self-adjoint operator on a complex Hilbert space $\mathcal{H}$. As is well known (e.g. [42, Sect. 10.1], [43, Theorem VII.24]), $\mathcal{H}$ has the orthogonal decomposition

$$\mathcal{H} = \mathcal{H}_{\mathrm{ac}}(H) \oplus \mathcal{H}_{\mathrm{sc}}(H) \oplus \mathcal{H}_{\mathrm{p}}(H), \tag{3.1}$$

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

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

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

$$H = H_{\mathrm{ac}} \oplus H_{\mathrm{sc}} \oplus H_{\mathrm{p}} \tag{3.2}$$

and

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

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 $\sigma_{\mathrm{disc}}(H)$ 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 3.2. *Suppose that each $H_{\#}$ has a time operator $T_{\#}$ with a CCR domain $\mathcal{D}_{\#}$. Then the direct sum*

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

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

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 $\psi_\# \in \mathcal{D}_\#$

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

Let $\psi = (\psi_{\rm ac}, \psi_{\rm sc}, \psi_{\rm p}) \in \mathcal{D}_{\rm ac} \oplus \mathcal{D}_{\rm sc} \oplus \mathcal{D}_{\rm p}$. Then, by (3.2), $\psi \in D(HT) \cap D(TH)$ 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 $\mathcal{D}_{\rm ac} \oplus \mathcal{D}_{\rm sc} \oplus \mathcal{D}_{\rm p}$. □

3.2. Strong Time Operators

3.2.1. A Summary of Known Results and Additional Results. We summarize some basic facts on strong time operators of H.

Proposition 3.3. *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 [1, 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 3.4. *Let T be a strong time operator of H and H' be a self-adjoint operator on a Hilbert space $\mathcal{H}'$ such that, for a unitary operator $U : \mathcal{H} \to \mathcal{H}'$, $UHU^{-1} = H'$. 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 3.3, 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 3.5 ([1]). *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 3.6. *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*

$$e^{itH}Se^{-itH} = S + t \tag{3.3}$$

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 3.3, we have operator equalities

$$e^{itH}T_ke^{-itH} = T_k + t, \quad t \in \mathbb{R}, k = 1, \ldots, n. \tag{3.4}$$

Since $e^{itH}Se^{-itH} = \sum_{k=1}^n e^{itH}a_kT_ke^{-itH}$ (operator equality), (3.4) implies (3.3). 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 (3.4). □

Proposition 3.6-(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 $\mathcal{H}$. Then $\sum_{j=1}^n H_j$ is essentially self-adjoint and, for all $t \in \mathbb{R}$,

$$e^{it\overline{\sum_{j=1}^n H_j}} = \prod_{j=1}^n e^{itH_j}, \tag{3.5}$$

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 3.7. *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 $e^{itH_k}T_je^{-itH_k} = T_j$ 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 3.3, we have operator equality $e^{itH_j}T_je^{-itH_j} = T_j + t$ for all $t \in \mathbb{R}$. Hence, by (3.5) and the commutativity of the operators e^{itH_k}, $k = 1, \ldots, n$, we have

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

Thus, the desired result follows. □

Proposition 3.7 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 3.7 is formulated as follows. Let $\{A_1, \ldots, A_n\}$ be a set of strongly commuting self-adjoint operators on $\mathcal{H}$ such that each A_j is injective. Suppose that each A_j has a strong time operator B_j such that, for all $j = 1, \ldots, n$, $\mathrm{D}(B_jA_j^{-1}) \cap \mathrm{D}(A_j^{-1}B_j)$ is dense and, for all $t \in \mathbb{R}$, $e^{itA_k}B_je^{itA_k} = B_j$, $k \neq j, k = 1, \ldots, n$. 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 3.8 ([1]). *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 [1, Sect. 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 $\mathcal{H}$. 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 [1, 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 3.9 ([27, Theorem 1.9]). *Let K be a closed null subset of $\mathbb{R}$ with respect to the Lebesgue measure. Assume that $f \in C^2(\mathbb{R}\backslash K)$ and $L := \{\lambda \in \mathbb{R}\backslash K | f'(\lambda) = 0\}$ 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*

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

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 $\mathcal{D} \subset \mathrm{D}(L)$, $L\lceil\mathcal{D}$ denotes the restriction of L to $\mathcal{D}$.

Example 3.10 (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 $\mathcal{H} = L^2(\mathbb{R}^d)$. 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 3.9 takes the form $D_{\mathrm{AB},j} := \mathrm{L.H.}\{g(P_j)\mathrm{D}(Q_j) | g \in C_0^\infty(\mathbb{R}\backslash\{0\})\}$. 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 3.8 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 [24]. Let

$$\Omega_j := \{k \in \mathbb{R}^d | k_j \neq 0\}, \quad D'_{\mathrm{AB},j} := \{f \in L^2(\mathbb{R}^d) | \hat{f} \in C_0^\infty(\Omega_j)\},$$

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 $g \in C_0^\infty(\mathbb{R}\backslash\{0\})$, $g(P_j)\mathrm{D}(Q_j) \supset g(P_j)D'_{\mathrm{AB},j}$. For any $g \in C_0^\infty(\mathbb{R}\backslash\{0\})$ 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* [4,32].

