Lieb-Thirring bound and generalized weak time operators associated with Schrödinger operators

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Abstract

This is a short version of [Hir15]. A weak time operator T associated with a given self-adjoint operator H is a symmetric operator such that $(H\phi, T\psi) - (T\phi, H\psi) = -i(\phi, \psi)$ for $\phi, \psi \in D$ with some domain D. In this paper we generalize weak time operators as a densely defined symmetric quadratic form, and a generalized weak time operator T_H associated with a Schrödinger operator of the form $H = -\Delta/2 + V$ on $\mathscr{H} = L^2(\mathbb{R}^d)$ is constructed. It is assumed that the quadratic moment of the negative eigenvalues $\{E_j\}_{j=1}^\infty$ of H is finite, i.e., $\sum_{j=1}^\infty E_j^2 < \infty$. This is ensured by the Lieb-Thirring inequality. Then we can construct $T_H(\cdot, \cdot) : \mathscr{H} \times \mathscr{H} \to \mathbb{C}$ such that

$$T_H(H\phi, \psi) - T_H(\phi, H\psi) = -i(\phi, \psi)$$

for all $\phi, \psi \in \mathscr{D}$ with some domain $\mathscr{D}$.

1 Introduction

1.1 Preliminaries

Canonical commutation relations (CCR) are a fundamental tool in quantum physics. In one-dimensional quantum mechanics the momentum operator $P = -id/dx$ and the position operator $Q = x$ satisfy CCR:

$$[P, Q] = -i\mathbb{1} \tag{1.1}$$

on some dense subspace. FROM CCR the position-momentum uncertainty relation (so-called Robertson inequality) is derived. On the other hand the energy of a quantum system can be realized as a Hamiltonian which is a self-adjoint operator on a Hilbert

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space, whereas time t is treated as a parameter, and not as an operator. It is however there is a physical folklore such that the pair of position-momentum corresponds to that of time-energy.

From a mathematical point of view we are interested in finding an operator T associated with a given self-adjoint operator H such that

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

on $\mathrm{D}(HT) \cap \mathrm{D}(TH)$, and we call T as " time operator". As far as we know, a firm mathematical investigation of time operators (so-called strong time operators) are initiated by [Miy01], and investigated and generalized in [Ara05, Ara07]. When pair (H, T) satisfies (1.2), it is known that either H or T is unbounded. Hence it may occur that $\mathrm{D}(HT) \cap \mathrm{D}(TH)$ is not dense or empty. The so-called weak CCR is introduced in [Ara09], where commutation relations (1.2) are replaced by a bilinear form:

$$(H\phi, T\psi) - (T\phi, H\psi) = -i(\phi, \psi). \tag{1.3}$$

A weak time operator T associated with H is a symmetric operator satisfying (1.3).

In this paper we generalize a weak time operator to a symmetric quadratic form (Definition 1.1), which we call a generalized weak time operator (GWTO), and are concerned with a weak time operator associated with a Schrödinger operator

$$H_V = -\frac{1}{2}\Delta + V \tag{1.4}$$

in Hilbert space $L^2(\mathbb{R}^d)$. Here Δ denotes the d-dimensional Laplacian and $V : \mathbb{R}^d \to \mathbb{R}$ is the multiplication operator describing an external potential. $V(x) = -1/|x|$ is a typical example.

Definition 1.1 (Generalized weak time operator and CCR domain) A densely defined symmetric quadratic form $T(\cdot, \cdot) : \mathscr{H} \times \mathscr{H} \to \mathbb{C}$ is a weak time operator associated with a self-adjoint operator H if and only if

$$T(H\psi, \phi) - T(\psi, H\phi) = -i(\psi, \phi) \tag{1.5}$$

for all $\psi, \phi \in \mathscr{D}$ with some domain $\mathscr{D}$. $\mathscr{D}$ is called a CCR domain for (H, T)

Remark 1.2 Note that $\mathscr{D}$ in Definition 1.1 is not necessarily dense.

