Gauss's Theorem and the self-adjointness of Schrödinger operators

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1. An introductory survey

Let us not too quickly pass in review those proofs of the self-adjointness of Schrödinger operators that in one way or another bear upon our subject. We recommend Chapter X of [41] for an account of self-adjointness questions that takes a wider view and that also discusses their physical relevance, and we refer to [26] for an extensive bibliography. The expert reader may immediately proceed to p. 22.

If $\Omega \subset \mathbf{R}^n$ is an open (and in general an unbounded) set, and q a real-valued measurable function defined on Ω, we put

(1.1) $$\tau := -\Delta + q.$$

It is usually very easy to find a subspace $\mathfrak{S}$ of the Hilbert space $\mathfrak{H} := L^2(\Omega)$ such that $\tau \restriction \mathfrak{S}$ is a symmetric operator in $\mathfrak{H}$. One can take, for example,

(1.2) $$\mathfrak{S} := C_0^\infty(\Omega)$$

if (and only if)

(1.3) $$q \in L^2_{\text{loc}}(\Omega)$$

holds.

Let us assume (1.3) for the time being. We write

(1.4) $$T_{\min} := \tau \restriction \mathfrak{S}$$

because this is so to speak the smallest operator that can be associated with (1.1) in $\mathfrak{H}$. Since $T_{\min}$ is real, it has self-adjoint extensions [41, p. 143]. Of particular interest is the case that $T_{\min}$ has exactly one self-adjoint extension ($T_{\min}$ is then called essentially self-adjoint) in which case it is $\overline{T}_{\min}$, the closure of $T_{\min}$, that describes the dynamics of the underlying physical system (one or several particles in nonrelativistic quantum mechanics which are subject to external electrostatic forces or which interact with each other). If there are several self-adjoint extensions, each of these describes a different physical situation (See the excellent discussion in [41, pp. 141—145]), which can be specified by a certain "boundary condition" to be imposed on the elements of the domain of the adjoint of (1.4) given by

$$D\big((T_{\min})^*\big) = \{u \mid u,\ \tau u \in \mathfrak{H}\} \tag{1.5}$$

("$\tau u \in \mathfrak{H}$" means that τu is a distribution on $C_0^\infty(\Omega)$ which is generated by an $L^2(\Omega)$-function).

It is clear from (1.5) that $(T_{\min})^*$ is the largest operator pertaining to (1.1) in $\mathfrak{H}$. It is very easy to see that $T_{\min}$ is essentially self-adjoint if and only if $(T_{\min})^*$ is a symmetric operator, which is the case if and only if $\big((T_{\min})^* u, u\big)$ is real-valued for all $u \in D\big((T_{\min})^*\big)$. A self-adjointness proof suggesting itself is therefore the following. Use partial integration on $K \subset\subset \Omega'$[1] to obtain

$$\int_K (-\Delta u + qu)\bar{u} = -\int_{\partial K} \bar{u} \frac{\partial u}{\partial n} + \int_K (|\nabla u|^2 + q\,|u|^2) \tag{1.6}$$

$$\big(u \in D((T_{\min})^*)\big)$$

$\left(\text{"}\dfrac{\partial}{\partial n}\text{"}\right.$ denotes as usual the outer normal derivative on $\left.\partial K\right)$ and show that

$$\int_{\partial K} \bar{u} \frac{\partial u}{\partial n} \quad \big(u \in D((T_{\min})^*)\big)$$

tends to zero when K exhausts Ω.

Two questions, however, immediately obtrude themselves.

(Q.1) *Does the volume integral on the r.h.s. of* (1.6) *exist for all* $u \in D\big((T_{\min})^*\big)$?

(Q.2) *Has every* $u \in D\big((T_{\min})^*\big)$ *a representative for which the surface integral in* (1.6) *exists and for which Gauss's theorem is applicable*?

(Since ∂K will be a set of n-dimensional Lebesgue measure zero, it is clear that the surface integral in (1.6) does not make sense for the whole equivalence class $u \in D\big((T_{\min})^*\big)$.)

It was Carleman who in 1934 in the predecessor of this journal [5] and with the tools laid down in his memoir of 1923 [4] answered both questions positively for $q \in C^0(\mathbf{R}^3)$. Furthermore, he showed by a reasoning to be refined by Friedrichs [14, 15] that the surface integral in (1.6) tends to zero on a sequence of spheres the radii of which tend to infinity if q is in addition assumed to be bounded from below. (At the same time Friedrichs had established the essential self-adjointness of $T_{\min}$ under basically the same conditions in a seemingly different way [14][2]. We shall

[1] For open sets Ω_1, Ω_2 we write, following [1], $\Omega_1 \subset\subset \Omega_2$ if $\bar{\Omega}_1$ is compact and $\bar{\Omega}_1 \subset \Omega_2$.

[2] Satz 2, p. 691, in conjunction with his Footnote 6 (he assumes besides semiboundedness of q piecewise continuity if $n=1$ and $q \in C^1(\mathbf{R}^n)$ if $n \in \{2, 3\}$ [14, p. 777]), Cf. our Footnote 6.

come back to both proofs in § 6.) Dealing with $(T_{\min})^*$, i.e. with a closed operator, requires the notion of a generalized derivative, and it must be recalled that it was not until a few years later that such a notion was systematically developed by Sobolev [51] and Friedrichs [16]. Carleman's (and Friedrichs's) restriction to lower dimensions is today clear from eq. (1.8) below together with the Sobolev embedding theorems. It is only in dimensions up to three that every $u\in D\big((T_{\min})^*\big)$ contains a representative which is continuous [52, p. 69 f.].