Example 3.11. 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 [44]. See [1, Sect. 11]) for the details.

3.2.2. 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 Hilbert space $\mathcal{H}$, a nonzero 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 $\mathcal{H}$, where, for a subset $\mathcal{D}$ of $\mathcal{H}$, L.H.$\mathcal{D}$ denotes the algebraic linear hull of vectors in $\mathcal{D}$.

We denote by E_H the spectral measure of H. For a nonzero vector $\psi \in \mathcal{H}$, a measure μ_ψ on $\mathbb{R}$ is defined by

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

where $\mathcal{B}$ 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 3.12. *Assume that $\mathcal{H}$ is separable. Suppose that H has a cyclic vector ϕ. Then there exists a unitary operator U from $\mathcal{H}$ 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* 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 [43, Sect. VII.2] to the case of unbounded self-adjoint operators [31, Theorem 1.8]. To prove the second half of the lemma, we note that, by the cyclicity of ϕ for H, L.H.$\{H^n\phi | n \in \{0\} \cup \mathbb{N}\}$ is dense in $\mathcal{H}$. 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 L.H.$\{e^{itH}\phi | t \in \mathbb{R}\}$ is dense in $\mathcal{H}$. By the first half of the lemma, we have $Ue^{itH}\phi = e^{itX}$. Hence, L.H.$\{e^{itX} | t \in \mathbb{R}\}$ is dense in $L^2(\mathbb{R}, d\mu_\phi)$. □

Let $\psi \in \mathcal{H}$. 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 $\mu_\psi(B) = \int_B \rho_\psi(\lambda) d\lambda$, $B \in \mathcal{B}$.

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

Definition 3.13. We say that a self-adjoint operator H on $\mathcal{H}$ is in the class $S_0(\mathcal{H})$ 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

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

Let $\mathcal{H}$ be separable and $H \in S_0(\mathcal{H})$ 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 3.14. *The operator Y is a symmetric operator.*

Proof. By Lemma 3.12, $D(Y)$ 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 3.15. *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 3.16. *Assume that $\mathcal{H}$ is separable and that $H \in S_0(\mathcal{H})$. Then H has a strong time operator.*

Proof. We have $U^{-1}M_XU = H$. By Lemma 3.15, Y is a strong time operator of M_X. Hence, by an application of Proposition 3.4, $U^{-1}YU$ is a strong time operator of H. □

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

3.3. 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 $\mathcal{H}$ and $\mathcal{H}'$, respectively. If $\mathcal{H} = \mathcal{H}'$, 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 $\mathcal{H}_{\mathrm{ac}}(H)$ of H. For a linear operator A, we denote by $\mathrm{Ran}(A)$ the range of A.

Lemma 3.17. *Assume the following (A.1)–(A.3):*

(A.1) *The wave operators*

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

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

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

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

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

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

Proof. See textbooks of quantum scattering theory (e.g. [45,46]). □

Theorem 3.18. *Assume (A.1)–(A.3) in Lemma 3.17. 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 3.17 and an application of Proposition 3.4. □

Theorem 3.18 can be used to construct strong time operators of H' from those of H.

4. Time Operators of a Self-Adjoint Operator with Purely Discrete Spectrum

4.1. Case (I)

If $\sigma_{\mathrm{disc}}(H) \neq \emptyset$, then no strong time operator of H exists by Proposition 3.5-(3). But, even in that case, H may have time operators or weak time operators. We first recall basic results on this aspect.

Proposition 4.1 ([13,16]). *Suppose that $\sigma(H) = \sigma_{\mathrm{disc}}(H) = \{E_n\}_{n=1}^{\infty}$ ($E_n \neq E_m$ 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*

$$T\phi = i \sum_{n=1}^{\infty} \left(\sum_{m \neq n} \frac{(e_m, \phi)}{E_n - E_m} \right) e_n, \quad \phi \in \mathrm{D}(T) \tag{4.1}$$

with domain

$$\mathrm{D}(T) := \mathcal{F} := \mathrm{L.H.}\{e_n | n \in \mathbb{N}\}, \tag{4.2}$$

Then T is a symmetric operator and $[H, T] = -i\mathbb{1}$ holds on

$$\mathcal{E} := \mathrm{L.H.}\{e_n - e_m | n, m \in \mathbb{N}\}.$$

Furthermore, $\mathcal{E}$ is dense.

This proposition shows that T is a time operator of H with a dense CCR domain $\mathcal{E}$ and hence T is a weak time operator of H too with a weak-CCR domain $\mathcal{E}$. 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 2.6) (note that $\mathcal{E}$ contains no eigenvectors of H).