While we can also define the strong time operator associated with H. To define a strong time operator we introduce weak Weyl relations. We call that the pair of self-adjoint operators (A, B) satisfies the Weyl relation if and only if

$$e^{-isA}e^{-itB} = e^{ist}e^{-itB}e^{-isA} \tag{1.6}$$

holds for all $s, t \in \mathbb{R}$. A Weyl relation implies CCR, and pair (P, Q) satisfies the Weyl relation. Conversely it is known as the von Neumann uniqueness theorem that if pair (A, B) satisfies Weyl relation (1.6) and there is no invariant domain with respect to e^{-isA} and e^{-itB}, then $A \cong P$ and $B \cong Q$. Here $\cong$ describes a unitary equivalence. When H is bounded from below, this theorem tells us that there exists no symmetric operator T such that pair (H, T) satisfies the Weyl relation, since $H \ncong P$. Thus instead of Weyl relation the so-called weak Weyl relation is introduced to define the strong time operator.

Definition 1.3 (Weak Weyl relation) The pair (A, B) satisfies weak Weyl relation (WWR) if and only if A is self-adjoint and B is symmetric, $e^{-itA}\mathrm{D}(B) \subset \mathrm{D}(B)$ and $Be^{-itA}\psi = e^{-itA}(B + t)\psi$ hold for all $\psi \in \mathrm{D}(B)$ and all $t \in \mathbb{R}$.

It is clear that the Weyl relation implies WWR, and WWR does CCR.

Definition 1.4 (Strong time operator) A symmetric operator T is a strong time operator associated with a self-adjoint operator H if and only if the pair (H, T) satisfies WWR.

When T is a strong time operator, T defines a weak time operator $\hat{T} : \mathscr{H} \times \mathscr{H} \to \mathbb{C}$ by $\hat{T}(\phi, \psi) = (\phi, T\psi)$ for $\phi, \psi \in \mathrm{D}(T)$.

Strong time operators (resp. weak time operator) associated with an abstract self-adjoint operator with purely absolutely continuous spectrum (resp. purely discrete spectrum) are studied in [Ara05, Ara07, AM08, AM09, HKM09, Miy01] (resp. [Gal02, GCB04, Ara09]). Representations of CCR are also studied in [Sch83a, Sch83b, Dor84]. The spectrum of Schrödinger operator H_V considered in this paper is of the form $\{E_j\}_{j=1}^{N} \cup [0, \infty)$, and under conditions:

$$N = \infty \quad \text{and} \quad \sum_{j=1}^{\infty} E_j^2 < \infty, \tag{1.7}$$

we construct a weak time operator associated with H_V. Here (1.7) is ensured by the Lieb-Thirring inequality

$$\sum_{j=1}^{\infty} E_j^2 \leq a \int_{\mathbb{R}^d} |V_-(x)|^{2+\frac{d}{2}} dx \tag{1.8}$$

with some constant a, where V_- is the negative part of V.

1.2 Strong time operators

The proposition on strong time operators below is well known.

Proposition 1.5 *Suppose that a strong time operator T associated with a self-adjoint operator H exits. Then assertion (1)-(3) below follow.*

(1) *The closure $\bar{T}$ is also a strong time operator.*

(2) *T has no self-adjoint extension.*

(3) *$\sigma(H)$ must be purely absolutely continuous spectrum, i.e., $\sigma(H) = \sigma_{\rm ac}(H)$.*

Proof: See [Ara05]. **qed**

By this proposition we may assume that the strong time operator is a closed symmetric operator in what follows.

Assume that (H, T) satisfies WWR. We are interested in constructing a strong time operator associated with $f(H)$, where $f : \mathbb{R} \to \mathbb{R}$. Actually this is established in the proposition below.

Proposition 1.6 *Let T_H be a strong time operator associated with a self-adjoint operator H. Let $f \in C^2(\mathbb{R} \setminus K)$ and $L = \{\lambda \in \mathbb{R} \setminus K; f'(\lambda) = 0\}$, where K is a closed subset of $\mathbb{R}$, and both of the Lebesgue measures of K and L are zero. Let $D = \{\rho(H){\rm D}(T); \rho \in C_0^\infty(\mathbb{R} \setminus L \cup K)\}$. Then*

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

is a strong time operator associated with $f(H)$.