It must be admitted that Carleman's paper is rather sketchy, and a more detailed investigation of $D\big((T_{\min})^*\big)$ was not taken up until after the war by Povzner [40], Stummel [54] and N. Nilsson [39]. The first two, however, are not concerned with questions (Q.1) and (Q.2). Nilsson answered (Q.1) in the affirmative if

$$q\in L^p_{\mathrm{loc}}(\Omega)\quad\text{for some}\quad p>\max\left\{2,\frac{n}{2}\right\},\tag{1.7}$$

but did not look into (Q.2). Instead he proved that $(T_{\min})^*$ is symmetric (under the additional requirement that q does not fall off at infinity faster than — const$\cdot r^2$) by using cut-off functions in order to avoid the surface term in (1.6). With the help of Stummel's results Ikebe—Kato [19] showed (see [44, Chapter 6] and [55] in this context) that

$$D\big((T_{\min})^*\big)=\{u\,|\,u\in H^2_{\mathrm{loc}}(\Omega)\cap\mathfrak{H},\ \tau u\in\mathfrak{H}\}^{3)}\tag{1.8}$$

if

$$q\in Q^\alpha_{\mathrm{loc}}(\Omega)\quad\text{for some}\quad\alpha\in(0,4]\tag{1.9}$$

where $Q^\alpha_{\mathrm{loc}}(\Omega)$ is a class of potentials that had been introduced by Stummel ((1.7) is a sufficient condition for q to be in this class).

Under condition (1.9) the answer to (Q.1) is therefore yes and so it is for (Q.2) owing to Sobolev's embedding theorem [16, p. 69 f.]. Using these results we proved in [22] that $(T_{\min})^*$ is symmetric (the underlying domain being $\Omega=\mathbf{R}^n\setminus\{0\}$) for potentials which may have a certain strong singularity at the origin and at most — const$\cdot r^2$ — behaviour at infinity by showing the vanishing of the surface terms in (1.6) along the lines drawn by Carleman and Friedrichs. Ikebe—Kato [19] and Jörgens [20], on the other hand, had established the symmetry of the adjoint of a general class of second-order elliptic operators by using cut-off functions.

In 1972 Kato [30] proved a distributional inequality (see Lemma 1 below) with the help of which he showed that $T_{\min}$ is essentially self-adjoint if q satisfies (1.3) with $\Omega=\mathbf{R}^n$ and is bounded from below. (This result had been conjectured by Simon [49]; for extensions to general second-order elliptic operators see [7, 8, 11,

[3)] For $m\in\mathbf{N}$ we write as usual "$H^m_{\mathrm{loc}}(\Omega)$" for the set of all (equivalence classes of) L^2_{loc}-functions whose generalized derivatives up to the order m belong to $L^2_{\mathrm{loc}}(\Omega)$.

27, 28, 33, 35, 45].) Kato remarks loc. cit. p. 139 that in the presence of such singularities of q it is a priori not clear whether a positive answer can be given to (Q.1). As a consequence his self-adjointness proof is not a symmetry proof of $(T_{\min})^*$. Rather he shows that $\overline{R(T_{\min}+c)}=\mathfrak{H}$ for some suitable $c>0$ using the fact that $(-\Delta+c)^{-1}$ is "positivity preserving" [41, p. 185 f.]. It will be one of the results of the present paper that even if the singularities of q are as strong as in [30] the answer to (Q.1), (Q.2) will still be yes, so that the indicated symmetry proof of $(T_{\min})^*$ can be accomplished.

As a matter of fact we shall show that this is true under even extremer circumstances like those envisaged by Kato in his 1974 paper [32]. It was in this paper that he even relaxed assumption (1.3). When doing this one faces the problem that there is no longer an obvious candidate for the set $\mathfrak{S}$ mentioned at the beginning. There is, however, a "largest" subspace of $\mathfrak{H}$ on which (1.1) can be considered, viz. the set of all those $u\in\mathfrak{H}$ for which the function qu generates a distribution on $C_0^\infty(\Omega)$ (so that τu also makes sense as a distribution) and for which $\tau u\in\mathfrak{H}$. A sufficient condition for qu to generate a distribution is, of course, $qu\in L^1_{\mathrm{loc}}(\Omega)$[4], and that is why Kato suggested

(1.10) $$\mathcal{M} := \{u \mid u\in\mathfrak{H},\ qu\in L^1_{\mathrm{loc}}(\Omega),\ \tau u\in\mathfrak{H}\}$$

as domain of the "largest"[5] operator to be associated with (1.1). Taking $\Omega=\mathbf{R}^n$, Kato established the self-adjointness of

$$T_{\max} := \tau \restriction \mathcal{M}$$

if

(1.11) $$q\in L^1_{\mathrm{loc}}(\Omega)$$

is bounded from below (for generalizations see [6, 9, 27, 28]). Knowles recently showed [34] that the q-dependent subspace

(1.12) $$\mathfrak{S} := \{u \mid u\in\mathcal{M},\ \operatorname{supp} u \text{ is compact in } \Omega\}$$

can replace (1.2) just as in the one-dimensional case if (1.3) no longer holds. That is to say, he assumes that q satisfies (1.11) with $\Omega=\mathbf{R}^n$ and is locally bounded from below and then proves that (1.4) with the $\mathfrak{S}$ given by (1.12) defines a symmetric operator with the property

(1.13) $$(T_{\min})^* = T_{\max}.$$

Now at last we can describe the contents of the present paper. Using Kato's

[4] In the one-dimensional case where (1.11) has long been the usual assumption rather than (1.3) [53, p. 458] no such requirement is necessary since a function u with a weak L^1-derivative is automatically locally absolutely continuous [46, p. 54; 52, p. 34].

