EXPLICIT FORMULAE FOR THE WAVE OPERATORS OF PERTURBED SELF-ADJOINT OPERATORS

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Abstract. We give explicit formulae for the wave operators of the position operator H_0 and the operator H obtained from H_0 by a rank one perturbation. Then by the spectral theorem, we deduce a general formula for wave operators of unbounded self-adjoint operators with absolute continuous spectrum.

1. Introduction

Let A and B be two unbounded self-adjoint operators. Consider the one-parameter family of unitary operators

$$W(t) = e^{itA}e^{-itB},\ t \in \mathbb{R}.$$

The physicists are interested in the asymptotic behavior of $W(t)$ as $t \to \mp\infty$ since $W(t)$ is used to describe the motion of a quantum mechanical system. The strong limits $W_\pm$ of $W(t)$ as $t \to \mp\infty$ (see [13] for this apparently odd looking notation) when they exist, are called proper wave operators. There are the generalized ones which are defined by $W_\pm = s - \lim_{t\to\mp\infty} W(t)P_{ac}(B)$ where $P_{ac}(B)$ denotes the projection onto the absolutely continuous subspace H_{ac} of B.

It is, however, worth mentioning that if B has an absolutely continuous spectrum then the proper and generalized wave operators coincide since in this case one has $P_{ac} = I$.

The beginning of the theory of wave operators dates back to late forties of the last century and the pioneering papers are [4] and [10]. For further results on scattering theory, the reader may consult [8, 9, 13]. For some recent advance in this theory especially for the perturbed Schrödinger operator one may consult, among others, [1, 2, 15] where it is proved under some conditions on the perturbed operators that the wave operators are L^p-bounded with $1 < p < \infty$.

So, what we will be doing in this paper is to actually give explicit formulae for the wave operators of two other operators H_0 and H where H_0 is the position operator (in some references this is more known as the coordinate operator) defined on $L^2(\mathbb{R})$ by $H_0f(x) = xf(x)$ and H is defined by $Hf(x) = xf(x) + \langle f, \varphi\rangle \varphi$ where φ is in $L^2(\mathbb{R})$. It is a well known fact that H_0 is an unbounded self-adjoint operator with domain $\{f \in L^2(\mathbb{R}) : xf \in L^2(\mathbb{R})\}$ and so is H as a perturbed self-adjoint operator by a bounded symmetric operator (see, e.g., the Kato-Rellich theorem in [12]).

The question asked in this paper is: what is $W_\pm = s - \lim_{t\to\mp\infty} e^{itH}e^{-itH_0}$?

We claim that the wave operators for H and H_0 can be written explicitly as

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$$W_{\pm}f(x)=\int_{-\infty}^{\infty}K_{\pm}(x,y)f(y)dy+\gamma_{\pm}(x)f(x)$$

where $K_{\pm}$ and $\gamma_{\pm}$ are two functions yet to be found.

And in the very end of this article, we generalize this result to general unbounded self-adjoint operators A (with absolute continuous spectrum) and A_0 also obtained from A by a rank one perturbation.

Before we finish this introduction, let us just say that there is a known example in the literature concerning this type of questions. In [8], the wave operator (for example W_+) for the self-adjoint operators $H_1=-i\frac{d}{dx}$ and $H_2=-i\frac{d}{dx}+q(x)$, with domain $H^1(\mathbb{R})$ (the Sobolev space) and where the function q is real-valued and bounded, is given by the operator of multiplication by the function

$$\exp\left(i\int_x^{\infty}q(y)dy\right),$$

provided the integral $\int_0^{\infty}q(y)dy$ exists.

Finally, we assume the reader is familiar with notions, definitions and results about unbounded operators. The reader may consult [8, 11] where these subjects are well treated.

Notations. $C_0^{\infty}(\mathbb{R})$ is the set of smooth functions in $\mathbb{R}$ with compact support.

We introduce the following set

$$M:=\{\varphi\in C_0^{\infty}(\mathbb{R}):\varphi(x)\text{ and }F(x)-1\text{ do not vanish simultaneously}\},$$

where

$$F(x):=\int_{\mathbb{R}}\frac{|\varphi(y)|^2}{x-y}dy,\ x\in\mathbb{R}.$$

The wave operators of two operators A and B will be denoted by $W_{\pm}(A,B)$ or just $W_{\pm}$ when the context is clear.