Proof: See [HKM09, Theorem 1.9]. **qed**

We give some examples. Let $P_j = -id/dx_j$ and Q_j be the multiplication by x_j for $j = 1, ..., d$ in $L^2(\mathbb{R}^d)$. A strong time operator associated with P_j is Q_j for $j = 1, ..., d$. Proposition 1.6 can be applied to construct a strong time operator associated with $f(P_1, ..., P_d)$. An important example includes Aharonov-Bohm operator $T_{\rm AB}$ [AB61], which is a strong time operator associated with $\frac{1}{2}\sum_{j=1}^d P_j^2$ and defined by

$$T_{\rm AB} = \frac{1}{2}\sum_{j=1}^d \overline{(Q_j P_j^{-1} + P_j^{-1} Q_j)\lceil_{D_j}}, \tag{1.9}$$

with $D_j = \{\rho(P_j^2){\rm D}(Q_j); \rho \in C_0^\infty(\mathbb{R}^d \setminus \{0\}\}$.

1.3 Canonical commutation relations

We review a weak time operator associated with a self-adjoint operator H such that $\sigma(H) = \sigma_{\rm disc}(H) = \{E_j\}_{j=1}^\infty$, where $E_1 < E_2 < \cdots$. Note that $E_n \ni E_m$ if $n \ni m$. In this case there exists no strong time operator by Proposition 1.5.

Assumption 1.7 *Suppose that* $\sigma(H) = \sigma_{\rm disc}(H) = \{E_j\}_{j=1}^\infty$, $E_1 < E_2 < \cdots$, *and* $\displaystyle\sum_{j=J}^\infty \frac{1}{E_j^2} < \infty$ *for some* $J \geq 1$.

In [Ara09] a symmetric operator T such that $[H,T] = -i\mathbb{1}$ is defined for H satisfying Assumption 1.7. Let $He_{n\alpha} = E_n e_{n\alpha}$, $\alpha = 1, ..., M_n$, and $(e_{n\alpha}, e_{m\beta}) = \delta_{nm}\delta_{\alpha\beta}$, where M_n denotes the multiplicity of E_n. Let

$$\bar{e}_n = \frac{1}{\sqrt{M_n}} \sum_{\alpha=1}^{M_n} e_{n\alpha}. \tag{1.10}$$

Note that $(\bar{e}_n, \bar{e}_m) = \delta_{nm}$. Set

$$\mathscr{F} = \text{span}\ \{\bar{e}_n; n \in \mathbb{N}\}. \tag{1.11}$$

Definition 1.8 Suppose Assumption 1.7. Then we define T by

$$T\phi = i\sum_{n=1}^\infty \left(\sum_{m \neq n} \frac{(\bar{e}_m, \phi)}{E_n - E_m} \right) \bar{e}_n \tag{1.12}$$

with $\mathrm{D}(T) =$ span $\{\psi = \psi_1 + \psi_2; \psi_1 \in \mathscr{F}, \psi_2 \in \mathscr{F}^\perp\}$.

By the definition of T above we have $Tf = 0$ for $f \in \mathscr{F}^\perp$. We set

$$\mathscr{E} = \text{ span }\{\bar{e}_n - \bar{e}_m; n, m \in \mathbb{N}\}. \tag{1.13}$$

Proposition 1.9 *Suppose Assumption 1.7. Let* T *be in (1.12). Then* $[H,T] = -i\mathbb{1}$ *holds on* $\mathscr{E}$.

Proof: See [Ara09]. **qed**

We give remarks. It is not necessarily that $\mathscr{E}$ is dense.

2 Generalized weak time operators

2.1 Assumptions

By applying results introduced in the previous section we construct generalized weak time operators associated with Schrödinger operators. Let

$$H_0 = -\frac{1}{2}\Delta \tag{2.1}$$

and set

$$H_V = H_0 + V. \tag{2.2}$$

Let $\mathscr{H} = \mathscr{H}_{\rm ac} \oplus \mathscr{H}_{\rm sing}$ be the decomposition of $\mathscr{H}$ into the absolutely continuous part and singular part of H. We set $\mathscr{H}_{\rm sing} = \mathscr{H}_{\rm sc} \oplus \mathscr{H}_{\rm p}$, where $\mathscr{H}_{\rm p}$ denotes the closure of the span eigenvectors of H_V. Let $H_{\rm ac} = H_V\lceil_{\mathscr{H}_{\rm ac}}$, $H_{\rm sc} = H_V\lceil_{\mathscr{H}_{\rm sc}}$, and $H_{\rm p} = H_V\lceil_{\mathscr{H}_{\rm p}}$. Then $H_V = H_{\rm ac} \oplus H_{\rm p} \oplus H_{\rm sc}$. Conditions we assume on H_V are as follows:

Assumption 2.1

(1) $\sigma_{\rm sc}(H_V) = \emptyset$, i.e., $H_V = H_{\rm ac} \oplus H_{\rm p}$.

