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On Some Schrödinger Operators with a Singular Complex Potential.

TOSIO KATO (*)

dedicated to Hans Lewy

1. – Introduction.

Consider the differential operator

$$L = -\Delta + q(x) \tag{1.1}$$

In R^n, where Δ is the Laplacian and q is a complex-valued, measurable function. Suppose that

$$\operatorname{Re} q \geqslant 0 . \tag{1.2}$$

Then L is formally accretive (or $-L$ is formally dissipative), and it is expected that L has an *m-accretive realization* A in the Hilbert space $L^2(R^n)$. (A is m-accretive if $-A$ is the infinitesimal generator of a strongly continuous, contraction semigroup $\{\exp[-tA]; t \geqslant 0\}$.) Moreover, one may expect that the semigroup is given by the *Trotter product formula*

$$\exp[-tA] = \operatorname*{strong\,lim}_{n\to\infty} (\exp[t\Delta/n] \exp[-tq/n])^n . \tag{1.3}$$

In a remarkable paper [1], Nelson showed (among other things) that the above results are true if $\operatorname{Re} q = 0$ and if q is only continuous on $R^n \setminus F$, where F is a closed subset of R^n with capacity zero; no assumption is made on the behavior of q near F. Furthermore, it is interesting to note, he proves first that the limit in (1.3) exists and forms a semigroup, and then that the (negative) generator A of this semigroup is indeed a realization of L in $L^2(R^n)$. In the convergence proof he makes an essential use of the Wiener integral. It will be noted that Nelson does not give a direct characterization of A,

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but he does show that $D(A) \subset H^1(R^n)$, where D denotes the domain and H^1 the Sobolev space of L^2-type.

The purpose of the present paper is to generalize Nelson's results, using more conventional operator theory without recourse to the Wiener integral. We shall consider the operator L on an arbitrary open set $\Omega \subset R^n$ and construct a distinguished m-accretive realization A of L in $\boldsymbol{H} = L^2(\Omega)$, with a complete characterization of $D(A)$. Our assumption on q is that

$$q \in L^p_{\mathrm{loc}}(\Omega)\,, \tag{1.4}$$

where $p = 2n(n+2)^{-1}$ if $n \geqslant 3$, $p > 1$ if $n = 2$ and $p = 1$ if $n = 1$, in addition to (1.2). Roughly speaking, A is the realization of L with the Dirichlet boundary condition (see Definition 2.1 and Theorem I below).

We shall then show that the Trotter product formula (1.3) holds, where Δ should also be taken as the realization of the formal Laplacian with the Dirichlet boundary condition (see Theorem II).

Nelson's results for $\Omega = R^n \setminus F$ can easily be recovered as special cases of these results (see Remark 2.5).

Our proof depends only on the familiar theories of monotone and accretive operators, except that an essential use is made of a lemma which the author proved in another occasion [2].

[Note]. In this paper we distinguish between accretive and monotone operators, even when the underlying spaces are Hilbert spaces. Accretive operators act within a space, while monotone operators act from a space into its adjoint (anti-dual) space.

2. – The main results.

In what follows we assume (1.2) and (1.4) for q.

Definition 2.1. We define an operator A in $\boldsymbol{H} = L^2(\Omega)$ by

$$Au = Lu = -\Delta u + qu \tag{2.1}$$

with the domain $D(A)$ consisting of all $u \in \boldsymbol{H}$ such that

$$u \in H^1_0(\Omega) \quad \text{and} \quad Lu \in L^2(\Omega)\,. \tag{2.2}$$

Remark 2.2. $H^1_0(\Omega)$ is the usual Sobolev space defined as the completion of $C^\infty_0(\Omega)$ under the H^1-norm

$$\|u\|_1 = (\|u\|^2 + \|\operatorname{grad} u\|^2)^{\frac{1}{2}}\,, \tag{2.3}$$

where $\| \;\|$ denotes the $L^2(\Omega)$-norm (for scalar and vector functions). Thus A satisfies the Dirichlet boundary condition in a generalized sense.

REMARK 2.3. If $u \in H_0^1(\Omega)$, then $u \in L^{p'}(\Omega)$ by the Sobolev embedding theorem, where $p'^{-1} = 1 - p^{-1}$, so that $qu \in L^1_{\mathrm{loc}}(\Omega)$ by (1.4). Hence Lu is a distribution in Ω, and condition (2.2) makes sense.