We loosely use L^2 to mean $L^2(\mathbb{R})$.

Finally, the abbreviation SOT stands for "strong operator topology".

2. Main Results

T. Kato [5] proved that for any two self-adjoint operators A and B satisfying $A=B+<\cdot,\varphi>\varphi$ ($\varphi\in L^2(\mathbb{R})$), the generalized wave operators exist. In fact, if $A-B$ is trace class then the corresponding generalized wave operators are guaranteed to exist and this is called the Kato-Rosenblum theorem (see [5, 14]).

Accordingly, since $\sigma(H_0)=\sigma_{ac}(H_0)=\mathbb{R}$, then $W_{\pm}(H,H_0)$ exist.

The following lemmas are standard. Their proofs can be found in either [8] or [13].

Lemma 1. *The two operators H and H_0 obey*

$$HW_{\pm}=W_{\pm}H_0.$$

Lemma 2. *We have*

$$\lim_{t\to\mp\infty}||W_{\pm}e^{-itH_0}f-e^{-itH_0}f||=0.$$

Before stating the result in a general form, we first prove it in a restricted form.

Proposition 1. *Let H_0 be the position operator defined on $L^2(\mathbb{R})$ by $H_0 f(x) = xf(x)$. Let H be defined by $Hf(x) = xf(x) + < f, \varphi > \varphi$ where $\varphi \in M$. Then the wave operator $W_+ f(x) = s - \lim_{t \to -\infty} e^{itH} e^{-itH_0} f(x)$ has the form*

$$W_+ f(x) = \varphi(x) \int_{-\infty}^{\infty} \frac{\overline{\varphi(y)} f(y)}{(y-x)(1 - F(y) + i\pi|\varphi(y)|^2)} dy + \frac{1 - F(x)}{1 - F(x) + i\pi|\varphi(x)|^2} f(x)$$

where f belongs to $C_0^\infty(\mathbb{R})$ and F is defined in the notations.

Proof. As alluded to in the introduction, we want to write the wave operators of H and H_0 as

$$W_\pm f(x) = \int_{-\infty}^{\infty} K_\pm(x,y) f(y) dy + \gamma_\pm(x) f(x)$$

where $\gamma_\pm$ and $K_\pm$ are two functions yet to be determined in terms of the fixed φ (although the formula above is for W_+ but the proof is essentially the same for W_-). We also assume for the present that such an expression for $W_\pm$ holds, and justify this later.

Let $f \in C_0^\infty(\mathbb{R})$ and $\varphi \in M$. By Lemma 1, we already know that

$$HW_\pm = W_\pm H_0.$$

This tells us that

$$HW_\pm f(x) = W_\pm H_0 f(x), \text{ for all } f.$$

Then

$$H(W_\pm) f(x) = xW_\pm f(x) + < W_\pm f, \varphi > \varphi$$

and

$$W_\pm (H_0 f)(x) = \int_{-\infty}^{\infty} K_\pm(x,y) y f(y) dy + x\gamma_\pm(x) f(x).$$

Hence one gets

$$x \int_{\mathbb{R}} K_\pm(x,y) f(y) dy + x\gamma_\pm(x) f(x) + \varphi(x) \int_{\mathbb{R}^2} K_\pm(x,y) f(y) \overline{\varphi(x)} dx dy$$
$$+ \varphi(x) \int_{\mathbb{R}} \gamma_\pm(x) f(x) \overline{\varphi(x)} dx = \int_{\mathbb{R}} K_\pm(x,y) y f(y) dy + x\gamma_\pm(x) f(x).$$

Or equivalently

$$\int_{\mathbb{R}} K_\pm(x,y)(y-x) f(y) dy = \varphi(x) \int_{\mathbb{R}} \gamma_\pm(y) f(y) \overline{\varphi(y)} dy + \varphi(x) \int_{\mathbb{R}} \left(\int_{\mathbb{R}} K_\pm(x,y) \overline{\varphi(x)} dx \right) f(y) dy.$$