(2) $\sigma_{\rm ac}(H_V) = [0, \infty)$, and there exists a strong time operator $T_{\rm ac}$ associated with $H_{\rm ac}$ in $\mathscr{H}_{\rm ac}$.

(3) $\sigma(H_{\rm p})(= \overline{\sigma_{\rm p}(H_V)}) = \{0\} \cup \{E_j\}_{j=1}^N$, where $N = \infty$, $E_1 < E_2 < \cdots < 0$, $\{E_j\}_{j=1}^\infty = \sigma_{\rm disc}(H_V)$, and

$$\sum_{j=1}^\infty E_j^2 < \infty.$$

2.2 Discrete spectrum

In Assumption 2.1 (3), $0 \in \sigma(H_{\rm p})$ is possibly an eigenvalue of $H_{\rm p}$. When 0 is an eigenvalue of $H_{\rm p}$ we denote the set of vectors e_0 such that $H_{\rm p} e_0 = 0$ by $\mathscr{H}_0$. Let $H_{\rm p} e_{n\alpha} = E_n e_{n\alpha}$, $\alpha = 1, ..., M_n$, and $(e_{n\alpha}, e_{m\beta}) = \delta_{nm}\delta_{\alpha\beta}$. Subspaces $\mathscr{F}$ and $\mathscr{E}$ of $\mathscr{H}_{\rm p}$ are defined in the same way as (1.11) and (1.13), respectively. In particular $\mathscr{H}_0 \subset \mathscr{F}^\perp$. Let $\mathscr{H}_{\rm p} = \mathscr{H}_- \oplus \mathscr{H}_0$ (possibly $\mathscr{H}_0 = \emptyset$).

Lemma 2.2 *Suppose (3) of Assumption 2.1. Then*

$$T_{\rm d}\phi = i\sum_{n=1}^\infty \left(\sum_{m\neq n} \frac{(\bar{e}_m, \phi)}{\frac{1}{E_n} - \frac{1}{E_m}} \right) \bar{e}_n \tag{2.3}$$

with

$$\mathrm{D}(T_{\rm d}) = \mathrm{span}\, \{\psi = \psi_1 + \psi_2; \psi_1 \in \mathscr{F}, \psi_2 \in \mathscr{F}^\perp\} \tag{2.4}$$

is a generalized weak time operator associated with $(H_{\rm p}\lceil_{\mathscr{H}_-})^{-1}$.

Proof: We see that $\sigma(H_{\rm p}\lceil_{\mathscr{H}_-}^{-1}) = \{1/E_j\}_{j=1}^\infty$. Then the lemma follows from Proposition 1.9. **qed**

We define the symmetric quadratic form $T_{\rm p} : \mathrm{D}(T_{\rm d}) \times \mathrm{D}(T_{\rm d}) \to \mathbb{C}$ on $\mathscr{H}_{\rm p}$ by

$$T_{\rm p}(\phi, \psi) = \begin{cases} -\dfrac{1}{2}\left((T_{\rm d}\phi, H_{\rm p}^{-2}\psi) + (H_{\rm p}^{-2}\phi, T_{\rm d}\psi) \right), & \phi, \psi \in \mathscr{F}, \\ 0, \quad \text{otherwise.} \end{cases} \tag{2.5}$$

Note that $\mathscr{F} \cap \mathscr{H}_0 = \emptyset$, $\mathscr{F} \subset \mathrm{D}(H_{\rm p}^{-k})$ for all $k \geq 0$.

Remark 2.3 We formally write $T_{\rm p}(\phi,\psi)=(\phi,T_{\rm p}\psi)$ and

$$T_{\rm p}=-\frac{1}{2}(T_{\rm d}H_{\rm p}^{-2}+H_{\rm p}^{-2}T_{\rm d}). \tag{2.6}$$

Notice that however it is not clear whether $D(H_{\rm p}^{-2})\supset T_{\rm d}D(T_{\rm d})$ or not. Hence we can not define $T_{\rm p}$ as a nontrivial symmetric operator.

