**Carleman's sufficency theorem for the Schrödinger equation**

The theory about unbounded densely defined self-adjoint operators on Hilbert spaces and their associated spectral functions was created by Torsten Carleman. His monograph *Sur les equations singuliers à noyeaux réel et symmetrique* published by Uppsala University in 1923 contains a wealth of results which Carleman for example used to study monent problems and spectral of densely defined partial differential operators. One example is the operator defiuned in $\mathbf{R}^3$ by

$$(*) \qquad L = \Delta + \sum \frac{m_k}{|x - p_k|}$$

where the last term is a a finite sum of Newton's potentials, i.e. $\{m_k\}$ are positive real numbers and $\{p_k\}$ a finite set of points in the 3-dimensional $x$-space, where $|x - y|$ denotes the euclidian distance between a pait of points $x$ and $y$ in $\mathbf{R}^3$. At the Scandinavian congess in mathematics held in Cpenhagen 1925, the relevance of this PDE was put forward by Niels Bohr while he presented the new-born quantum mehcanics. Here we shall not discuss physical background but refer to Bohr's article in [xxx]. The mathemactical problem is to find eigenvalues for $L$ when it acts as a densey defined linear operator on $L^2)\mathbf{R}^3)$. A solution was given by Carleman in his plenary lecture at the cited congress. The result is that there exists a non-decreasing sequence $\{\lambda_\nu\}$ of positive real eigenvalues, i.e for every $\lambda_\nu$ one finds a real-valued $L^2$-function $\phi_\nu$ for which $\Delta(\phi_n u)$ also is square integrable and

$$L(\phi_\nu) + \lambda_\nu \cdot \phi_\nu = 0$$

We prove this result in § xx and remark only that it is quite straightforward because one deals with a special poltential function in (*). More generally, consider a real-valued function $c(x, y, z)$ in the 3-dimensional $(x, y, z)$-space which is at locally square integrable and the differential operator

$$L = \Delta + c(x, y, z)$$

When $u$ and $v$ are test-functions in $\mathbf{R}^3$ one has the equality:

$$(*) \qquad \int L(u) \cdot v \, dm = \int u \cdot L(v) \, dm$$

where $dm$ denotes the Lebesgue measure. Since test-functions give a dense subspace of $L^2(\mathbf{R}^3)$ this means that $L$ is a densely defined and symmetric operator on the Hilbert space $L^2(\mathbf{R}^3$. Next, the $L$-operator has a domain of definition $\mathcal{D}(L)$ which by definition consists of $L^2$-functions in $\mathbf{R}^3$ for which

$$\Delta(u) + cu \in L^2$$

Since we assume that $c$ is in $L^2_{\text{loc}}$ this entails that $\Delta(u)$ is at least in $L^1_{\text{loc}}$ and thrn Newton's fundamental solution to the Laplace operstor implie thst $u$ is of class $C^1$, i.e. its partial derivatives exist as continuous functions. With $\mathcal{D}(L)$ chosen as above it also holds that $L$ has a closed graph, and by the genersl theory in the cited monograph the closed and densely defined operator $L$ is self-adjoint if and only if (*) hold for every pair $u, v$ in $\mathcal{D}(L)$. We shall prove the following sufficncy result.

**Theorem.** *The operator Lis self-adjoint if*

$$\limsup_{|p| \to +\infty} c(p) < \infty$$

The proof requires several steps. To begin with we need a result sbout $L^2$-functions of class $C^1$.

**1 Proposition.** *For every $L^2$-funtcion $f$ of class $C^1$ there exists an increasing sequence $\{r_k\}$ of positive real numbers which tends to $+\infty$, such that*

$$\lim \int_{|x|=r_k} f \cdot \frac{\partial f}{\partial n} \, d\sigma = 0$$

*where integration is taken over the sphere $|x| = r_k$ on which $d\sigma$ is the area measure and $\frac{\partial f}{\partial n}$ the normal derivative.*

*Proof.* Introducing polar coordinates in $\mathbf{R}^3$ one has

$$\int f^2\,dm = \int_0^\infty [\int_{S^2} f^2(r\omega)\,d\omega]\,r^2\,dr$$

where $S^2$ is the unit sphere with spherical coordinates $\omega$. When $r > 0$ we put

$$\phi(r) = \int_{S^2} f^2(r\omega)\,d\omega$$

The derivative becomes

$$\phi'(r) = \int_{S^2} f(r\omega)\cdot\frac{\partial f}{\partial n}(r\omega)\,d\omega$$