Set

$$\psi_\pm(y) = \int_{\mathbb{R}} K_\pm(x,y) \overline{\varphi(x)} dx.$$

Then one has

$$\int_{\mathbb{R}} \left[K_{\pm}(x,y)(y-x) - \varphi(x)\psi_{\pm}(y) - \varphi(x)\gamma_{\pm}(y)\overline{\varphi(y)}\right] f(y)dy = 0.$$

The previous being true for all f, we deduce that

$$K_{\pm}(x,y)(y-x) = \varphi(x)[\psi_{\pm}(y) + \gamma_{\pm}(y)\overline{\varphi(y)}]. \tag{1}$$

By Lemma 2 we know that

$$\lim_{t\to\mp\infty} \|W_{\pm}e^{-itH_0}f - e^{-itH_0}f\| = 0$$

and since $H_0 f(x) = xf(x)$ then $e^{-itH_0}f = e^{-itx}f$ (by the spectral theorem) and hence

$$W_{\pm}e^{-itH_0}f - e^{-itH_0}f = \int_{\mathbb{R}} K_{\pm}(x,y)e^{-ity}f(y)dy + (\gamma_{\pm}(x)-1)e^{-itx}f(x).$$

Since the modulus of e^{itx} is one, we get

$$\|W_{\pm}e^{-itH_0}f - e^{-itH_0}f\| = \left\| \int_{\mathbb{R}} K_{\pm}(x,y)e^{it(y-x)}f(y)dy + (\gamma_{\pm}(x)-1)f(x)\right\| \to 0 \text{ as } t\to\mp\infty.$$

Setting $G(y) = [\psi_{\pm}(y) + \gamma_{\pm}(y)\overline{\varphi(y)}]f(y)$ and using the previous equation give us

$$\varphi(x)\int_{\mathbb{R}} \frac{G(y)e^{it(y-x)}}{y-x}dy + (\gamma_{\pm}(x)-1)f(x) \to 0. \tag{2}$$

The change of variables $y - x = z$ allows us to write the integral in the previous equation in the following way

$$\int_{\mathbb{R}} \frac{G(y)e^{it(y-x)}}{y-x}dy = \int_{\mathbb{R}} \frac{G(x+z)-G(x)}{z}e^{-itz}dz + G(x)\int_{\mathbb{R}} \frac{e^{-itz}}{z}dz.$$

Now since both f and φ are in $C_0^{\infty}(\mathbb{R})$ then the quantity $\frac{G(x+z)-G(x)}{z}$ is easily seen to be in $L^1(\mathbb{R})$. It then follows from the Riemann-Lebesgue lemma (see [3]) that

$$\lim_{t\to\mp\infty} \int_{\mathbb{R}} \frac{G(x+z)-G(x)}{z}e^{-itz}dz = 0.$$

The previous equality, when combined with (2), yields

$$\varphi(x)G(x)\int_{\mathbb{R}} \frac{e^{-itz}}{z}dz + (\gamma_{\pm}(x)-1)f(x) \to 0. \tag{3}$$

A simple application of the residues theorem gives us

$$\int_{-\infty}^{\infty} \frac{e^{-itz}}{z} dz = i\pi \text{ when } t \to -\infty \text{ and } -i\pi \text{ when } t \to +\infty.$$

From now on we will only consider the case $t \to -\infty$ (the corresponding formula for the case $t \to +\infty$ will be given in a remark below). We denote γ_+ (respectively K_+ and ψ_+) by γ (respectively K and ψ).