[5] This should be taken with a grain of salt. If q is "very singular" $\mathcal{M}$ might consist solely of the null element.

distributional inequality (Lemma 1) we show in § 2 that all elements of $\mathcal{M}$ have locally finite energy integrals if q is locally bounded from below (Theorem 1). This answers (Q.1) in the affirmative. In § 3 we prove two versions of Gauss's theorem which are tailored to the needs of spectral theory. The first (Theorem 2) involves an integrand with compact support and therefore does not presuppose anything of the underlying domain. The second (Theorem 3) answers (Q.2) positively for almost every open set whose boundary is the level set of a "regular" function. In § 4 we combine our first version of Gauss's theorem with an idea due to Simader ([48]; see Lemma 5) to establish (1.13) for very general situations (see Theorem 4). The resulting proof is more elementary than Knowles's proof [34] in the sense that it avoids use of the anti-dual of certain Sobolev spaces, an avoidance which we believe increases its clarity.

The remaining Sections 5 and 6 are devoted to the special case

$$\Omega = \mathbf{R}^n_+ := \mathbf{R}^n \setminus \{0\} \tag{1.14}$$

with $q \in L^1_{\mathrm{loc}}(\mathbf{R}^n_+)$ locally bounded from below (but possibly not bounded from below at the origin or at infinity). This case has been studied extensively under conditions (1.9) [20, 21, 22, 26] or (1.3) [6, 25, 47, 50] ([6] contains also a result under assumption (1.11)). With relation (1.13) at our disposal, we can use our second version of Gauss's theorem to give a characterization of the Friedrichs extension of $T_{\min}$ [41, p. 177; 56, p. 317] by showing that a certain "distinguished" restriction of $T_{\max}$ is symmetric (Theorem 5) just as we did earlier under more stringent assumptions on q [21, 26] or in the one-dimensional case [24]. Under additional requirements on q, the Friedrichs extension of $T_{\min}$ turns out to coincide with $T_{\max}$, so that $T_{\min}$ is essentially self-adjoint[6] (Theorem 6).

Academic examples can, of course, be constructed which subordinate to our Theorems 5 or 6, but for which self-adjointness has not been established previously, but this is not our point. Our point is to show that even under condition (1.11) a self-adjointness proof can be reduced to a simple symmetry proof involving surface integrals. Concerning our preference to deal with surface terms rather than to avoid them by using cut-off functions, we find that it reduces the amount of technicalities in the proper self-adjointness proof and thus adds to its transparency when the use of cut-off function is restricted to preparatory theorems such as Theorems 1 to 4, where they are probably indispensable. Moreover, such theorems can be used in situations where surface integrals are not so easy to avoid, e.g. in questions about the absence of eigenvalues of Schrödinger operators (see [23] and the literature cited there). It is also with this idea of a building-block system in mind that we

[6] This is actually the way in which Friedrichs proved the essential self-adjointness of $T_{\min}$ under the conditions mentioned in Footnote 2.

do not try to avoid Kato's distributional inequality by truncating $u \in \mathcal{M}$ (as Frehse [13] in his proof of Theorem 1 does and as Simader does in his beautifully elementary self-adjointness proof in [47]).

We have being working intermittently on this paper for a couple of years starting in Princeton in the academic year of 1974/75. We acknowledge with pleasure that we are indebted to B. Simon for inviting us to Princeton University, to G. Hellwig for supporting leave of absence from Technische Hochschule Aachen, to Ministerium für Wissenschaft und Forschung des Landes Nordrhein-Westfalen for granting it, and to Deutsche Forschungsgemeinschaft for subsidizing it. Our thanks are also due to T. Kato for making [31] available to us, for permitting us to reproduce his result here (Theorem 7), and for pointing out to us (at the occasion of a visit of ours at Berkeley in 1975) that Theorem 1 had already been found by J. Frehse. They are due to J. Frehse for giving us his proof of Theorem 1 prior to its publication in [13], and in particular to J. Walter for countless stimulating discussions throughout our years in Aachen. They are due to H. Cycon and R. Wüst for spotting an error in the original manuscript and last, but not least to H. Leinfelder, now at the University of Bayreuth, for many vivid talks in connection with our lectures about the topic of the present paper at the University of Munich during the summer term of 1977, discussions that resulted in great simplifications of our original proofs of Theorems 1 and 2.