On $|x| = r$ we have $d\sigma = r^2\cdot d\omega$ and hence

$$\phi'(r) = r^{-2}\cdot\int_{|x|\approx r} f\cdot\frac{\partial f}{\partial n}\,d\sigma$$

Next, if no sequence $\{r_k\}$ exists the continuity of $r\mapsto\phi'(r)$-function gives a positiive constant and some $r_* > 0$ such that

$$r\geq r_* \implies r\phi'(r)\geq\frac{c}{r^2}$$

where we if necesssry only have replaced $f$ by $-f$. Now (xx) gives another constant $C$ such thst

$$r\geq r_* \implies \phi(r)\geq\frac{c}{r}$$

At the same time $f$ is square integrable so that

$$\int_0^\infty r^2\cdot\phi(r)\,dr < \infty$$

Next, apply Green's formula in a ball $B(R) = \{|x| < R\}$which gives the equation below for every $u\in\mathcal{D}(L)$:

$$\int_{B(R)} u\cdot L(u)\,dm + \int_{B(R)} |\nabla(u)|^2\,dm + \int_{|x|=R} u\cdot\frac{\partial u}{\partial n}\,d\sigma = \int_{B(R)} c\cdot u^2\,dm \tag{1.2}$$

Since $u$ and $L(u)$ are square-integrable over $\mathbf{R}^3$, the function $u\cdot L(u)$ is absolutely integrable by the Cauchy-Schwarz inequality. Together with Proposition 1 we conclude that the non-negative function $|\nabla(u)|^2$ belongs to $L^2)\mathbf{R}^3$ if

$$\limsup_{R\to\infty}\int_{B(R)} c\cdot u^2\,dm < +\infty \tag{1.3}$$

It is clear that (1.3) holds if the $c$-function satisfies (**) in Theorem xx. So when (**) holds one has the implication:

$$u\in\mathcal{D}(L) \implies \int_{\mathbf{R}^3} |\nabla(u)|^2\,dm < +\infty \tag{1.4}$$

Using (1.4) we can show that $L$ is self-adjoint. For let $u$ and $v$ be a pair in $\mathcal{D}(L)$. For every $R > 0$, Green's formula gives

$$\int_{B(R)} (uL(v) - vL(u))\,dm = \int_{S(R)} (v\frac{\partial u}{\partial n} - u\frac{\partial v}{\partial n})\,d\sigma$$

Since $u\cdot L(v)$ nd $L(u)\cdot u$ both belong to $L^1)\mathbf{R^3})$ we get (*) if there exists a sequence $\{R_k\}$ with $R_k\to+\infty$ such that

$$\lim_{k\to\infty}\int_{S(R_k)} (v\frac{\partial u}{\partial n} - u\frac{\partial v}{\partial n})\,d\sigma = 0 \tag{1.5}$$

There remains to prove (1.5). Passing to polar coordinates we first notice that (1.4) gives:

$$\int_0^\infty [\int_{S(r)} (\frac{\partial u}{\partial n})^2 \, d\sigma \,] \, dr < \infty$$

The same conclusion holds for $v$ and since both $u$ and $v$ also are in $L^2(\mathbf{R}^3)$ we get:

$$\int_0^\infty [\int_{S(r)} \big(u^2 + v^2 + (\frac{\partial u}{\partial n})^2 + (\frac{\partial v}{\partial n})^2\big) \, d\sigma \,] \, dr < \infty$$

This entails that

$$\liminf_{r \to +\infty} \int_{S(r)} \big(u^2 + v^2 + (\frac{\partial u}{\partial n})^2 + (\frac{\partial v}{\partial n})^2\big) \, d\sigma = 0 \tag{6}$$

Finally applying the Cauchy-Schwarz inequality to the pairs $u, \frac{\partial v}{\partial n}$ and $v, \frac{\partial u}{\partial n}$ we get (1.5) which finishes the proof of the Theorem.