Example 4.2. (One-dimensional quantum harmonic oscillator) The Hamiltonian of a 1-dimensional quantum harmonic oscillator is given by

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

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_{osc} is self-adjoint, $\sigma(H_{\mathrm{osc}}) = \sigma_{\mathrm{disc}}(H_{\mathrm{osc}}) = \{\omega(n+\frac{1}{2})\}_{n=0}^{\infty}$ and each eigenvalue $\omega(n+\frac{1}{2})$ is simple. Since $\sum_{n=1}^{\infty} \frac{1}{(n+\frac{1}{2})^2} < \infty$, the assumption in Proposition 4.1 holds. Hence, H_{osc} has a time operator T_{osc} given by

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

One can show that T is bounded and $\sigma(\overline{T}) = [-\pi/\omega, \pi/\omega]$ (see [17, Example 4.2]).

Corollary 4.3. *Suppose that* $\sigma(H)\backslash\{0\} = \sigma_{\rm disc}(H) = \{E_n\}_{n=1}^\infty$*, 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*

$$T_{\rm d}\phi := i\sum_{n=1}^\infty \left(\sum_{m\neq n} \frac{(e_m,\phi)}{\frac{1}{E_n}-\frac{1}{E_m}} \right) e_n, \quad \phi \in {\rm D}(T_{\rm d}) := \mathcal{F} \tag{4.3}$$

is a time operator of H^{-1}*, where* $\mathcal{F}$ *is given by* (4.2)*, i.e.* $[H^{-1}, T_{\rm d}] = -i\mathbb{1}$ *on* $\mathcal{E}$*.*

Proof. We see that $\sigma(H^{-1}) = \sigma_{\rm disc}(H^{-1}) = \{1/E_n\}_{n=1}^\infty$ and $\sum_{n=1}^\infty \frac{1}{(1/E_n)^2} < \infty$. Hence, the corollary follows from Proposition 4.1. □

4.2. Case (II)

In Corollary 4.3, 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 4.1 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 $\mathcal{H}$ into the direct sum of appropriate mutually orthogonal closed subspaces [47].

Lemma 4.4. *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:*

$$A_k \cap A_l = \emptyset \text{ for } k \neq l,\ k, l = 1, \ldots, N;$$

$$A = \cup_{k=1}^N A_k;$$

$$\sum_{n=1}^\infty |a_{kn}|^p < \infty, \quad k = 1, \ldots, N.$$

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 $A' := A \backslash A_1$. 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 $A'' := A' \backslash A_2 = A \backslash (A_1 \cup A_2)$. 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 $\mathcal{K}$ is reduced by a closed subspace $\mathcal{D}$ of $\mathcal{K}$, then we denote by $S_{\mathcal{D}}$ the reduced part of S to $\mathcal{D}$, unless otherwise stated.

Lemma 4.5. *Let $\sigma(H) = \sigma_{\rm disc}(H) = \{E_n\}_{n=1}^\infty$, $E_1 < E_2 < \cdots < 0$, $\lim_{n\to\infty} E_n = 0$ and $0 \notin \sigma_{\rm p}(H)$. Then there exist mutually orthogonal closed subspaces $\mathcal{H}_j$ of $\mathcal{H}$ ($j = 1, \ldots, N$, $N \le \infty$) such that $\mathcal{H}$ is decomposed as $\mathcal{H} = \oplus_{j=1}^N \mathcal{H}_j$ ($N \le \infty$) and (1)–(3) below are satisfied.*

(1) *Each $\mathcal{H}_j$ reduces H and $\sigma(H_j)\backslash\{0\} = \sigma_{\rm disc}(H_j)) = \{F_{jk}\}_{k=1}^\infty$, where $H_j := H_{\mathcal{H}_j}$.*
(2) *Each eigenvalue F_{jk} ($1 \le j \le N, 1 \le k \le \infty$) is simple.*
(3) *$\sum_{k=1}^\infty F_{jk}^2 < \infty$ for each $1 \le j \le N$.*

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

$$\sup_{n\ge1} M_n = M \quad \text{and} \quad \limsup_{n\to\infty} M_n = m.$$

We consider two cases: (A) $m = \infty$ and (B) $m < \infty$.

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

$$\mathcal{G}_k = {\rm L.H.}\{e_j^k |\ M_j \ge k\}$$

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

$$\mathcal{H} = \oplus_{k=1}^\infty \overline{\mathcal{G}_k}. \tag{4.4}$$

Fix k and consider $\mathcal{G}_k$. Let $\mathcal{A} := \sigma_{\rm disc}(H_{\mathcal{G}_k}) = \{a_j | j \in \mathbb{N}\}$ ($= \{E_n | M_n \ge k\}$). Then each eigenvalue a_j is simple and $a_j \ne a_k$ for $j \ne k$, $\lim_{j\to\infty} a_j = 0$. Hence, we can apply Lemma 4.4 with $p = 2$ to conclude that there exist an $N_k \le \infty$ and subsets $\mathcal{A}_l := \{a_j^l \in \mathcal{A} | j \in \mathbb{N}, \sum_{j=1}^\infty |a_j^l|^2 < \infty\}$ of $\mathcal{A}$ such that $\mathcal{A} = \cup_{l=1}^{N_k} \mathcal{A}_l$ (a disjoint union). Hence, we can decompose $\overline{\mathcal{G}_k}$ as

$$\overline{\mathcal{G}_k} = \oplus_{l=1}^{N_k} \overline{\mathcal{G}_k^l}, \tag{4.5}$$

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

$$\mathcal{H} = \oplus_{k=1}^\infty \oplus_{l=1}^{N_k} \overline{\mathcal{G}_k^l} \tag{4.6}$$

and the lemma follows.