2. A local Dirichlet type result

In order to see what can be expected we start with the following

Example 1. Let $x \in \mathbf{R}^n$ and $r := |x|$. For $\nu > 0$ we define

$$q(r) := \begin{cases} \left[\nu^2 - \left(\frac{n-2}{2}\right)^2\right] r^{-2} & \text{if} \quad r > 0 \\ 0 & \text{if} \quad r = 0 \end{cases}$$

and

$$u_{\pm\nu}(r) := \begin{cases} r^{-\frac{n-2}{2} \pm \nu} & \text{if} \quad r > 0 \\ 0 & \text{if} \quad r = 0. \end{cases} \tag{2.1}$$

Then

$$-\Delta u_{+\nu} + q u_{+\nu} = 0 \quad (\nu > 0) \tag{2.2}$$

and

$$-\Delta u_{-\nu} + q u_{-\nu} = 0 \quad \left(\nu \in \left(0, \frac{n-2}{2}\right)\right) \tag{2.3}$$

hold in the sense of distributions on $\mathbf{R}^n$. Let $\mathcal{M}_{\mathrm{loc}}$ be the "localization" of (1.10) defined in eq. (2.6) below. We deduce from (2.1) and (2.2) for $n \neq 4$ and $\nu = 1$ that

$$u_{+\nu} \in \mathcal{M}_{\mathrm{loc}}, \quad \text{but} \quad qu_{+\nu}, \Delta u_{+\nu} \notin L^2_{\mathrm{loc}}(\mathbf{R}^n), \tag{2.4}$$

and from (2.1) and (2.3) for $n \geqq 3$ and $\nu \in \left(0, \min\left\{1, \frac{n-2}{2}\right\}\right)$ that

$$u_{-\nu} \in \mathcal{M}_{\mathrm{loc}},$$

but $\nabla u_{-\nu} \notin L^2_{\mathrm{loc}}(\mathbf{R}^n)$ and $|\nabla u_{-\nu}|^2 + q\,|u_{-\nu}|^2 \notin L^1_{\mathrm{loc}}(\mathbf{R}^n)$.

This example shows that the answer to (Q.1) will be no if q has strong negative singularities. If q is, however, locally bounded from below, the elements in the domain of the maximal operator will have locally finite kinetic and potential energies (which implies in particular that (Q.1) can be answered positively). This is the contents of Theorem 1.

Theorem 1 was found by J. Frehse as early as 1973 but was not published until recently [13]. (A "semilocal" version for $q \in L^2_{\mathrm{loc}}(\mathbf{R}^n)$ bounded from below can already be found in [30, Proposition 5]; the proof uses, however, the essential self-adjointness of $T_{\min}$ [30, Proposition 3]). We arrived at this theorem in 1974 and learned of Frehse's result in the following year as we mentioned in the introduction. The proof we shall give uses the following inequality of Kato's [30] (see [45, 10] for generalizations) the underlying geometric idea of which is very simple [41, p. 183].

Recall $(\operatorname{sign} f)(x) := \begin{cases} \dfrac{f(x)}{|f(x)|} & \text{if } f(x) \neq 0 \\ 0 & \text{if } f(x) = 0 \end{cases}$ $(x \in \Omega)$ for a function $f\colon \Omega \to \mathbf{C}$.

Lemma 1. *Let $\Omega \subset \mathbf{R}^n$ be open and u, $\Delta u \in L^1_{\mathrm{loc}}(\Omega)$. Then*

$$\Delta\,|u| \geqq \operatorname{Re}(\operatorname{sign} \bar{u} \cdot \Delta u)$$

in the distributional sense, i.e.

$$\int_\Omega |u|\,\Delta\varphi \geqq \int_\Omega \operatorname{Re}(\operatorname{sign} \bar{u} \cdot \Delta u)\,\varphi \tag{2.5}$$

for all $0 \leqq \varphi \in C_0^\infty(\Omega)$.

Theorem 1. *Assume that*

(2.i) *$\Omega \subset \mathbf{R}^n$ is open*

and

(2.ii) *$q\colon \Omega \to \mathbf{R}$ is measurable and bounded from below on every compact subset of Ω.*

Then

$$\nabla u, \sqrt{|q|}\,u \in L^2_{\mathrm{loc}}(\Omega)$$

for all

$$u \in \mathcal{M}_{\mathrm{loc}} := \{v \mid v \in L^2_{\mathrm{loc}}(\Omega),\ qv \in L^1_{\mathrm{loc}}(\Omega),\ \tau v \in L^2_{\mathrm{loc}}(\Omega)\}. \tag{2.6}$$

Proof. The difficulty one has to face is that there will be cancellations between the singularities of $-\Delta u$ and those of qu (see (2.4)). We proceed as follows. Let $K \subset\subset \Omega$ and K_1 such that $K \subset\subset K_1 \subset\subset \Omega$, and let $\zeta \in C_0^\infty(K_1)$ be a function with $0 \leqq \zeta \leqq 1$ and $\zeta(x)=1$ for $x \in K$. Suppose without loss of generality that $u \in \mathcal{M}_{\mathrm{loc}}$ is real-valued and $q \geqq 0$ on K_1.

Proof of $\sqrt{q}\,u \in L^2_{\mathrm{loc}}$. Let $\varrho \in (0, \operatorname{dist}(\bar{K}_1, \partial\Omega))$. Then, writing $v_\varrho := J_\varrho |u|$ where J_ϱ is the usual Friedrichs—Sobolev mollifier [16, 52] with kernel j_ϱ (see e.g. [1, 56] for its properties), we have

$$\int_{K_1} J_\varrho q|u| \cdot v_\varrho \zeta^2 = \int_{K_1} (-\Delta v_\varrho + J_\varrho q|u|) v_\varrho \zeta^2 - \int_{K_1} (\nabla v_\varrho)^2 \zeta^2$$
$$-2\int_{K_1} v_\varrho \nabla v_\varrho \cdot \zeta \nabla \zeta \leqq \int_{K_1} (-\Delta v_\varrho + J_\varrho q|u|) v_\varrho \zeta^2 + \int_{K_1} v_\varrho^2 (\nabla\zeta)^2.$$