We set $H_{\rm p}^{-1}\mathscr{E}={\rm span}\,\{\frac{1}{E_n}\bar{e}_n-\frac{1}{E_m}\bar{e}_m; n,m\in\mathbb{N}\}$. Note that $H_{\rm p}^{-k}\mathscr{E}\subset\mathscr{F}$ for $k\in\mathbb{Z}$.

Lemma 2.4 *Let* $\phi,\psi\in H_{\rm p}^{-1}\mathscr{E}$. *Then* $T_{\rm p}(H_{\rm p}\phi,\psi)-T_{\rm p}(\phi,H_{\rm p}\psi)=-i(\phi,\psi)$ *follows. I.e.,* $T_{\rm p}$ *is a generalized weak time operator associated with* $H_{\rm p}$ *with CCR domain* $H_{\rm p}^{-1}\mathscr{E}$.

Proof: Let $T'=-2T_{\rm p}$. Let $\phi'=H_{\rm p}^{-1}\phi,\psi'=H_{\rm p}^{-1}\psi\in H_{\rm p}^{-1}\mathscr{E}$. We see that

$$T'(H_{\rm p}\phi',\psi')-T'(\phi',H_{\rm p}\psi')=T'(\phi,H_{\rm p}^{-1}\psi)-T'(H_{\rm p}^{-1}\phi,\psi).$$

By the definition of T' we have

$$\begin{aligned}&T'(H_{\rm p}\phi',\psi')-T'(\phi',H_{\rm p}\psi')\\&=(T_{\rm d}\phi,H_{\rm p}^{-3}\psi)+(H_{\rm p}^{-2}\phi,T_{\rm d}H_{\rm p}^{-1}\psi)-(H_{\rm p}^{-3}\phi,T_{\rm d}\psi)-(T_{\rm d}H_{\rm p}^{-1}\phi,H_{\rm p}^{-2}\psi)\\&=(H_{\rm p}^{-1}T_{\rm d}\phi,H_{\rm p}^{-2}\psi)-(H_{\rm p}^{-2}\phi,H_{\rm p}^{-1}T_{\rm d}\psi)+(H_{\rm p}^{-2}\phi,T_{\rm d}H_{\rm p}^{-1}\psi)-(T_{\rm d}H_{\rm p}^{-1}\phi,H_{\rm p}^{-2}\psi).\end{aligned}$$

Then the first two terms of the most right-hand side above can be computed by using $[H_{\rm p}^{-1},T_{\rm d}]=-i\mathbb{1}$ on $\mathscr{E}$ as

$$\begin{aligned}&(H_{\rm p}^{-1}T_{\rm d}\phi,H_{\rm p}^{-2}\psi)-(H_{\rm p}^{-2}\phi,H_{\rm p}^{-1}T_{\rm d}\psi)\\&=2i(H_{\rm p}^{-1}\phi,H_{\rm p}^{-1}\psi)+(T_{\rm d}H_{\rm p}^{-1}\phi,H_{\rm p}^{-2}\psi)-(H_{\rm p}^{-2}\phi,T_{\rm d}H_{\rm p}^{-1}\psi).\end{aligned}$$

Hence we conclude that $T'(H_{\rm p}\phi',\psi')-T'(\phi',H_{\rm p}\psi')=2i(\phi',\psi')$ and the lemma follows. **qed**

2.3 Main results

We state the main result. Suppose Assumption 2.1. We define the densely defined symmetric quadratic form $T_{H_V}(\cdot,\cdot):\mathscr{H}\times\mathscr{H}\to\mathbb{C}$ ($\mathscr{H}=\mathscr{H}_{\rm ac}\oplus\mathscr{H}_{\rm p}$) by

$$T_{H_V}(\phi_1\oplus\phi_2,\psi_1\oplus\psi_2)=(\phi_1,T_{\rm ac}\psi_1)+T_{\rm p}(\phi_2,\psi_2) \tag{2.7}$$

for $\phi_1,\psi_1\in D(T_{\rm ac})$ and $\phi_2,\psi_2\in D(T_{\rm d})$.

Theorem 2.5 (Generalized weak time operator) *Suppose Assumption 2.1. Then* T_{H_V} *is a generalized weak time operator associated with* H_V *with a CCR domain* $D(T_{\rm ac})\oplus H_{\rm p}^{-1}\mathscr{E}$. *I.e.,*

$$T_{H_V}(H_V\phi,\psi)-T_{H_V}(\phi,H_V\psi)=-i(\phi,\psi). \tag{2.8}$$

Proof: From Proposition 3.2 and Lemma 2.4 the theorem follows. **qed**

3 Examples

In the previous section we can construct generalized weak time operators associated Schrödinger operators H_V. In this section we give examples of external potential V such that generalized weak time operator can be constructed.