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

(a) $M = m = 1$. In this case, $\mathcal{H} = \overline{\mathcal{G}_1}$ and $\overline{\mathcal{G}_1}$ can be decomposed as (4.5). Then the lemma follows.

(b) $M \ge 2$ **and** $M = m$. In this case, for all $k = 1, \ldots, M$, $\mathcal{G}_k$ is infinite dimensional. Hence, in the same way as in the case $m = \infty$ we can see that $\mathcal{H} = \oplus_{k=1}^M \overline{\mathcal{G}_k}$ and $\overline{\mathcal{G}_k}$ can be decomposed as (4.5). 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 $\mathcal{B}_k = \text{L.H.}\{e_j^k | j < j_0, k \leq M_j\}$, $k = 1, \cdots, M$ and $\mathcal{C} := \text{L.H.}\{e_j^1 | j \geq j_0\}$. Then we can decompose $\mathcal{C}$ as $\overline{\mathcal{C}} = \oplus_{k=1}^M \overline{\mathcal{C}_k}$, where $\mathcal{C}_k = \text{L.H.}\{e_{j_k}^1 | j_k \geq j_0, j_k = j_0 + k - 1 + Mr, r \in \{0\} \cup \mathbb{N}\}$ $(k = 1, \ldots, M)$. Define $\mathcal{D}_k = \mathcal{B}_k \oplus \overline{\mathcal{C}_k}$, $k = 1, \cdots, M$. Then we have $\mathcal{H} = \oplus_{k=1}^M \mathcal{D}_k$. In the same way as in the case (A), we can decompose $\mathcal{D}_k$ like (4.5). 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 $j = 1, \ldots, m$, $\mathcal{G}_j$ is infinite dimensional. We have the orthogonal decomposition

$$\mathcal{H} = \left(\oplus_{j=1}^{m-1} \overline{\mathcal{G}_j}\right) \oplus \mathcal{K}, \tag{4.7}$$

where $\mathcal{K} = \left(\oplus_{j=1}^{m-1} \overline{\mathcal{G}_j}\right)^{\perp}$. The closed subspace $\mathcal{K}$ reduces H. Since $\mathcal{G}_m \subset \mathcal{K}$, it follows that $\sigma(H_{\mathcal{K}}) \backslash \{0\} = \sigma_{\text{disc}}(H_{\mathcal{K}})$ is an infinite set. Let $\sigma_{\text{disc}}(H_{\mathcal{K}}) = \{b_j\}_{j=1}^{\infty}$ 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 $\mathcal{K}$ as $\mathcal{K} = \oplus_{j=1}^{M-m+1} \mathcal{K}_j$, where $\mathcal{K}_j$ is an infinite dimensional closed subspace of $\mathcal{K}$. Hence,

$$\mathcal{H} = \left(\oplus_{j=1}^{m-1} \overline{\mathcal{G}_j}\right) \oplus \left(\oplus_{j=1}^{M-m+1} \mathcal{K}_j\right). \tag{4.8}$$

In the same way as in the case (A), we can decompose $\overline{\mathcal{G}_j}$ and $\mathcal{K}_j$ like (4.5). Thus, the lemma follows. □

Combining Corollary 4.3 and Lemma 4.5, we can prove the following lemma.

Theorem 4.6 (Time operator of H^{-1}). *Suppose that* $\sigma(H) \backslash \{0\} = \sigma_{\text{disc}}(H) = \{E_j\}_{j=1}^{\infty}$, $E_1 < E_2 < \cdots < 0$, $\lim_{j \to \infty} E_j = 0$, *and* $0 \notin \sigma_{\text{p}}(H)$. *Then there exists a time operator* T_{-1} *of* H^{-1} *with a dense CCR domain for* (H^{-1}, T_{-1}).

Proof. By Lemma 4.5, $\mathcal{H}$ can be decomposed as $\mathcal{H} = \oplus_{j=1}^N \mathcal{H}_j$ with $N \leq \infty$. By Proposition 4.1, a time operator S_j of H_j^{-1} exists:

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

on $\mathcal{E}_j := \text{L.H.}\{e_n^j - e_m^j, n, m \in \mathbb{N}\}$, 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 $\text{D}(S_j) = \text{L.H.}\{e_n^j | n \in \mathbb{N}\}$. Define T_{-1} by $T_{-1} := \oplus_{j=1}^N S_j$ with $\text{D}(T_{-1}) := \oplus_{j=1}^N \text{D}(S_j)$ (algebraic direct sum). Then T_{-1} is a time operator of H^{-1} with a CCR domain given by $\oplus_{j=1}^N \mathcal{E}_j$ (algebraic direct sum), which is dense in $\mathcal{H}$. □

4.3. Case (III)

We next consider an extension of Proposition 4.1 to the case where no restriction is imposed on the growth order of the discrete eigenvalues $\{E_n\}_{n=1}^{\infty}$ of H.