Then Equation (3) is equivalent to

$$\gamma(x)[i\pi|\varphi(x)|^2 + 1] = 1 - i\pi\varphi(x)\psi(x).$$

Or simply

$$\gamma(x) = \frac{1 - i\pi\varphi(x)\psi(x)}{i\pi|\varphi(x)|^2 + 1}.$$

In order to find K and γ in terms of φ we only need find ψ in terms of φ. After elementary calculations using previous equations one obtains

$$\psi(y) = \frac{\overline{\varphi(y)} \int\limits_{\mathbb{R}} \frac{|\varphi(x)|^2}{y-x} dx}{1 - \int\limits_{\mathbb{R}} \frac{|\varphi(x)|^2}{y-x} dx + i\pi|\varphi(y)|^2}.$$

Or by adopting the notation of F

$$\gamma(x) = \frac{1 - F(x)}{1 - F(x) + i\pi|\varphi(x)|^2}$$

and in a similar way

$$K(x,y) = \frac{\varphi(x)\overline{\varphi(y)}}{y - x} \left[\frac{1}{1 - F(y) + i\pi|\varphi(y)|^2} \right].$$

Thus, we get

(4)
$$W_+ f(x) = \varphi(x) \int\limits_{\mathbb{R}} \frac{\overline{\varphi(y)} f(y)}{(y-x)(1 - F(y) + i\pi|\varphi(y)|^2)} dy + \frac{1 - F(x)}{1 - F(x) + i\pi|\varphi(x)|^2} f(x).$$

Now since φ belongs to M then Formula (4) is well defined. But this is essentially motivation rather than proof. To close this gap, we define a bounded operator by Formula (4), W say, then we must show that $W = W_+$.

To come to this end we have to check that W verifies $HW = WH_0$ and

$$\lim_{t \to -\infty} ||We^{-itH_0} f - e^{-itH_0} f|| = 0,$$

then we must deduce that $W = W_+$.

By going backwards in the proof we see easily that W satisfies the above two conditions. The only step that needs a bit of justification is Equation (2) which is just Lemma 2 applied to W (and for $t \to -\infty$). The left hand side of (3) is 0 for $t < 0$. Since G is smooth with compact support, then the displayed line before (3) holds with convergence in L^2.

Having shown that W satisfies the two conditions we now verify that $W = W_+$.

For all $f \in C_0^\infty(\mathbb{R})$ we have
$\|(W - W_+)f\| = \|(W - W_+)e^{itH_0}e^{-itH_0}f\| = \|We^{itH_0}e^{-itH_0}f - W_+e^{itH_0}e^{-itH_0}f\|$.
Since $HW = WH_0$, then one has $We^{itH_0} = e^{itH}W$ (and the same for W_+). Hence

$$\|We^{itH_0}e^{-itH_0}f - W_+e^{itH_0}e^{-itH_0}f\| = \|e^{itH}(We^{-itH_0}f - W_+e^{-itH_0})f\|$$

$$= \|We^{-itH_0}f - W_+e^{-itH_0}f\| \leq \|We^{-itH_0}f - e^{-itH_0}f\| + \|W_+e^{-itH_0}f - e^{-itH_0}f\|,$$

which tends to zero, as t goes to $-\infty$.

□

Before giving Formula (4) a sense for $f, \varphi \in L^2(\mathbb{R})$, we have the following

Lemma 3. *The integral in Formula (4) can be singular. In particular, the eigenvalues of H are the points λ for which $\varphi(\lambda) = 0$ and $F(\lambda) = 1$ where $\varphi \in C_0^\infty(\mathbb{R})$.*

Proof. To illustrate this we try to solve $Hf(x) = \lambda f(x)$. It follows that

$$(\lambda - x)f(x) = \left(\int_{\mathbb{R}} f(x)\overline{\varphi(x)}dx\right)\varphi(x) = \alpha\varphi(x)$$

where α is nothing but the inner product of f and φ . So $f(x) = \frac{\alpha\varphi(x)}{\lambda - x}$. Multiplying the previous equation by $\overline{\varphi(x)}$ and integrating with respect to t over $\mathbb{R}$ give us $F(\lambda) = 1$. If we want λ to be an eigenvalue we need f to be in $L^2(\mathbb{R})$ which is possible if for instance $\varphi(\lambda) = 0$. □

First, let us get round the small problem encountered in the previous lemma.

Lemma 4. *The set M is dense in L^2.*

Proof. Let φ is in $C_0^\infty(\mathbb{R})$. Then we can approximate φ by ψ_n which has a finite number of zeros inside suppψ_n with the corresponding F (which we denote by F_{ψ_n}) different from one, i.e., $\psi_n \in M$.