REMARK 2.4. It is not at all obvious that $D(A)$ contains elements other than 0. Actually $D(A)$ is dense in $\boldsymbol{H}$. In fact we have a stronger result.

THEOREM I. *A is m-accretive.*

THEOREM II. *The Trotter product formula* (1.3) *holds for our A, where Δ on the right is the special case of $-A$ for $q = 0$.* (In other words, Δ is the realization of the Laplacian in $\boldsymbol{H}$ with the Dirichlet boundary condition.)

REMARK 2.5. Suppose that $\Omega = R^n \setminus F$ as in Nelson's case, where F is a closed set with capacity zero. Then $\boldsymbol{H} = L^2(R^n)$ because F has measure zero. Furthermore, $H_0^1(\Omega) = H^1(R^n)$ in an obvious sense (see Lemma 2.6 below). It follows that Δ extends, and therefore coincides with, the canonical realization of the Laplacian in $L^2(R^n)$ (with domain $H^2(R^n)$). Then (1.3) shows that our semigroup $\{\exp[-tA]\}$ coincides with Nelson's and, consequently, our A with his generator. In this way we recover Nelson's results for a wider class of potentials q.

LEMMA 2.6. *$H_0^1(\Omega) = H^1(R^n)$ if and only if $R^n \setminus \Omega = F$ has capacity zero.*

PROOF. Since $C_0^\infty(\Omega) \subset H^1(R^n)$ in an obvious sense, $H_0^1(\Omega)$ may be identified with a subspace of $H^1(R^n)$. Then $H_0^1(\Omega) = H^1(R^n)$ if and only if $v \in H^1(R^n)$ and $(v, \varphi)_1 = 0$ for all $\varphi \in C_0^\infty(\Omega)$ together imply $v = 0$. [$(\;,\;)_1$ denotes the inner product in the Hilbert space $H^1(R^n)$.] But the latter condition is equivalent to that the distribution $w = (1 - \Delta)v$ annihilates $C_0^\infty(\Omega)$, that is, w is supported on F. Since $w \in H^{-1}(R^n)$, this implies $w = 0$, hence $v = 0$, if and only if F has capacity zero (see Hörmander and Lions [3]).

3. – Proof of Theorem I.

Besides the realization A in $\boldsymbol{H} = L^2(\Omega)$ of L, it is convenient to introduce another realization of L between the Hilbert space $H_0^1(\Omega)$ and its adjoint space $H^{-1}(\Omega)$.

DEFINITION 3.1. We define an operator T from $H_0^1(\Omega)$ into $H^{-1}(\Omega)$ by $Tu = Lu$, with $D(T)$ characterized by

$$u \in H_0^1(\Omega) \quad \text{and} \quad Lu \in H^{-1}(\Omega)\,. \tag{3.1}$$

REMARK 3.2. T is the maximal realization of L between these two Hilbert spaces. Note that condition (3.1) makes sense because Lu is a distribution in Ω if $u \in H_0^1(\Omega)$ (see Remark 2.3). Since $\Delta u \in H^{-1}(\Omega)$ then, the second condition in (3.1) is equivalent to $qu \in H^{-1}(\Omega)$.

PROPOSITION 3.3. $C_0^\infty(\Omega) \subset D(T)$.

PROOF. $\varphi \in C_0^\infty(\Omega)$ implies $q\varphi \in L^p(\Omega)$ by (1.4). But $L^p(\Omega) \subset H^{-1}(\Omega)$ because $H_0^1(\Omega) \subset L^{p'}(\Omega)$ (see Remark 2.3). Hence $q\varphi \in H^{-1}(\Omega)$ and (3.1) is satisfied. |||

DEFINITION 3.4. We denote by T_0 the restriction of T with $D(T_0) = C_0^\infty(\Omega)$. ($T_0$ is densely defined.)

REMARK 3.5. T_0 may be called the minimal realization of L between $H_0^1(\Omega)$ and $H^{-1}(\Omega)$. In this connection, it should be noted that there is no minimal realization of L in $\boldsymbol{H}$. Indeed, $D(A)$ need not contain $C_0^\infty(\Omega)$ (see Remark 2.4).