Now,

$$0 \leqq j_\varrho(x-\cdot) \in C_0^\infty(\Omega)$$

for every $x \in K_1$. Using $j_\varrho(x-\cdot)$ as a test function in (2.5), we get (note $\Delta u \in L^1_{\mathrm{loc}}(\Omega)$ because of $-\Delta u + qu,\ qu \in L^1_{\mathrm{loc}}(\Omega)$)

$$-(\Delta v_\varrho)(x) = -(J_\varrho \Delta |u|)(x) \leqq -(J_\varrho(\operatorname{sign} u \cdot \Delta u))(x)$$

for all $x \in K_1$. Writing $w := -\Delta u + qu$ and observing

$$|J_\varrho(\operatorname{sign} u \cdot w)| \leqq J_\varrho |w| =: w_\varrho,$$

we therefore have

$$0 \leqq \int_{K_1} J_\varrho q|u| \cdot v_\varrho \zeta^2 \leqq \int_{K_1} w_\varrho v_\varrho \zeta^2 + \int_{K_1} v_\varrho^2 (\nabla\zeta)^2. \tag{2.7}$$

Since

$$\lim_{\varrho\to 0} \|J_\varrho f - f\|_{L^p(K_1)} = 0 \tag{2.8}$$

for every $f \in L^p_{\mathrm{loc}}(\Omega)$ $(p \geqq 1)$, the limit $\varrho \to 0$ on the r.h.s. of (2.7) exists. Hence

$$0 \leqq \limsup_{\varrho\to 0} \int_K J_\varrho q|u| \cdot v_\varrho \leqq \limsup_{\varrho\to 0} \int_{K_1} J_\varrho q|u| \cdot v_\varrho \zeta^2 < \infty. \tag{2.9}$$

In view of (2.8) and Riesz's lemma there exists a sequence $\{\varrho_n\}$ with $\varrho_n \to 0$ as $n \to \infty$ such that

$$J_{\varrho_n} q|u| \to q|u| \quad \text{a.e. on } K_1.$$

$$\lim_{n\to\infty} \|v_{\varrho_n} - |u|\|_{L^2(K_1)} = 0$$

then implies the existence of a subsequence $\{\sigma_n\}$ of $\{\varrho_n\}$ with $\sigma_n \to 0$ as $n \to \infty$ and

$$v_{\sigma_n} \to |u| \quad \text{a.e. on } K_1.$$

On account of (2.9) the sequence defined by $f_n := J_{\sigma_n} q|u| \cdot v_{\sigma_n}$ $(n \in \mathbf{N})$ satisfies the hypotheses of Fatou's lemma. Hence $q|u| \cdot |u| \in L^1(K)$.

Proof of $\nabla u \in L^2_{\mathrm{loc}}$. From

$$\int_{K_1} (\nabla J_\varrho u)^2 \zeta^2 = \int_{K_1} (-\Delta J_\varrho u + J_\varrho qu) J_\varrho u \cdot \zeta^2 - \int_{K_1} J_\varrho qu \cdot J_\varrho u \cdot \zeta^2 - 2\int_{K_1} J_\varrho u \cdot \nabla J_\varrho u \cdot \zeta \nabla \zeta$$

we infer

$$\tfrac{1}{2} (\nabla J_\varrho u)^2 \zeta^2 \leqq \int_{K_1} J_\varrho w \cdot J_\varrho u \cdot \zeta^2 + \int_{K_1} J_\varrho q |u| \cdot v_\varrho \zeta^2 + 2\int_{K_1} (J_\varrho u)^2 (\nabla \zeta)^2.$$

Hence

$$\limsup_{\varrho\to 0} \int_K (\nabla J_\varrho u)^2 \leqq \limsup_{\varrho \to 0} \int_{K_1} (\nabla J_\varrho u)^2 \zeta^2 < \infty \tag{2.10}$$

because of (2.9).

Let $j \in \{1, \dots, n\}$. It is clear from (2.10) and from the fact that $C_0^\infty(K)$ is dense in $L^2(K)$ that

$$f_j(v) := \lim_{\varrho \to 0} (v, \partial_j J_\varrho u) \quad (v \in L^2(K))$$

defines a continuous linear functional on $L^2(K)$. According to the Riesz representation theorem there exists therefore an element $w_j \in L^2(K)$ with the property

$$f_j(v) = (v, w_j) \quad (v \in L^2(K)).$$

Sending $\varrho \to 0$ in

$$-(\partial_j \varphi, J_\varrho u) = (\varphi, \partial_j J_\varrho u) \quad (\varphi \in C_0^\infty(K))$$

we obtain

$$-(\partial_j \varphi, u) = (\varphi, w_j) \quad (\varphi \in C_0^\infty(K)).$$

Thus $\partial_j u$ exists in the generalized sense, and we have $\partial_j u = w_j \in L^2(K)$. ▮

Remark 1. For $q=0$ Theorem 1 reduces to a special case of V. I. Krylov's embedding theorem [46, pp. 181 f., 190]. It is not difficult to see $\mathcal{M}_{\mathrm{loc}} = H^2_{\mathrm{loc}}(\Omega)$ in this case.

Remark 2. For $q \in L^2_{\mathrm{loc}}(\Omega)$ locally bounded from below and $u \in L^2_{\mathrm{loc}}(\Omega)$ satisfying $\tau u = 0$ in the distributional sense Frehse [13] derives the sharp result to be expected from Example 1 that $u \in L^\infty_{\mathrm{loc}}(\Omega) \cap H^2_{\mathrm{loc}}(\Omega)$.