Lemma 4.7. *Suppose that* $\sigma(H) = \sigma_{\text{disc}}(H) = \{E_n\}_{n=1}^{\infty}$ *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 $\mathcal{H}_j$ of $\mathcal{H}$ ($j = 1, \ldots, N, N \leq \infty$) such that $\mathcal{H} = \oplus_{j=1}^N \mathcal{H}_j$ and (1)–(3) below are satisfied:*

(1) *Each $\mathcal{H}_j$ reduces H and $\sigma(H_{\mathcal{H}_j}) = \sigma_{\mathrm{disc}}(H_{\mathcal{H}_j}) = \{F_{jk}\}_{k=1}^\infty$.*
(2) *Each F_{jk} ($1 \leq j \leq N, k \in \mathbb{N}$) is simple.*
(3) $\displaystyle\sum_{k=1}^\infty \frac{1}{F_{jk}^2} < \infty$ *for each $1 \leq j \leq N$.*

Proof. Let $K = H^{-1}$. Then K is self-adjoint and $\sigma(K)\setminus\{0\} = \sigma_{\mathrm{disc}}(K) = \{1/E_n\}_{n=1}^\infty$, $1/E_1 > 1/E_2 > \cdots > 0$, $\lim_{j\to\infty} 1/E_j = 0$ and $0 \notin \sigma_{\mathrm{p}}(K)$. Hence, by applying Lemma 4.5 to the case where H and E_n there are replaced by $-K$ and $-1/E_n$, respectively, we see that $\mathcal{H}$ has an orthogonal decomposition $\mathcal{H} = \oplus_{j=1}^N \mathcal{H}_j$ ($N \leq \infty$) with closed subspaces $\mathcal{H}_j$ of $\mathcal{H}$ such that (1)–(3) above are satisfied. □

Theorem 4.8 (Time operator of H). *Let $\sigma(H) = \sigma_{\mathrm{disc}}(H) = \{E_n\}_{n=1}^\infty$, $E_1 < E_2 < \cdots$ 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 4.6. By Lemma 4.7, $\mathcal{H}$ can be decomposed as $\mathcal{H} = \oplus_{j=1}^N \mathcal{H}_j$ with $N \leq \infty$. By Proposition 4.1 a time operator T_j of $H_{\mathcal{H}_j}$ exists: $[H_{\mathcal{H}_j}, T_j] = -i\mathbb{1}$ on $\mathcal{E}_j = \mathrm{L.H.}\{e_n^j - e_m^j, n, m \in \mathbb{N}\}$, where $\{e_n^j\}_{n=1}^\infty$ denotes the eigenvectors of $H_{\mathcal{H}_j}$ 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 $\oplus_{j=1}^N \mathcal{E}_j$ (algebraic direct sum), which is dense in $\mathcal{H}$. □

Example 4.9 (d-dimensional quantum harmonic oscillator). Let $\omega_j > 0$ ($j = 1, \ldots, d$) be a constant and

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

acting in $L^2(\mathbb{R}^d)$ (see Example 4.2). Then the Hamiltonian of a d-dimensional quantum harmonic oscillator is given by

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

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

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

Hence, by Theorem 4.8, $H_{\mathrm{osc}}^{(d)}$ has a time operator with a dense CCR domain.

Example 4.10 (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 [48] is defined by the self-adjoint operator

$$H(\alpha, \beta) = A \otimes \left(-\frac{1}{2}\Delta + \frac{1}{2}x^2 \right) + J \otimes \left(xD + \frac{1}{2} \right) \tag{4.9}$$

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 [18] that $\sigma(H(\alpha, \beta)) = \sigma_{\text{disc}}(H(\alpha, \beta)) = \{\lambda_n\}_{n=1}^\infty$ and the multiplicity of each λ_n is not greater than 2 with $\lambda_n \to \infty$ $(n \to \infty)$. Hence, by Theorem 4.8, $H(\alpha, \beta)$ has a time operator with a dense CCR domain.

Example 4.11 (Rabi model). Let $\mathbb{Z}_+ := \{0\} \cup \mathbb{N}$ be the set of non-negative 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 $\mathcal{F}_\text{b}(\mathbb{C})$ over $\mathbb{C}$ (e.g. [43, p. 53, Example 2] and [49, Sect. X.7]): $\ell^2(\mathbb{Z}_+) = \mathcal{F}_\text{b}(\mathbb{C})$. We denote by a the annihilation operator on $\mathcal{F}_\text{b}(\mathbb{C})$:

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

We have $(a^*\psi)_0 = 0$, $(a^*\psi)_n = \sqrt{n}\psi_{n-1}$, $n \geq 1$ for all $\psi \in \mathrm{D}(a^*)$. 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

$$H_{\text{Rabi}} := \mu\sigma_z \otimes \mathbb{1} + \omega \mathbb{1} \otimes a^*a + g\sigma_x \otimes (a + a^*) \tag{4.10}$$

on $\mathbb{C}^2 \otimes \mathcal{F}_\text{b}(\mathbb{C})$, where $\mu > 0$, $\omega > 0$ and $g \in \mathbb{R}$ are constants. The model whose Hamiltonian is given by H_{Rabi} is called the Rabi model [19,21,22]. 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