PROPOSITION 3.6. $T = \overline{T}_0^*$, *where* $\overline{T}_0$ *is the operator* T_0 *for* q *replaced by its complex conjugate* $\bar{q}$ *and* $*$ *denotes the adjoint operator*. (Thus T is closed.)

PROOF. We have to show that given $u \in H_0^1(\Omega)$ and $f \in H^{-1}(\Omega)$, $Tu = f$ is true if and only if $\langle u, \overline{T}\varphi\rangle = \langle f, \varphi\rangle$ for all $\varphi \in C_0^\infty(\Omega)$, where $\langle\ ,\ \rangle$ denotes the pairing between H_0^1 and H^{-1}. But this is obvious from the definition of T. |||

PROPOSITION 3.7. T_0 *is monotone.*

PROOF. This is obvious because for $\varphi \in C_0^\infty(\Omega)$,

$$\operatorname{Re}\langle T_0\varphi, \varphi\rangle = \operatorname{Re}\Big(\langle -\Delta\varphi, \varphi\rangle + \int q|\varphi|^2\Big) \geqslant \|\operatorname{grad}\varphi\|^2 \geqslant 0\,. \quad ||| \tag{3.2}$$

PROPOSITION 3.8. $1 + T_0$ *is monotone and coercive in the sense that* $\|(1+T_0)\varphi\|_{-1} \geqslant \|\varphi\|_1$ *for* $\varphi \in D(T_0)$, *where* $\|\ \|_{-1}$ *denotes the* $H^{-1}(\Omega)$*-norm.*

PROOF. (3.2) implies that

$$\operatorname{Re}\langle (1+T_0)\varphi, \varphi\rangle \geqslant \|\varphi\|^2 + \|\operatorname{grad}\varphi\|^2 = \|\varphi\|_1^2\,. \tag{3.3}$$

Since the left member does not exceed $\|(1+T_0)\varphi\|_{-1}\|\varphi\|_1$, the desired result follows. |||

PROPOSITION 3.9. *T_0 is closable, with closure T_0^{**}. $R(1+T_0^{**})$ is closed.* (R denotes the range.)

PROOF. Since $T_0^* = \overline{T}$ by Proposition 3.6 and since $\overline{T} \supset \overline{T}_0$ is densely defined, T_0^{**} exists and equals the closure of T_0. Since $1 + T_0^{**}$ is coercive with $1 + T_0$, $R(1+T_0^{**})$ is closed by a well-known result. |||

PROPOSITION 3.10. *$R(1+T_0^{**})$ is the whole space $H^{-1}(\Omega)$, so that T_0^{**} is maximal monotone.* [This is our key proposition. Note that the Lax-Milgram theorem is not useful here, since T_0^{**} is not a bounded operator.]

PROOF. In view of Proposition 3.9, it suffices to show that $u \in H_0^1(\Omega)$ and $\langle (1+T_0)\varphi, u\rangle = 0$ for all $\varphi \in C_0^\infty(\Omega)$ together imply $u = 0$.

The stated condition implies $\langle (\varphi - \Delta\varphi + q\varphi, u\rangle = 0$ or $u - \Delta u + \bar{q}u = 0$ in the distribution sense (recall that $\bar{q}u \in L^1_{\mathrm{loc}}(\Omega)$ by Remark 2.3). Since this implies that $\Delta u = u + \bar{q}u \in L^1_{\mathrm{loc}}(\Omega)$, it follows from a lemma in [2] that

$$\Delta|u| \geqslant \mathrm{Re}[(\operatorname{sign}\bar{u})\Delta u] = \mathrm{Re}\,(|u| + \bar{q}|u|) \geqslant |u|$$

in the distribution sense, which means that

$$\langle (1-\Delta)|u|, \varphi\rangle \leqslant 0 \quad \text{for } 0 \leqslant \varphi \in C_0^\infty(\Omega)\,. \tag{3.4}$$