**Neumann's calculus.**

For the less experienced reader we recall Carl Neumann's spectral calculcus for unbounded linear operators. In general, let $T$ be a linear operator from a Banach space $X$ in to itself whose domain of definition $\mathcal{D}_T$ is dense. We alsom assume that the graph

$$\Gamma(T) = \{(x, Tx) \quad : x \in \mathcal{D}_T\}$$

is a closed subset of $X \times X$. One says that $T$ is invertible in Neumann's sense if the following two conditions hold:

$$\text{(i)} \qquad T(\mathcal{D}_T) = X$$

There exists a constant $c > 0$ such that

$$\text{(ii)} \qquad ||T(x)|| \geq c \cdot ||x|| \quad : x \in \mathcal{D}_T$$

**Exercise.** Show that (i-ii) gives the existence of aa unique bounded liunear operator $R$ on $X$ whose range is equal to $\mathcal{D}_T$ and

$$(*) \qquad R(Tx) = x \quad : x \in \mathcal{D}_T \quad \& \quad T(Rx) = x : \ \forall \ x \in X$$

We put $R = T^{-1}$ and refer to this operator as Neumann's inverse of $T$. Notice that the operator in (*) is not invertible since $T$ is assumed to be unbounded. So the spectrum $\sigma(T^{-1})$ contains $\lambda = 0$. Next, the bounded linear operator $\sigma(T^{-1})$ has a compact spectrum in the complex $\lambda$-plane. It turns out thst it determines the spectrum of $T$.

**1. The position of $T$.** Assume as above that the densely defined and unbounded linear operator $T$ has a bounded inverse $R = T^{-1}$. The second equation in (*) means that the composed operator $T \circ R$ is the identity $E$. So if $\lambda$ is a non-zero complex number it follows that

$$(1.1) \qquad (T - \lambda \cdot E) \circ R = E - \lambda \cdot R$$

If the right hsnd side is invertible we get the bounded linear operator

$$(1.2) \qquad R \circ (E - \lambda \cdot R)^{-1}$$

The reader should check that (1.2) yields Neumann's inverse to the densely defined operator $T - \lambda \cdot E$ and conclude that

$$(1.3) \qquad \sigma(T) = \{\lambda \neq 0 \quad : \lambda^{-1} \in \sigma(R)\}$$

**Remark.** In general a densely defined operator $t$ with a closed graph may be "ugly" in the sense that $T - \lambda \cdot E$ fails to be invertible in Neumann'ssense for all complex numbers $\lambda$. But in many applications one enconters unbounded operators where Neumann's inverse exists on a non-empty open set of $\lambda$-values. of course, in contrast to bounded operators, the spectrum of an unbounded operator is in general not a compact set in the complex $\lambda$-plane. It is instructive to see examples. In $\mathbf{R}^3$ the Laplace operator $\Delta$ is densely defined on the Hilbert space $L^2(\mathbf{R}^3$. Plancherels formula gives

$$\Delta(f)(x) = -(2\pi i)^{-3} \int e^{i(x,\xi)} \cdot |\xi|^2 \cdot \widehat{f}(\xi)\, d\xi$$

where $f$ to begin with varies over text-functions. If $\lambda$ is a complex number it follows that

$$(\Delta - \lambda \cdot E)(f) = -(2\pi i)^{-3} \int e^{i(x,\xi)} \cdot (|\xi|^2 + \lambda) \cdot \widehat{f}(\xi)\, d\xi$$

if $\lambda$ stays outside $(-\infty, 0]$ the function $\xi \mapsto (|\xi|^2 + \lambda)^{-1}$ is bounded. Form this the reader should check that $\Delta - \lambda \cdot E$ is invertible and conclude that

$$\sigma(\Delta) = (-\infty, 0]$$

In particular the spectrum is real. Notice that the spectrum is not reduced to a discrete set of points.

Recal the major result from [ibid]. Let $\mathcal{H}$ be a separable Hilbert space whose Hermitian inner priodict assigns complex numbers $\langle x, y\rangle >$ for each pair of vectors $x, y$ in $\mathcal{H}$. Let $T\colon \mathcal{H} \to \mathcal{H}$ be a densely defined linear operator, i.r. the domain of definition for $T$ is a dense subspace $\mathcal{D}(T)$. One says that $T$ is symmetric if

$$(*) \qquad \langle Tx, y\rangle = \langle x, Ty\rangle \quad : x, y \in \mathcal{D}(T)$$

When (*) holds we define a subspace $\mathcal{H}_*$ of $\mathcal{H}$ which consists of vevtors $\xi$ such that there exists a constant $C(\xi)$ and

$$(1) \qquad |\langle Tx, \xi\rangle| \leq C(\xi) \cdot ||x|| \quad : x \in \mathcal{D}(T)$$