3. Gauss's theorem for functions in $D(T_{\max})$

We begin with a version of Gauss's theorem that does not require any well-behaviour of the open set $\Omega \subset \mathbf{R}^n$ since the integrand has compact support.

Theorem 2. *Under the hypotheses of Theorem* 1 *we have*

$$-\int_\Omega u \, \Delta v = \int_\Omega \nabla u \, \nabla v \tag{3.1}$$

for all $u, v \in \mathcal{M}_{\mathrm{loc}}$ *if* u *or* v *has compact support in* Ω.

Proof. Suppose that v has compact support in Ω. Let $\operatorname{supp} v \subset K \subset\subset \Omega$ be a set with $\delta := \operatorname{dist}(\operatorname{supp} v, \partial K) > 0$ and $0 < \varrho,\ \sigma < \min\{\delta,\ \operatorname{dist}(K, \partial\Omega)\}$. Then

$$-\int_K J_\varrho u \cdot \Delta J_\sigma v = \int_K \nabla J_\varrho u \cdot \nabla J_\sigma v \tag{3.2}$$

by the usual Gauss theorem, since $J_\sigma v$ has compact support in K. Applying Theorem 1 we see that the r.h.s. of (3.2) tends to the r.h.s. of (3.1) as $\varrho, \sigma \to 0$. The l.h.s. of (3.2), however, is somewhat more difficult to handle. On account of $\Delta v \in L^1(K)$ it tends to

$$-\int_K J_\varrho u \cdot \Delta v$$

as $\sigma \to 0$. To perform the limit $\varrho \to 0$ we have to find an integrable dominating function. Let u_m be the truncation of u,

$$u_m := \begin{cases} u & \text{if } |u| \leqq m \\ m \operatorname{sign} u & \text{if } |u| > m \end{cases} \quad (m \in \mathbf{N}).$$

Theorem 1 then implies $u_m \in H^1_{\mathrm{loc}}(\Omega)$ for all $m \in \mathbf{N}$ and

$$\lim_{m\to\infty} \|u - u_m\|_{L^2(K)} = \lim_{m\to\infty} \|\nabla u - \nabla u_m\|_{L^2(K)} = 0$$

(cf. [47, p. 56]). This allows us to conclude

$$-\int_K u_m \Delta v = \int_K \nabla u_m \cdot \nabla v \quad (m \in \mathbf{N})$$

from (3.2) with "u" replaced by "u_m". (The limit $\sigma \to 0$ is uncritical; for the limit $\varrho \to 0$ Riesz's lemma and $|J_\varrho u_m| \leqq m$ have to be used.) To handle the l.h.s. of this equation (the r.h.s. again being easy), we note $|u_m| \leqq |u|$ and $u\Delta v \in L^1(K)$ this latter relation following from $quv \in L^1(K)$ (by Theorem 1) and $(-\Delta v + qv)u \in L^1(K)$. Hence

$$\lim_{m\to\infty} \int_K u_m \Delta v = \int_K u \Delta v$$

by the dominated convergence theorem. ∎

The open set $\Omega \subset \mathbf{R}^n$ on which the differential expression (1.1) is to be considered will in quantum mechanical applications usually be of a very simple nature. It will, for example, be $\mathbf{R}^n$ itself, or the exterior of a ball, or $\mathbf{R}^n$ with some isolated points or some easily describable submanifolds left out. Accordingly the subset K in (1.6) will also be a very simple one, e.g. a ball or an annulus. It will therefore be of sufficient generality to assume (cf. [43]) that

(3.i) *Ω is a finitely connected domain such that there exists a compact set $B \subset \Omega$ and a real-valued function $f \in C^1(\Omega \setminus B)$ with $|\nabla f| > 0$ and $\lim_{x \to \partial\Omega} f(x) = \infty$. (We regard ∞ as a point of $\partial\Omega$ in case Ω is unbounded.)*

It follows from (3.i) that there exists a number t_0 with the property that

$$\Omega_t := \{x \mid x \in \Omega \setminus B,\ f(x) < t\} \quad (t \geqq t_0) \tag{3.3}$$

is a finitely connected bounded domain the boundary of which consists of smooth $(n-1)$-dimensional closed surfaces which permit application of the classical Gauss theorem. (We note in passing that Gauss's theorem was proved in a very general setting by de Giorgi and Federer [12, p. 478].)

Theorem 3. *Suppose that condition* (3.i) *holds in addition to those of Theorem* 1. *Then*

$$-\int_{\Omega_t} u\,\Delta v = -\int_{\partial\Omega_t} u\,\nabla v \frac{\nabla f}{|\nabla f|} + \int_{\Omega_t} \nabla u\,\nabla v \tag{3.4}$$

for all $u, v \in \mathcal{M}_{\mathrm{loc}}$ *and almost all* $t \geqq t_0$ $(\Omega_t$ *and* t_0 *as in* (3.3)$)$.