Now it is known that $|u|$ belongs to $H_0^1(\Omega)$ with u (see Stampacchia [4]). Since $|u| \geqslant 0$, there is a sequence $\varphi_j \in C_0^\infty(\Omega)$ with $\varphi_j \geqslant 0$ such that $\varphi_j \to |u|$ in $H_0^1(\Omega)$ as $j \to \infty$, a nontrivial result due to Stampacchia (private communication). Then

$$(|u|, \varphi_j)_1 = \lim_k\,(\varphi_k, \varphi_j)_1 = \lim_k\,\langle (1-\Delta)\varphi_k, \varphi_j\rangle = \langle (1-\Delta)|u|, \varphi_j\rangle \leqslant 0\,,$$

where we have used the fact that $(1-\Delta)\varphi_k \to (1-\Delta)|u|$ in the distribution sense; the last inequality is due to (3.4). Letting $j \to \infty$, we obtain $(|u|, |u|)_1 \leqslant 0$, hence $u = 0$. |||

PROPOSITION 3.11. $T = T_0^{**}$. *Hence T is maximal monotone.*

PROOF. $T_0 \subset T$ implies $T_0^{**} \subset T$ because T is closed by Proposition 3.6. But $1 + T_0^{**}$ already has the whole space $H^{-1}(\Omega)$ as its range by Proposition 3.10, while $1 + T = 1 + \bar{T}_0^*$ has trivial null space because its adjoint $1 + \bar{T}_0^{**}$ has range $H^{-1}(\Omega)$ by the same proposition. Hence T cannot be a proper extension of T_0^{**}. This shows that $T = T_0^{**}$, and T is maximal monotone by Proposition 3.10. |||

We can now complete the proof of Theorem I. A is the *part* of T in $\boldsymbol{H} = L^2(\Omega)$, in the sense that $u \in D(A)$ if and only if $u \in D(T)$ and $Tu \in L^2(\Omega)$, in which case $Au = Tu$. Since $R(1 + T)$ covers all of $H^{-1}(\Omega)$, it is obvious that $R(1 + A)$ covers all of $L^2(\Omega)$. Furthermore, $\mathrm{Re}(Au, u) = \mathrm{Re}\langle Tu, u\rangle \geqslant 0$ because T is monotone. It follows that A is m-accretive (see e.g. Kato [5]).

4. – Proof of Theorem II.

First we note that in (1.3) we may replace A by $1 + A$ and Δ by $\Delta - 1$ without affecting the theorem.

As is usually the case with the Trotter formula, we base the proof of the modified formula (1.3) on Chernoff's lemma (see [5, 6]). According to this lemma, it suffices to show that

$$(4.1) \quad t\big(1 - \exp[t(\Delta - 1)]\exp[-tq]\big)^{-1} \to (1 + A)^{-1} \quad \text{strongly in } \boldsymbol{H}$$

as $t\downarrow 0$. For our purpose, it is convenient to modify (4.1) slightly and prove that

$$(4.2) \quad t\big(\exp[t(1 - \Delta)] - \exp[-tq]\big)^{-1} \to (1 + A)^{-1} \quad \text{strongly in } \boldsymbol{H}.$$

The equivalence of (4.1) and (4.2) will be seen from Lemma 4.1 given at the end of this section.

To this end we first note that the inverse operator on the left of (4.2) exists for $t > 0$ because $\exp[t(1 - \Delta)]$ is an (unbounded) selfadjoint operator majorizing $e^t \geqslant 1 + t$ while $\exp[-tq]$ is a contraction operator.

For any $u \in \boldsymbol{H}$ let

$$(4.3) \quad w_t = t\big(\exp[t(1 - \Delta)] - \exp[-tq]\big)^{-1} u \in D\big(\exp[-t\Delta]\big) \subset H_0^1(\Omega) \subset \boldsymbol{H}.$$

This implies that

$$(4.4) \qquad t^{-1}\big(\exp[t(1 - \Delta)] - \exp[-tq]\big)\, w_t = u\,.$$

Taking the inner product in $\boldsymbol{H}$ of (4.4) with w_t, we obtain

$$t^{-1}\big((\exp[t(1 - \Delta)] - 1)\, w_t, w_t\big) + t^{-1}\big((1 - \exp[-tq])\, w_t, w_t\big) = (u, w_t)\,.$$