Let us denote suppφ by Ω. Let

$$\Omega_0 = \{x \in \mathbb{R} : \inf_{y\in\Omega} |x - y| \leq \beta\},$$

where β is a real number bigger than 1 and yet to be chosen.

Let χ a smooth function with compact support Ω_0 such that $\chi(x) = 1$ on Ω.

By applying the Stone-Weierstrass theorem to φ on Ω_0 there exists a polynomial P_n that approximates φ uniformly.

Then we take $\psi_n(x) = \chi(x)P_n(x)$ and see easily that this ψ_n also approximates φ uniformly. Then this ψ_n has only a finite number of zeros inside supp$\psi_n = \Omega_0$. We claim that $|F_{\psi_n}(x)| < 1$ for x outside suppψ. For if $x \in \mathbb{R}\setminus\Omega_0$ (hence $|x-y| > \beta$ for all $y \in \Omega$) then

$$|F_{\psi_n}(x)| = \left|\int_{\Omega_0} \frac{|\psi_n(y)|^2}{x - y}dy\right| \leq \int_{\Omega_0} \frac{|\psi_n(y)|^2}{|x - y|}dy = \int_{\Omega} \frac{|\psi_n(y)|^2}{|x - y|}dy + \int_{\Omega_0\setminus\Omega} \frac{|\psi_n(y)|^2}{|x - y|}dy.$$

But for $x \in \mathbb{R}\setminus\Omega_0$ and $y \in \Omega_0\setminus\Omega$ the function $y \mapsto \frac{|\chi(y)|^2}{x-y}$ is bounded and since P_n converges uniformly to φ then for given $\varepsilon > 0$ one has for n large enough

$$\int_{\Omega_0\setminus\Omega} \frac{|\psi_n(y)|^2}{|x - y|}dy < \varepsilon m,$$

where m is a positive constant.

This yields

$$|F_{\psi_n}(x)| < \frac{1}{\beta}\int_\Omega |\psi_n(y)|^2 dy + m\varepsilon.$$

Hence by choosing β big enough we obtain $|F_{\psi_n}(x)| < 1$.

To conclude the proof we multiply ψ_n by a number $\alpha < 1$ (and very close to 1), so that if x_1, x_2,..., x_p are the zeros of ψ_n (inside its support) then one has

$$F_{\alpha\psi_n}(x_i) = \alpha^2 F_{\psi_n}(x_i) \neq 1,\ \forall i \in \{1, 2, ..., p\}.$$

Thus $\alpha\psi_n \in M$ and one deduces easily that M is then dense in L^2. □

We said above that the formula for W_+ is well-defined for $f \in C_0^\infty(\mathbb{R})$ and $\varphi \in M$. First we extend it to functions f belonging to $L^2(\mathbb{R})$. The term γf in the formula is easily extended to f in $L^2(\mathbb{R})$ since $\gamma \in L^\infty(\mathbb{R})$ and since $C_0^\infty(\mathbb{R})$ is dense in $L^2(\mathbb{R})$. The "integral" part is not any harder since one just uses the L^2-boundedness of the Hilbert transform (see e.g. [3]). So as L^2-limits, we can set for $f \in L^2(\mathbb{R})$ and $\varphi \in M$

$$I(f,\varphi) = \varphi(x)\int_{\mathbb{R}} \frac{\overline{\varphi(y)}f(y)}{(y-x)(1-F(y)+i\pi|\varphi(y)|^2)}dy$$

and

$$NI(f,\varphi) = \frac{1-F(x)}{1-F(x)+i\pi|\varphi(x)|^2}f(x).$$

In fact, the formula for $NI(f,\varphi)$ holds for $\varphi \in L^2$ as well.

In order to finish off this discussion we need the following lemma (which is an immediate consequence of the Corollary to Theorem XI.8 in [13])

Lemma 5. *Set $H_n f(x) = xf(x) + < f, \varphi_n > \varphi_n$. Then $W_\pm(H_n, H_0) \to W_\pm(H, H_0)$ in* SOT *as $\varphi_n \to \varphi$ in L^2.*

Since M is dense in L^2, then there exist $\varphi_n \in M$ such that $\varphi_n \to \varphi$ in L^2, then $NI(f,\varphi_n) \to NI(f,\varphi)$ (also in L^2) and since $W_+(H_n, H_0) \to W_+(H, H_0)$ in SOT then $I(f,\varphi_n)$ converges to a limit. If we denote that limit by $I(f,\varphi)$ we extend the definition of $I(f,\varphi)$ by continuity to all φ in L^2.