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

where $H_\pm := \omega a^* a \pm g(a + a^*)$ and we have used the natural identification $\mathbb{C}^2 \otimes \mathcal{F}_{\rm b}(\mathbb{C}) = \mathcal{F}_{\rm b}(\mathbb{C}) \oplus \mathcal{F}_{\rm b}(\mathbb{C})$. 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 [19,20] for studies on spectral properties of $H_{\rm Rabi}$). Hence, we can apply Theorem 4.8 to conclude that $H_{\rm Rabi}$ has a time operator with a dense CCR domain.

5. Ultra-Weak Time Operators

5.1. Ultra-Weak Time Operators of a Self-Adjoint Operator

In this subsection, we consider the case where a self-adjoint operator H obeys the assumption of Theorem 4.6 and ask if H has a time operator. We first give a formal heuristic argument. By Theorem 4.6, 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 4.1 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 3.9 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 4.6. 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

$$\mathfrak{t}_j[\phi, \psi] := -\frac{1}{2}\left\{(S_j\phi, H_j^{-2}\psi) + (H_j^{-2}\phi, S_j\psi)\right\}, \quad \phi, \psi \in \mathrm{D}(S_j). \tag{5.1}$$

Lemma 5.1. *Let*

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

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

$$\mathfrak{t}_j[H_j\phi, \psi] - \mathfrak{t}_j[\phi, H_j\psi] = -i(\phi, \psi). \tag{5.2}$$

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

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

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

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

Thus, (5.2) follows. □

Lemma 5.1 shows that $\mathfrak{t}_j$ is an ultra-weak time operator of H_j with $H_j^{-1}\mathcal{E}_j$ being an ultra-weak CCR domain.

We introduce

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

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

Theorem 5.2. *Under the same assumption as in Theorem 4.6, there exists an ultra-weak time operator* $\mathfrak{t}_{\mathrm{p}}$ *of* H *with* $\widetilde{\mathcal{E}}$ *being an ultra-weak CCR domain.*

Proof. Let T_{-1} be as in Theorem 4.6 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 5.1 that, for all $\psi, \phi \in \widetilde{\mathcal{E}}$, $H\psi, H\phi \in \mathcal{E} \subset \mathrm{D}(T_{-1})$ 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 $\widetilde{\mathcal{E}}$ 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 5.3 (Class $S_1(\mathcal{H})$). A self-adjoint operator H on $\mathcal{H}$ is said to be in the class $S_1(\mathcal{H})$ 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 $\mathcal{H}_{\mathrm{ac}}(H)$.

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

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

By (H.3), we can apply Theorem 5.2 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 $\mathcal{E}_{\mathrm{p}}$ such that

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

We denote by $\mathcal{D}_{\mathrm{p}}$ the subspace $\mathrm{D}(T_{-1})$ in the proof of Theorem 5.2. Hence, $\mathfrak{t}_{\mathrm{p}} : \mathcal{D}_{\mathrm{p}} \times \mathcal{D}_{\mathrm{p}} \to \mathbb{C}$ with $\mathcal{E}_{\mathrm{p}} \subset \mathrm{D}(H_{\mathrm{p}}) \cap \mathcal{D}_{\mathrm{p}}$ and $H_{\mathrm{p}}\mathcal{E}_{\mathrm{p}} \subset \mathcal{D}_{\mathrm{p}}$. By (H.4), there exists a dense CCR domain $\mathcal{D}_{\mathrm{ac}}$ for $(H_{\mathrm{ac}}, T_{\mathrm{ac}})$. Let $\widetilde{\mathcal{E}}_{\mathrm{p}} := H_{\mathrm{p}}^{-1}\mathcal{E}_{\mathrm{p}}$ and

$$\mathcal{D}_H := \mathcal{D}_{\mathrm{ac}} \oplus \widetilde{\mathcal{E}}_{\mathrm{p}}, \tag{5.3}$$

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

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

$$\begin{aligned}\mathfrak{t}_H[\phi_1 \oplus \phi_2, \psi_1 \oplus \psi_2] =& (\phi_1, T_{\mathrm{ac}}\psi_1) + \mathfrak{t}_{\mathrm{p}}[\phi_2, \psi_2],\\ & \phi_1 \in \mathcal{H}_{\mathrm{ac}}(H), \psi_1 \in \mathrm{D}(T_{\mathrm{ac}}), \phi_2, \psi_2 \in \mathcal{D}_{\mathrm{p}}.\end{aligned} \tag{5.4}$$

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

Theorem 5.4 (Abstract ultra-weak time operator 1). *Let $H \in S_1(\mathcal{H})$. Then the sesquilinear form $\mathfrak{t}_H$ defined by (5.4) is an ultra-weak time operator of H with $\mathcal{D}_H$ being an ultra-weak CCR domain.*