Since the first term on the left dominates $((1-\Delta)w_t, w_t) = \|w_t\|_1^2$ and the second term has nonnegative real part, we have

$$\|w_t\|_1^2 \leqslant \mathrm{Re}(u, w_t)\,, \qquad \text{hence } \|w_t\|_1 \leqslant \|u\|\,. \tag{4.5}$$

Given any sequence $t_j \downarrow 0$, we can therefore pick up a subsequence along which w_t converges weakly to a $w \in H_0^1(\Omega)$ in H_0^1-topology. We shall show that $w = (1+A)^{-1}u$. To this end, we apply $\exp[t(\Delta-1)]$ (a bounded operator) to (4.4), obtaining

$$t^{-1}\big(1-\exp[t(\Delta-1)]\exp[-tq]\big)w_t = \exp[t(\Delta-1)]u\,. \tag{4.6}$$

Taking the inner product in $\boldsymbol{H}$ of (4.6) with a $\varphi \in C_0^\infty(\Omega)$, we obtain, after a simple computation,

$$\begin{aligned} t^{-1}(w_t, (1-\exp[-t\bar{q}])\varphi) &+ \\ &+ t^{-1}\big(w_t, \exp[-t\bar{q}](1-\exp[t(\Delta-1)])\varphi\big) = \big(u, \exp[t(\Delta-1)]\varphi\big)\,. \end{aligned} \tag{4.7}$$

Now the following relations hold.

$$t^{-1}(1-\exp[-t\bar{q}])\varphi \to \bar{q}\varphi \quad \text{in } L^p(\Omega)\,, \tag{4.8}$$

$$t^{-1}\exp[-t\bar{q}](1-\exp[t(\Delta-1)])\varphi \to (1-\Delta)\varphi \quad \text{in } L^2(\Omega)\,, \tag{4.9}$$

as $t\downarrow 0$. (4.8) follows from the facts that the left member is majorized pointwise by $|\bar{q}\varphi|$, which is in $L^p(\Omega)$ by (1.4), and converges pointwise to $\bar{q}\varphi$, so that the convergence takes place also in $L^p(\Omega)$ by Lebesgue's theorem. (4.9) follows from the facts that $t^{-1}\big(1-\exp[t(\Delta-1)\big)\varphi \to (1-\Delta)\varphi$ in $L^2(\Omega)$ and that $\exp[-t\bar{q}] \to 1$ strongly as an operator on $L^2(\Omega)$.

Since both $L^p(\Omega)$ and $L^2(\Omega)$ are continuously embedded in $H^{-1}(\Omega)$ (see the proof of Proposition 3.3) and since w_t tends to w weakly in $H_0^1(\Omega)$ along the subsequence considered, it follows from (4.7), (4.8), and (4.9) that

$$\langle w, \bar{q}\varphi + (1-\Delta)\varphi\rangle = \langle u, \varphi\rangle\,. \tag{4.10}$$

Since this is true for every $\varphi \in C_0^\infty(\Omega)$, we have $(1-\Delta)w + qw = u$ in the distribution sense, where it should be noted again that $qw \in L^1_{\mathrm{loc}}(\Omega)$. It follows from Definition 2.1 that $w \in D(A)$ with $(1+A)w = u$. Hence $w = (1+A)^{-1}u$.

Since w is thus independent of the subsequence of t_j chosen, we have proved that

$$w_t \to w = (1+A)^{-1}u \quad \text{weakly in } H_0^1(\Omega) \text{ as } t\downarrow 0\,. \tag{4.11}$$

To prove (4.2), it remains to show that

$$w_t \to (1+A)^{-1}u \quad \text{strongly in } \boldsymbol{H} = L^2(\Omega)\,. \tag{4.12}$$

To this end, we first note that (4.11) already implies (4.12) *locally* due to Rellich's lemma. Thus the desired result will follow if we show that w_t is « small at infinity in L^2-sense, uniformly in t. » (The precise meaning of this statement will be clear from the following proof.)