3.1 Absolutely continuous spectrum

We can construct a strong time operator associated with $H_{\rm ac}$ by through a wave operator.

Lemma 3.1 *Suppose that the wave operator* $\Omega^-(H_V, H_0) = \mathrm{s}\!-\!\lim_{t\to+\infty} e^{itH_V}e^{-itH_0}$ *exists. Then* $\Omega = \Omega^-(H_V, H_0)$ *fulfills (i)* $\Omega\mathscr{H} \subset \mathscr{H}_{\rm ac}$*, (ii)* $e^{-itH_V}\Omega = \Omega e^{-itH_0}$ *for all* $t \in \mathbb{R}$*, (iii)* $\Omega^*\Omega = 1\!\!1$*, and (iv)* $\Omega\Omega^* =$ *the projection onto* $\mathscr{H}_{\rm ac}$*.*

Proof: This is fundamental in the scattering theory in quantum physics. We omit it. **qed**

The strong time operator associated with $H_{\rm ac}$ can be constructed through Ω in Lemma 3.1 and Aharonov-Bohm operator given in (1.9).

Proposition 3.2 *Suppose Assumption 2.1. Let* $T_{\rm ac} = \Omega T_{\rm AB}\Omega^*$ *with* $\mathrm{D}(T_{\rm ac}) = \Omega\mathrm{D}(T_{\rm AB})$*. Then* $T_{\rm ac}$ *is the strong time operator associated with* $H_{\rm ac}$*.*

Proof: The proof is learned from [Ara06]. Let $\phi' = \Omega\phi \in \Omega\mathrm{D}(T_{\rm AB})$. Since $\Omega^*\Omega = 1\!\!1$, $T_{\rm ac}\phi' = \Omega T_{\rm AB}\phi$ is well defined. It is seen that

$$e^{-itH_V}T_{\rm ac}\phi' = \Omega e^{-itH_0}T_{\rm AB}\phi = \Omega(T_{\rm AB} - t)e^{-itH_0}\phi.$$

Since $e^{-itH_0}\phi = \Omega^* e^{-itH_V}\Omega\phi$, we have $e^{-itH_V}T_{\rm ac}\phi' = (\Omega T_{\rm AB}\Omega^* - t\Omega\Omega^*)e^{-itH_V}\phi'$. Since $\Omega\Omega^*$ is the projection to $\mathscr{H}_{\rm ac}$, which is denoted by $P_{\rm ac}$, and $\phi' = \Omega\phi \in \mathscr{H}_{\rm ac}$ and $\mathrm{Ran}T_{\rm ac} \subset \mathscr{H}_{\rm ac}$, we have $T_{\rm ac}e^{-itH_{\rm ac}}\phi' = e^{-itH_{\rm ac}}(T_{\rm ac} + t)\phi'$ and the proposition follows. **qed**

3.2 Short range potentials

In this section we consider short range potentials for which a generalized time operator can be constructed. It can be done however straightforwardly by the collection of known results concerning the spectrum of Schrödinger operators. In particular an upper bound of the quadratic moment of the negative eigenvalues of H_V is given by the Lieb-Thirring bound.

Suppose that V is of the form

$$V(x) = \frac{W(x)}{(|x|^2+1)^{1/2+\epsilon}} \tag{3.1}$$

for some $\epsilon > 0$, where $W : \mathbb{R}^d \to \mathbb{R}$ is a multiplication operator such that $W(-\Delta + i)^{-1}$ is compact. If V is of the form (3.1), V is called the Agmon potential. Agmon potentials form a linear space of $-\Delta$-bounded perturbations of relative bound zero. In particular H_V is self-adjoint on $\mathrm{D}(H_0)$. The perturbation by Agmon potential V leaves the essential spectrum of H_0 invariant, i.e., $\sigma_{\mathrm{ess}}(H_V) = \sigma_{\mathrm{ess}}(H_0) = [0,\infty)$. Following facts are known as Agmon-Kato-Kuroda theorem:

Proposition 3.3 (Absence of singular continuous spectrum and existence of wave operators) *Let V be an Agmon potential. Then (1) - (3) follow.*

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

(2) *The wave operator* $\Omega(H, H_0) = \mathrm{s}\text{–}\lim_{t\to\infty} e^{-itH_V} e^{itH_0}$ *exists and complete. In particular* $[0,\infty) = \sigma_{\mathrm{ac}}(H_V)$.