Proof. Let $\tau > t \geqq t_0$, $u, v \in \mathcal{M}_{\mathrm{loc}}$, and $\varrho, \sigma \in (0, \operatorname{dist}(\bar\Omega_t, \partial\Omega))$. Gauss's theorem then yields (see [43])

$$-\int_{\Omega_t} J_\varrho u \cdot \Delta J_\sigma v = -\int_{\partial\Omega_t} J_\varrho u \cdot \nabla J_\sigma v \frac{\nabla f}{|\nabla f|} + \int_{\Omega_t} \nabla J_\varrho u \cdot \nabla J_\sigma v.$$

Therefore

$$-\int_t^\tau \Big(\int_{\Omega_\lambda} J_\varrho u \cdot \Delta J_\sigma v\Big) d\lambda = -\int_{\Omega_\tau \setminus \bar\Omega_t} J_\varrho u \cdot \nabla J_\sigma v \cdot \nabla f + \int_t^\tau \Big(\int_{\Omega_\lambda} \nabla J_\varrho u \cdot \nabla J_\sigma v\Big) d\lambda \tag{3.5}$$

by Fubini's theorem. With the dominated convergence theorem and Theorem 1 at our disposal, there is no problem to perform the limits $\varrho, \sigma \to 0$ on the r.h.s. of (3.5). That the l.h.s. of (3.5) also tends to what one expects can be shown by the argument given in the proof of Theorem 2. Thus we arrive at

$$-\int_t^\tau \Big(\int_{\Omega_\lambda} u\,\Delta v\Big) d\lambda = -\int_{\Omega_\tau \setminus \bar\Omega_t} u\,\nabla v \cdot \nabla f + \int_t^\tau \Big(\int_{\Omega_\lambda} \nabla u \cdot \nabla v\Big) d\lambda. \tag{3.6}$$

In view of Theorem 1 and Fubini's theorem

$$\int_{\partial\Omega_\lambda} u\,\nabla v \frac{\nabla f}{|\nabla f|}$$

exists for almost all $\lambda \geqq t_0$ and is integrable. Moreover,

$$\int_{\Omega_\tau \setminus \bar\Omega_t} u\,\nabla v \cdot \nabla f = \int_t^\tau \Big(\int_{\partial\Omega_\lambda} u\,\nabla v \frac{\nabla f}{|\nabla f|}\Big) d\lambda.$$

We therefore obtain the desired relation (3.4) by using Lebesgue's theorem on differentiation in (3.6). ∎

Remark 3. Results related to Theorems 2 and 3, but with stronger stipulations on the functions and a weaker condition on the domain can be found in [2]. Both theorems are well-known if $D((T_{\min})^*)=D(T_{\max})$ can be described by (1.8) (cf. [37, p. 41 f.]). In case (1.8) holds, every class $u, v\in D(T_{\max})$ contains a representative with which (3.4) holds for all $t\geqq t_0$.

In order to perform partial integrations with the elements of $D(T_{\max})$ to our heart's content we need the following lemma at least part of which is well-known (cf. [52, p. 84]).

Lemma 2. *Suppose that assumption* (3.i) *is satisfied with a function* $f\in C^2(\Omega\setminus B)$ *and let* Ω_t *and* t_0 *be as in* (3.3). *Then every class* $\hat{u}\in H^1_{\mathrm{loc}}(\Omega)$ *has a representative* u *for which*

$$\psi_u(t):=\int_{\partial\Omega_t}|u|^2\quad(t\geqq t_0)$$

exists and defines a locally absolutely continuous function. Moreover,

$$\psi_u'(t)=\int_{\partial\Omega_t}2\,\mathrm{Re}\,(\bar{u}\nabla u)\frac{\nabla f}{|\nabla f|^2}+\int_{\partial\Omega_t}\frac{|u|^2}{|\nabla f|^2}\left[\Delta f-\frac{1}{2}\frac{\nabla f}{|\nabla f|^2}\nabla(|\nabla f|^2)\right]\tag{3.7}$$

for almost all $t\geqq t_0$.

Proof. Let $\varrho, \varrho'>0$ and $\tau>t\geqq t_0$. With the abbreviation $v_\varrho:=J_\varrho\hat{u}$ we have, as a consequence of Gauss's Theorem (cf. [43]),

$$\int_{\partial\Omega_t}\frac{|v_\varrho|^2}{|\nabla f|}\nabla f\frac{\nabla f}{|\nabla f|}=\int_{\Omega_t}\frac{|v_\varrho|^2}{|\nabla f|}\Delta f+\int_{\Omega_t}\nabla\frac{|v_\varrho|^2}{|\nabla f|}\cdot\nabla f$$

$$=\int_{\Omega_t}2\,\mathrm{Re}\,(\bar{v}_\varrho\nabla v_\varrho)\frac{\nabla f}{|\nabla f|}+\int_{\Omega_t}\frac{|v_\varrho|^2}{|\nabla f|}\left[\Delta f-\frac{1}{2}\frac{\nabla f}{|\nabla f|^2}\nabla(|\nabla f|^2)\right]$$

and therefore

$$\psi_{v_\varrho}(\tau)-\psi_{v_\varrho}(t)=\int_t^\tau\left(\int_{\partial\Omega_\lambda}2\,\mathrm{Re}\,(\bar{v}_\varrho\nabla v_\varrho)\frac{\nabla f}{|\nabla f|^2}\right)d\lambda\tag{3.8}$$

$$+\int_t^\tau\left(\int_{\partial\Omega_\lambda}\frac{|v_\varrho|^2}{|\nabla f|^2}\left[\Delta f-\frac{1}{2}\frac{\nabla f}{|\nabla f|^2}\nabla(|\nabla f|^2)\right]\right)d\lambda.$$