We have from (4.3)

$$\begin{aligned} w_t = t[&\exp[t(\Delta-1)]u + \\ &+ \exp[t(\Delta-1)]\exp[-tq]\exp[t(\Delta-1)]u + \ldots]\,, \end{aligned} \tag{4.13}$$

the series converging in $\boldsymbol{H}$-norm. Since $\exp[t(\Delta-1)]$ is positivity preserving, we have $|\exp[t(\Delta-1)]f| \leqslant \exp[t(\Delta-1)]|f|$ pointwise for each $f\in\boldsymbol{H}$. Since $|\exp[-tq]f|\leqslant|f|$ by (1.2), we see from (4.13) that

$$\begin{aligned} |w_t| \leqslant t[&\exp[t(\Delta-1)]|u| + \exp[2t(\Delta-1)]|u| + \ldots] = \\ &= t(\exp[t(1-\Delta)]-1)^{-1}|u|\,. \end{aligned} \tag{4.14}$$

Since the right member tends as $t\downarrow 0$ to $(1-\Delta)^{-1}|u|$ strongly in $\boldsymbol{H}$, it is clear that w_t is « uniformly small at infinity in the L^2-sense. » This completes the proof of Theorem II.

LEMMA 4.1. *Let $\{U_t\}$, $\{V_t\}$, $t>0$, be families of bounded operators on a Banach space X, such that $\|U_t\|\leqslant\exp[-t]$, $\|V_t\|\leqslant 1$, and $U_t\to 1$, $V_t\to 1$ strongly as $t\downarrow 0$. Assume, moreover, that U_t^{-1} exists as a (possibly) unbounded operator. Then the following three conditions are equivalent.*

(*a*) $t(1-U_tV_t)^{-1}\to C$,

(*b*) $t(1-V_tU_t)^{-1}\to C$,

(*c*) $t(U_t^{-1}-V_t)\to C$,

where C is a bounded operator on X and $\to$ means strong convergence.

PROOF. This is obvious from the identities:

$$(1-U_tV_t)^{-1} = 1 + (U_t^{-1}-V_t)^{-1}V_t\,, \qquad (1-V_tU_t)^{-1} = 1 + V_t(U_t^{-1}-V_t)^{-1}\,,$$

$$(U_t^{-1}-V_t)^{-1} = (1-U_tV_t)^{-1}U_t = U_t(1-V_tU_t)^{-1}\,.$$

5. – Supplementary remarks.

(*a*) If we strengthen condition (1.2) to

$$|\operatorname{Im} q(x)| \leqslant M \operatorname{Re} q(x), \qquad x \in \Omega, \tag{5.1}$$

then condition (1.4) can be weakened to

$$q \in L^1_{\mathrm{loc}}(\Omega). \tag{5.2}$$

In this case an m-accretive realization A of L in $\boldsymbol{H}$ can be constructed as before, with $D(A)$ characterized by (2.2) *and*

$$q|u|^2 \in L^1(\Omega). \tag{5.3}$$

Notice that (5.2) and (5.3) together imply $qu \in L^1_{\mathrm{loc}}(\Omega)$ so that Lu makes sense as a distribution in Ω.

The proof that A thus defined is m-accretive is essentially contained in [5, VI-§ 4.3]. There it is assumed that $\Omega = R^3$ and q is real, but these assumptions are not essential. It is interesting to note that the proof again depends on the lemma of [2] and Stampacchia's lemma, which are used in the proof of Proposition 3.10 above.

Trotter's formula (1.3) also holds in this case; it is a consequence of a general result given in Kato [7] (Simon's generalization of the author's theorem).

(*b*) One may also include in q a negative part q_-. If q_- is sufficiently weak relative to $-\Delta$, one can define the realization A in the same way as above. This was done (essentially) in [5, loc. cit.] when the main part of q satisfies (5.1) and (5.2) and q_- satisfies a certain condition of the Stummel type. A similar result is expected when the main part of q satisfies (1.2) and (1.4).

(*c*) These results may also be generalized to the case in which Δ is replaced by a general second-order differential operator of elliptic type with variable coefficients, under certain assumptions on the continuity and growth rate of the coefficients.

(*d*) When $\Omega = R^n$ and $0 \leqslant q \in L^1_{\mathrm{loc}}(\Omega)$, it is known (see Kato [8]) that the operator A considered in (*a*) is the only m-accretive realization of L in $\boldsymbol{H}$. This result can be extended to the case of a nonreal q satisfying either (1.2) and (1.4) or (5.1) and (5.2).

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