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

Proof: See [RS79, Theorem XIII.33]. **qed**

It is known that any $U \in L^p(\mathbb{R}^d)$ for $d/2 < p < \infty$ and $p \geq 2$, is relatively compact. Then $V(x) = (1+|x|^2)^{1/2+\epsilon} U(x)$, $\epsilon > 0$, is an Agmon potential. Another example is that $V(x) = \frac{U(x)}{(1+|x|^2)^{1/2+\epsilon}}$, $\epsilon > 0$, with $U \in L^\infty(\mathbb{R}^d)$ is an Agmon potential. See e.g. [RS79, p.439].

We introduce an assumption.

Assumption 3.4 (Infinite number of negative eigenvalues) *Let $d = 3$ and suppose that*

$$V(x) \leq -\frac{a}{|x|^{2-\delta}} \quad \text{for } |x| > R \tag{3.2}$$

with some $R > 0$, $a > 0$ and $\delta > 0$.

By Assumption 3.4 it can be seen that $\sigma_{\mathrm{disc}}(H_V) \subset (-\infty, 0)$ and $\#\sigma_{\mathrm{disc}}(H_V) = \infty$. See [RS78, Theorem XIII.6]. In particular 0 is a unique accumulation point of discrete spectrum of H_V.

Assumption 3.5 (Absence of strictly positive eigenvalues) Let V be spherically symmetric and

$$\int_a^\infty V(r)dr < \infty, \quad V \in L^2_{loc}(\mathbb{R}^d \setminus \{0\}). \tag{3.3}$$

Under Assumption 3.5 H_V has no strictly positive eigenvalues. See [RS78, Theorem XIII.56]. To construct a generalized weak time operator we need that the quadratic moment of negative eigenvalues is finite. This can be controlled by the Lieb-Thirring inequality [Lie76, Lie80]. It is known that

$$\sum_{j=1}^{\infty}|E_j|^\alpha \leq a_{d,\alpha}\int_{\mathbb{R}^d}|V(x)|^{\frac{d}{2}+\alpha}dx < \infty, \tag{3.4}$$

where $a_{d,\alpha}$ is a constant independent of V.

Assumption 3.6 (Finiteness of quadratic moment of negative eigenvalues) *Let $d=3$ and $V \leq 0$. Suppose that*

$$\int_{\mathbb{R}^3}|V(x)|^{7/2}dx < \infty. \tag{3.5}$$

Theorem 3.7 *Let $d=3$ and V be an Agmon potential. Suppose Assumptions 3.4, 3.5 and 3.6, Then the generalized weak time operator associated with H_V exists.*

Proof: By Proposition 3.3, $\sigma_{\rm sc}(H_V)=\emptyset$ and the wave operator $\Omega(H_V,H_0)$ exists. Then $T_{\rm ac}=\Omega T_{\rm AB}\Omega^*$ is a strong time operator associated with $H_{\rm ac}$ by Proposition 3.2. Under Assumptions 3.4 and 3.5 we can see that $\sigma(H_V)=\{E_j\}_{j=1}^\infty\cup[0,\infty)$, $E_1<E_2<\cdots<0$, $\overline{\sigma_{\rm p}(H_V)}=\{0\}\cup\{E_j\}_{j=1}^\infty$, and $\sigma_{\rm ac}(H_V)=[0,\infty)$. Furthermore Assumption 3.6 implies $\sum_{j=1}^\infty E_j^2<\infty$. Then the theorem follows from Theorem 2.5. **qed**

Example 3.8 Let $d=3$. Suppose that $U\in L^\infty(\mathbb{R}^3)$. Then

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

is an Agmon potential for all $\epsilon>0$. Suppose that U is negative, continuous, spherically symmetric and satisfies that $U(x)\sim 1/|x|^\alpha$ for $|x|\to\infty$ with $0<\alpha<1$. For each α, we can chose $\epsilon>0$ such that $2\epsilon+\alpha<1$. Hence V satisfies (3.2),(3.3) and (3.5). Hence a generalized weak time operator T_{H_V} associated with H_V exists.