Thus, we have just proved

Theorem 1. *The wave operator W_+ of H and H_0 is given by*

$$W_+ f(x) = I(f,\varphi) + NI(f,\varphi) \text{ for } f, \varphi \in L^2(\mathbb{R}).$$

Remark. The same arguments apply to show that for the case $t \to +\infty$ one obtains

$$W_- f(x) = \varphi(x)\int_{-\infty}^{\infty} \frac{\overline{\varphi(y)}f(y)}{(y-x)(1-F(y)-i\pi|\varphi(y)|^2)}dy + \frac{1-F(x)}{1-F(x)-i\pi|\varphi(x)|^2}f(x)$$

where $f, \varphi \in L^2(\mathbb{R})$.

Finally, we have the following theorem:

Theorem 2. *Let A_0 be an unbounded self-adjoint operator with absolute continuous spectrum defined on a Hilbert space $\mathcal{H}$ and let A be a rank one perturbation of A_0 defined by $Af = A_0 f + < f, \varphi > \varphi$ where $\varphi \in \mathcal{H}$. Then there exists a unitary* *operator $U:\mathcal{H}\longrightarrow L^2(E,dx)$ (E is some measurable subset of $\mathbb{R}$ and dx denotes the induced Lebesgue measure on E) such that $UW_{\pm}(A,A_0)U^{-1}f(x)$ is*

$$\varphi(x)\int_E \frac{\overline{\varphi(y)}f(y)}{(y-x)(1-F(y)\pm i\pi|\varphi(y)|^2)}dy+\frac{1-F(x)}{1-F(x)\pm i\pi|\varphi(x)|^2}f(x).$$

Proof. For the existence of $W_{\pm}(A,A_0)$ one has just to refer to [8]. As for the explicit formula, we just derive it from Theorem 1 as follows.

Let $\varphi\in\mathcal{H}$. Then let $\mathcal{K}$ be the smallest closed subspace containing φ and which reduces A_0 (see [8]). Then one can express $\mathcal{H}$ as $\mathcal{K}\oplus\mathcal{L}$ where $\mathcal{L}=\mathcal{K}^{\perp}$.

Then $A_0|\mathcal{K}$ is unitarily equivalent to multiplication by x on $L^2(\mu)$ for some measure μ on $\mathbb{R}$ (see again [8]).

Now, since A_0 has absolute continuous spectrum, then μ must be absolutely continuous with respect to Lebesgue measure and whence it can be taken to be Lebesgue measure on some measurable subset E of $\mathbb{R}$.

Since $Af=A_0f+<f,\varphi>\varphi$, then the wave operators are trivial on $\mathcal{L}$ (since for $f\in\mathcal{L}$ one has $Af=A_0f$ and whence $e^{itA}e^{-itA_0}f=f$) and the problem reduces to the case of multiplication by x on $L^2(E)$, which in turn is immediately reducible to the $L^2(\mathbb{R})$ case.

□

3. A question

It is well known (see [12]) that the Laplacian $B_0=-\triangle$, when considered as a self-adjoint operator on $L^2(\mathbb{R}^3)$ with domain $H^2(\mathbb{R}^3)$ (the Sobolev space), is unitarily equivalent to the multiplication operator by some nonnegative function. Hence it has a positive absolute continuous spectrum. So Theorem 2 may well be applied to the couple (B_0,B) where B is a rank one perturbation of B_0.

The question one can ask is can we still prescribe an explicit formula for the wave operators if, for instance, we change the perturbation term in B by some multiplication by a real $q(x)$, $x\in\mathbb{R}^3$, satisfying

$$|q(x)|\leq\frac{C}{(1+|x|)^{\beta}},\ \beta>1?$$

Since in this particular case the wave operators do exist (see, e.g., [7]).

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