Proof. Let $\mathfrak{t}_{\mathrm{ac}} : \mathcal{H}_{\mathrm{ac}}(H) \times \mathrm{D}(T_{\mathrm{ac}}) \to \mathbb{C}$ by

$$\mathfrak{t}_{\mathrm{ac}}[\phi, \psi] := (\phi, T_{\mathrm{ac}}\psi),\ \phi \in \mathcal{H}_{\mathrm{ac}}(H), \psi \in \mathrm{D}(T_{\mathrm{ac}}).$$

Then, by Remark 2.9-(2), $\mathfrak{t}_{\mathrm{ac}}$ is an ultra-weak time operator of H_{ac} with $\mathcal{D}_{\mathrm{ac}}$ being an ultra-weak CCR domain. Then, in the same way as in the proof of Theorem 5.2, one can show that $\mathfrak{t}_H$ is an ultra-weak time operator of H with $\mathcal{D}_H$ being an ultra-weak CCR domain. □

5.2. Ultra-Weak Time Operators of $f(H)$

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 $f(H_{\mathrm{ac}})$ is already constructed in Proposition 3.9. Hence, we need only to construct an ultra-weak time operator of $f(H_{\mathrm{p}})$. A set of conditions for that is as follows.

Assumption 5.5. Let $H \in S_1(\mathcal{H})$.

(1) The function $f : \mathbb{R} \to \mathbb{R}$ satisfies the same assumption as in Proposition 3.9.
(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 5.5 holds. Then $f(H)$ is self-adjoint and reduced by $\mathcal{H}_{\rm ac}(H)$ and $\mathcal{H}_{\rm p}(H)$ (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 $\mathcal{H}_{\rm ac}(H)$ and $\mathcal{H}_{\rm p}(H)$ 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

$$\sigma(f(H)) = \sigma(f(H_{\rm ac})) \cup \sigma(f(H_{\rm p})) = \overline{f([0,\infty))} \cup \overline{\{f(E_j)\}_{j=1}^{\infty}}. \tag{5.5}$$

Corollary 5.6 (Abstract ultra-weak time operator 2). *Under Assumption 5.5, 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 3.9, where $D := \{g(H_{\rm ac}) \mathrm{D}(T_{\rm ac}) | g \in C_0^\infty(\mathbb{R}\backslash L \cup K)\}$. 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 5.1, we can show that there is an ultra-weak time operator $\mathfrak{t}_{\rm p}^{\tilde{f}} : \mathcal{D}_{\rm p}^f \times \mathcal{D}_{\rm p}^f \to \mathbb{C}$ of $\tilde{f}(H_{\rm p})$, where $\mathcal{D}_{\rm p}^f$ is a dense subspace in $\mathcal{H}_{\rm p}(H)$. We define a sesquilinear form $\mathfrak{t}_H^f : (\mathcal{H}_{\rm ac}(H) \oplus \mathcal{D}_{\rm p}^f) \times (\mathrm{D}(T_{\rm ac}^f) \oplus \mathcal{D}_{\rm p}^f) \to \mathbb{C}$ by

$$\mathfrak{t}_H^f[\phi_1 \oplus \phi_2, \psi_1 \oplus \psi_2] = (\phi_1, T_{\rm ac}^f \psi_1) + \mathfrak{t}_{\rm p}^{\tilde{f}}[\phi_2, \psi_2] \tag{5.6}$$

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

6. Applications to Schrödinger Operators

6.1. Ultra-Weak Time Operators of Schrödinger Operators

In this subsection, we apply Theorem 5.4 to the Schrödinger operator H_V given by (2.8) 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

$$V(x) = \frac{W(x)}{(|x|^2+1)^{\frac{1}{2}+\varepsilon}}, \tag{6.1}$$

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* ([46, p. 439] or [50, p. 169]). It is easily shown that V is relatively compact with respect to the free Hamiltonian H_0 given by (2.9). Hence, by a general fact [50, p. 113, Corollary 2], H_V is self-adjoint with $\mathrm{D}(H_V) = \mathrm{D}(H_0)$ and

$$\sigma_{\mathrm{ess}}(H_V) = \sigma_{\mathrm{ess}}(H_0) = [0,\infty), \tag{6.2}$$

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

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

Proposition 6.1 (Absence of $\sigma_{\mathrm{sc}}(H)$, 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:* $\mathrm{Ran}(\Omega_\pm) = \mathcal{H}_{\mathrm{ac}}(H_V)$. *In particular* $\sigma_{\mathrm{ac}}(H_V) = [0,\infty)$.

Proof. See [50, 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 6.2. There are constants $R_0, a > 0$ and $\delta > 0$ such that

$$V(x) \le -\frac{a}{|x|^{2-\delta}} \quad \text{for } |x| > R_0. \tag{6.3}$$

Lemma 6.3 (Infinite number of negative eigenvalues). *Let V be an Agmon potential. Then, under Assumption 6.2, $\sigma_{\mathrm{disc}}(H_V) \subset (-\infty, 0)$ 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 $n \in \mathbb{N}$ [50, 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 (6.2) and the min-max principle imply the desired results. □

Assumption 6.4. The potential V is spherically symmetric, $V = V(|x|)$, and

$$\int_a^\infty |V(r)|dr < \infty \tag{6.4}$$

for some $a > 0$.