3.3 Long range potentials: Hydrogen atoms

In this section we show an example of long range potentials. Let $d=3$. The Schrödinger operator associated with a hydrogen atom is defined by

$$H_{\rm hyd}=H_0-\frac{1}{|x|}. \tag{3.6}$$

Theorem 3.9 *There exists a generalized weak time operator $T_{H_{\rm hyd}}$ associated with $H_{\rm hyd}$.*

Proof: It is well known that $\sigma_{\rm sc}(H_{\rm hyd}) = \emptyset$, $\sigma_{\rm p}(H_{\rm hyd}) = \{-\frac{1}{2}j^{-2}\}_{j=1}^\infty$ and $\sigma_{\rm ac}(H_{\rm hyd}) = [0, \infty)$. The modified wave operator $\Omega_D(H_{\rm hyd}, H_0)$ is defined by $\Omega_D(H_{\rm hyd}, H_0) = {\rm s}-\lim_{t\to\infty} e^{itH_{\rm hyd}}U_D(t)$ with some unitary operator $U_D(t)$. See [RS79, Theorem XI.71]. Then $\Omega = \Omega_D(H, H_0)$ plays a roll of Ω in Proposition 3.2. Then the theorem follows from Theorem 2.5. **qed**

4 Time operator associated with $f(H)$

In this section we construct a time operator associated with $f(H)$ with some function $f : \mathbb{R} \to \mathbb{R}$. The assumption we need is as follows.

Assumption 4.1 *(1) Let $f \in C^2(\mathbb{R} \setminus K)$ be injective and $L = \{\lambda \in \mathbb{R} \setminus K; f'(\lambda) = 0\}$, where K is a closed subset of $\mathbb{R}$, and both of the Lebesgue measures of K and L are zero. (2) $\sum_{j=1}^\infty f(E_j)^2 < \infty$*

Assume that f satisfies Assumption 4.1. Let $\sigma(H) = \{E_j\}_j \cup [0, \infty)$ and $\sigma_{\rm ac}(H) = [0, \infty)$. We define $f(H)$ by the spectral resolution of H. Then $\sigma(f(H)) = \{f(E_j)\}_{j=1}^\infty \cup \overline{f([0, \infty))}$. Let $T_{\rm ac}$ be a strong time operator associated with $H_{\rm ac}$. Then the strong time operator associated with $f(H_{\rm ac})$ is given by

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

by Proposition 1.6. Here $D = \{\rho(H_{\rm ac}){\rm D}(T); \rho \in C_0^\infty(\mathbb{R} \setminus L \cup K)\}$. Define $T_{\rm ac}^f$ by

$$T_{\rm ac}^f = \frac{1}{2}\overline{(T_{\rm ac}f'(H)^{-1} + f'(H)^{-1}T_{\rm ac})\lceil_D} \tag{4.1}$$

is a strong time operator associated with $f(H_{\rm ac})$. Let

$$T_{\rm d}^f\phi = i\sum_{n=1}^\infty \left(\sum_{m\neq n} \frac{(\bar{e}_m, \phi)}{f(E_n) - f(E_m)}\right)\bar{e}_n.$$

Then $T_{\rm d}^f$ is a weak time operator associated with $f(H_{\rm d})$. Define $T_{H_V}^f = T_{\rm d}^f \oplus T_{\rm ac}^f$.

Theorem 4.2 *Suppose Assumption 1.6. Then $T_{H_V}^f$ is a generalized weak time operator associated with $f(H_V)$ with a CCR domain ${\rm D}(T_{\rm ac}^f) \oplus H_{\rm p}^{-1}\mathscr{E}^f$. I.e.,*

$$T_{H_V}^f(f(H_V)\phi, \psi) - T_{H_V}^f(\phi, f(H_V)\psi) = -i(\phi, \psi). \tag{4.2}$$

We give examples. Let $f(x)=1-e^{-\beta x}$. Then

$$\sum_{j=1}^\infty (1-e^{-\beta E_j})^2 \leq c\sum_{j=1}^\infty E_j^2$$

with some constant c. Define $f(H)=\mathbb{1}-e^{-\beta H}$. Thus the generalized time operator associated with $f(H)$ exists.

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