When (1 holds the densiity of $\mathcal{D}(T)$ and eucldian geometey yields a uniquie vector $\xi^*$ such that

$$(2) \qquad \langle Tx, \xi\rangle = \langle x, \xi^*\rangle \quad : x \in \mathcal{D}(T)$$

This yields a linrar opeeator $S$ where $\mathcal{D}(S) = \mathcal{H}_*$ and

$$(2) \qquad \langle Tx, \xi\rangle = \langle x, S(\xi)\rangle \quad : x \in \mathcal{D}(T)$$

From (1) we see that $\mathcal{D}(T) \subset \mathcal{D}(S)$ and the restrictionm of $S$ to $\mathcal{D}(T)$ is equal to $T$, i.e. $S$ is an extension of $T$. It is denoted by $T^*$ and called the adjoint operator of $T$. Following Carleman one says that the symmetric operator $T$ is self-adjoint if $T^* = T$. Notice that the self-adjoint condition in particular means that $\mathcal{D}(T)$ is equal to the space $\mathcal{H}_*$ above. let us remark that there exist "ugly" densely defined symmetric operators where $T \neq T^*$ and the spectrum of $T^*$ is non-real. Such operators were construcuted by Carelan in an earlier article from 1920 and offers an instructive lesson about integral kernels. here we shall not dwell upon this but pay attention to the self-adjoint case. More orecsiely, if $T$ is self-adjoint one first roves that the sepctrum $\sigma(T)$ is rela, i.e. for every non-real complkex number $\lambda$ the range of $\lambda \cdot E - T$ is equal to $|mathcalH$ and there exists a positive constant $c = c(\lambda)$ such that

$$||\lambda \cdot x - Tx|| \geq c \cdot ||x|| \quad : x \in \mathcal{D}(T)$$

Or phrased in another way, the densely defined linear ioperator $\lambda \cdot E - T$ has a resolvent given by a bounded liunear ioperator $R_T(\lambda)$ such that the composed operator

$$R_T(\lambda) \circ (\lambda \cdot E - T)$$

restricts to the identity on $\mathcal{D}(T)$. helre $R_T(\lambda)$ is a resolvent operator in the sense of carl neuann whose pionering work from 1879 paved the way towards spectral theory of in general unbounded unear operators. We assume that the reader is familiar with Neumann's calculus which for example gives a fornua for the closed spectrum $\sigma(T)$ with the aid to $\sigma(R_T(\lambda)$ for an arbitrary point $\lambda \in \mathbf{C} \setminus \sigma(T)$. More precisley one has the set-theoretic equality below for each fixed $\alpha \in \mathbf{C} \setminus \sigma(T)$:

$$\sigma(T) = \{\lambda :$$

**The Bohr-Schrödinger equation.**

Soon after the new-born quantum mechanics, Niels Bohr presented some mathematical problems at the Scandianvian Congress held in Copehagen 1925 where one eigenvaliue problem emerges from his theory of atoms together with the new physical theories put forward by his former student Heisenberg. More precisely, let $L^2(\mathbf{R}^3)$ be the Hilbert space of complex-valued square integrable functions in $\mathbf{R}^3$ and consider a potential function

$$W(p)=\sum_{\nu=1}^{\nu=N}\frac{m_\nu}{|p-q_\nu|}+b \tag{0.1}$$

where $\{q_\nu\}$ is an $N$-tuple of distinct points in $\mathbf{R}^3$ while $\{m_\nu\}$ and $b$ are positive constants. One seeks pairs $(\phi,\lambda)$ where $\phi$ an $L^2$-function which solves the equation

$$\Delta(\phi)+W\cdot\phi+\lambda\cdot\phi=0 \tag{*}$$

Above $\Delta$ is the Laplace operator. To find eigenfunctions and their associated eigenvalues we shall regard the densely defined operator

$$T(f)=\Delta(f)+W\cdot f \tag{1}$$

whose domain of definition contains all test-functions $f$. Then we can find solutions to (*) following the classic device introduced by Carl Neumann in his pioneering work from 1879. Namely, we shall find a positive number $\kappa$ such that the densely defined operator $T-\kappa^2$ has a bounded inverse in Neumann's sense and after the spectrum of $T$ is recaptured from the bounded operator $(T-\kappa)^{-1}$ via Neumann's calculus. This device was used by Carleman to give a positive response about solutions to (*). Here follow the details. First we consider the symmetric function in $\mathbf{R}^6$ defined by:

$$H(p,q)=\frac{e^{-\kappa\cdot|p-q|}}{|p-q|} \tag{2}$$

defined for pairs of points $p$ and $q$ in $\mathbf{R}^3$, where $\kappa$ is a positive real number. This kernel function gives a linear operator $\mathcal{H}$ defined by

$$\mathcal{H}(\phi)(p)=\int_{\mathbf{R}^3}H(p,q)\cdot\phi(q)\,dq$$

Newton's formula for the fundamental solution of the Laplace operator gives:

$$(\Delta-W)\circ\mathcal{H}=-4\pi\cdot E \tag{2.1}$$

where $E$ is the identity operator on $L^2(\mathbf{R}^3)$. We shall choose $\kappa$ so large that

$$\max_{p\in\mathbf{R}^3}\int H(p,q)W(q)\,dq=k<4\pi \tag{3}$$

The reader can easily check that this is indeed possible. From now on $\kappa$ is fixed so that (3) holds and now we prove that (3) implies that the densely defined operator $T-\kappa^2$ has an inverse in Neumann's sense. To attain this inverse operator we shall construct a symmetric kernel function $G(p,q)$ which gives a bounded linear operator

$$\phi\mapsto\mathcal{G}(\phi)(p)=\int G(p,q)\cdot\phi(q)\,dq$$

where $\mathcal{G}$ satsfies the operator equation

$$\mathcal{G}=\mathcal{H}+\frac{1}{4\pi}\cdot\mathcal{H}\circ(W\cdot\mathcal{G}) \tag{4}$$

Notice that (4) expressed as an integral equation in Fredholm's sense means that

$$G(p,q)=H(p,q)+\frac{1}{4\pi}\cdot\int H(p,x)W(x)G(x,q)\,dx \tag{4.1}$$

**5. Proposition.** *When (3) holds the equation (4) has a solution where $\mathcal{G}$ is a bounded linear operator.*

Before the proof we show how the bounded operator $\mathcal{G}$ can be used to analyze eigenfunctions in the Bohr-Schrödinger equation (*). Namely, (2.1) and (4) give:

$$(\Delta - \kappa^2) \circ \mathcal{G} = -4\pi \cdot E - W \cdot \mathcal{G} \implies (T - \kappa) \circ \mathcal{G} = -4\pi \cdot E$$

This means that

$$-\frac{1}{4\pi} \cdot \mathcal{G} = (T - \kappa^2 \cdot E)^{-1} \tag{5.1}$$

where the last term is Neumann's inverse of the densely defined operator $T - \kappa^2 \cdot E$. Now Neumann's general spectral formula implies that a pair $(\phi, \lambda)$ solves (*) if and only if the $L^2$-function $\phi$ satisfies the integral equation

$$\phi(p) = \frac{\lambda + \kappa^2}{4\pi} \cdot \int G(p,q) \cdot \phi(q)\, dq \tag{**}$$

### Proof of Proposition 5

Since the $W$-function is everywhere positive we can take its square root and define the symmetric kernel

$$S(p,q) = \sqrt{W(p)} \cdot H(p,q) \cdot \sqrt{W(q)} \tag{i}$$

Notice that (3) gives the inequality

$$\int S(p,q)\sqrt{W(q)}\, dq \leq k \cdot \sqrt{W(p)} \tag{ii}$$

Since $\sqrt{W}$ is everywhere positive, it follows by a wellknown inequality due to Schur that the operator norm of $\mathcal{S}$ is bounded by $k$. here $k < 4\pi$ and hence $E - \frac{1}{4\pi}\mathcal{S}$ is invertible. This gives the bounded linear operator

$$\mathcal{L} = \mathcal{S} \circ (E - \frac{1}{4\pi}\mathcal{S})^{-1} = \mathcal{S} + \sum_{\nu=1}^{\infty} (4\pi)^{-\nu} \cdot \mathcal{S}^{\nu+1}$$

**Exercise.** The reader may confirm that the kernel function

$$G(p,q) = \frac{L(p,q)}{\sqrt{W(p)} \cdot \sqrt{W(q)}}$$

satisfies the requested equation (4) and that $\mathcal{G}$ is a *compact* linear operator on the Hilbert space $L^2(\mathbf{R}^3)$.