Lemma 6.5 (Absence of strictly positive eigenvalues). *Let V be an Agmon potential. Then, under Assumption 6.4, 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 [50, Theorem XIII.56] to derive the desired result. □

Theorem 6.6. *Let V be an Agmon potential such that $0 \notin \sigma_{\mathrm{p}}(H_V)$. Suppose that Assumptions 6.2 and 6.4 hold. Then H_V has an ultra-weak time operator with a dense ultra-weak CCR domain.*

Proof. By Proposition 6.1, $\sigma_{\mathrm{sc}}(H_V) = \emptyset$ and the wave operators $\Omega_\pm$ exist and are complete. Hence, by Theorem 3.18,

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

are strong time operators of $(H_V)_{\mathrm{ac}}$, where $\tau_j := \widetilde{T}_{\mathrm{AB},j}$ or $T'_{\mathrm{AB},j}$ denotes the Aharonov–Bohm time operators in Example 3.10. Under Assumptions 6.2 and 6.4, 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 5.4, we obtain the desired result. □

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

Proposition 6.7 (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 $S^{d-1} := \{w \in \mathbb{R}^d \,|\, |w| = 1\}$, 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) $$\lim_{r\to\infty} \frac{r^{-1} + r \sup_{w \in S^{d-1}} |V_2(rw)|}{h(r)} = 0.$$
 (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 $f \in D(H_V)$,*

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

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

Proof. This is due to [51, Theorem 2.4] and [52]. Also see [53]. □

A key fact to prove Proposition 6.7 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 [52].

Example 6.8. 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 6.7 (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 6.7, H_V has no zero eigenvalue. In particular, the hydrogen Schrödinger operator

$$H_{\mathrm{hyd}} := H_0 - \frac{\gamma}{|x|} \tag{6.5}$$

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

Example 6.9. 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 (6.3) and (6.4). Moreover, it is easy to see that V satisfies (1) and (2) in Proposition 6.7 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 6.7, $0 \notin \sigma_{\mathrm{p}}(H_V)$. Thus, by Theorem 6.6, H_V has an ultra-weak time operator with a dense ultra-weak CCR domain.

Example 6.10 (Hydrogen atom). It is known that the hydrogen Schrödinger operator H_{hyd} given by (6.5) 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 cannot apply Theorem 6.6 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

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

The fact that $0 \notin \sigma_{\mathrm{p}}(H_{\mathrm{hyd}})$ follows from Example 6.8 and Proposition 6.7. It is shown that the modified wave operators $\mathrm{s}\text{-}\lim_{t\to\pm\infty} e^{itH_{\mathrm{hyd}}} J e^{-itH_0}$ with some unitary operator J exist and are complete [46, Theorems XI. 71 and XI.72]. These facts imply that $H_{\mathrm{hyd}} \in S_1(L^2(\mathbb{R}^3))$. Thus, by Theorem 5.4, H_{hyd} has an ultra-weak time operator with a dense ultra-weak CCR domain.

6.2. Ultra-Weak Time Operators of $f(H_V)$

In this subsection, we assume that $H_V \in S_1(L^2(\mathbb{R}^d))$ (see Definition 5.3) 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 5.5 to hold.

Lemma 6.11. *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 $f(0) \notin \sigma_{\mathrm{p}}(H_V)$.*

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 $\psi = (\psi_{\mathrm{ac}}, \psi_{\mathrm{p}}) \in \mathcal{H}_{\mathrm{ac}}(H_V) \oplus \mathcal{H}_{\mathrm{p}}(H_V)$. We denote by ρ the Radon–Nykodým derivative of the absolutely continuous measure $\|E(\cdot)\psi_{\mathrm{ac}}\|^2$ with respect to the Lebesgue measure on $\mathbb{R}$. Then we have

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

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

Theorem 6.12. *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 3.9.*
(2) *The function f is continuous at $x = 0$.*
(3) *$f(\sigma_{\mathrm{disc}}(H_V))$ is an infinite set such that the multiplicity of each point in $f(\sigma_{\mathrm{disc}}(H_V))$ 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 6.11, property (4) in Assumption 5.5 is satisfied. Hence, by Corollary 5.6, the desired result is derived. □

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

Example 6.13. ($f(H_V) = e^{-\beta H_V}$) Let $f(x) = e^{-\beta x}$, $\beta \in \mathbb{R}\backslash\{0\}$. Then it is easy to see that the function f satisfies the assumption in Theorem 6.12. 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 6.14. ($f(H_V) = \sum_{j=0}^N a_j H_V^j$) 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 6.12. 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 6.15. ($f(H_V) = \sin(2\pi\beta H_V)$) Let $f(x) = \sin(2\pi\beta x)$, $\beta \in \mathbb{R}\backslash\{0\}$. 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 6.12 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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