By differentiation we obtain (3.7) for all $t\geqq t_0$ with "u" replaced by "v_ϱ". Insertion of $\psi_{v_\varrho-v_{\varrho'}}$ into the trivial identity

$$g(t)=\frac{1}{\tau-t}\left[\int_t^\tau(s-\tau)g'(s)\,ds+\int_t^\tau g(s)\,ds\right]\quad(g\in C^1([t,\tau]))$$

therefore yields

$$\int_{\partial\Omega_t}|J_\varrho\hat{u}-J_{\varrho'}\hat{u}|^2\leqq\mathrm{const}\int_{\Omega_\tau\setminus\bar{\Omega}_t}(|J_\varrho\hat{u}-J_{\varrho'}\hat{u}|^2+|\nabla J_\varrho\hat{u}-\nabla J_{\varrho'}\hat{u}|^2)$$

Thus $\{J_\varrho \hat{u} \upharpoonright \partial\Omega_t\}$ is a Cauchy sequence in $L^2(\partial\Omega_t)$ the limit element of which defines the desired representative $u \in \hat{u}$. Now we can take the limit $\varrho \to 0$ in (3.8) (using Fubini's theorem on the r.h.s.). The resulting relation shows (using Fubini again) that ψ_u can be written as the indefinite integral over a summable function. This proves that ψ_u is locally absolutely continuous. (3.7) then follows by differentiation. ▮

We conclude this section with an observation we need in the proof of Theorem 4.

Remark 4. Let $\Omega \subset \mathbf{R}^n$ be open. With the help of the Friedrichs—Sobolev mollifiers one can immediately prove [37, p. 42] that Gauss's theorem holds good in the form

$$\int_\Omega \nabla u \cdot v = -\int_\Omega u \nabla v$$

for all $u, v \in H^1_{\mathrm{loc}}(\Omega)$ when u or v has compact support in Ω.

4. $(T_{\min})^* = T_{\max}$

Relation (1.13), which we let also occur in the heading of this section, is an immediate consequence of the notion of a generalized derivative if (1.3) holds, but it seems to be unknown whether this relation persists if (1.3) is weakened to (1.11). It is well-known, but not all obvious that it does if $n=1$ [53, p. 458; 38, p. 68]. One problem is to ascertain that $T_{\min}$ is in fact densely defined. It was Kato [32] who showed that the theory of sesquilinear forms provides a convenient tool to see that $T_{\max}$ is densely defined which result he proved under the assumptions that $\Omega = \mathbf{R}^n$ and that

(4.i) $\qquad q \in L^1_{\mathrm{loc}}(\Omega)$ is locally bounded from below.

Once $T_{\min}$ has been introduced, which was first done for $n>1$ under condition (4.i) (and $\Omega = \mathbf{R}^n$) by Knowles [34], it is not difficult to see that it is also densely defined. As we mentioned in the introduction, Knowles then established (1.13) by using the antidual of $H^1(\Omega)$ (or rather of some modified Sobolev space because he dealt with general second-order elliptic operators). Applying our version of Gauss's theorem laid down in Theorem 2 in conjunction with an idea of Simader [48] (the regularity result of Lemma 5 below is basically due to him), we shall show that this part of his proof can be replaced by a much more elementary argument.

We shall assume throughout this section (without repeating this again) that the underlying domain Ω has property (3.i) and that q satisfies (4.i). To prove that

$T_{\min}$ is densely defined under these conditions, we mimic an argument of Kato's [32]. Let t_0 be as in (3.3), $t_0 \leqq k \in \mathbf{N}$, and $\varphi_k \in C_0^\infty(\Omega)$ a function with

$$0 \leqq \varphi_k \leqq 1 \quad \text{and} \quad \varphi_k = \begin{cases} 1 & \text{on} \quad \Omega_k \\ 0 & \text{on} \quad \Omega \diagdown \Omega_{k+1} \end{cases}$$

Let $c \in \mathbf{R}$. Then

$$q_k := \begin{cases} q & \text{on} \quad \Omega_{k+1} \\ c & \text{on} \quad \Omega \diagdown \Omega_{k+1} \end{cases} \tag{4.1}$$

belongs to $L^1_{\mathrm{loc}}(\Omega)$ and is bounded from below. The sesquilinear form

$$h_k(u, v) := \int_\Omega q_k u \bar{v} \quad (u, v \in \{w | w, \sqrt{|q_k|}\, w \in \mathfrak{H}\})$$

is therefore densely defined, closed, and bounded from below [29, p. 348]. These properties are shared by the sesquilinear form

$$h_0(u, v) := \int_\Omega \nabla u \overline{\nabla v} \quad (u, v \in H_0^1(\Omega))^{7)}$$

(cf. [29, pp. 347, 352]). Hence $h_0 + h_k$ is also densely defined, closed, and bounded from below [29, p. 319]. Let H_k be the self-adjoint operator determined by this form. Then

$$D(H_k) \subset D(h_0 + h_k) \tag{4.2}$$

and

$$(H_k u, u) = \|\nabla u\|^2 + \int_{\mathbf{R}^n} q_k |u|^2 \quad (u \in D(H_k)) \tag{4.3}$$

[29, p. 322]. Moreover, it follows immediately from [29, p. 348 f.] or [32, p. 197] that

$$H_k \subset T_{\max}^{(k)} \tag{4.4}$$

where $T_{\max}^{(k)}$ is the maximal Schrödinger operator associated with $-\Delta + q_k$ in $\mathfrak{H}$

Lemma 3. *Let* $u \in D(H_k)$. *Then*

$$\varphi_k u \in D(H_k) \cap D(T_{\min})$$

and

$$H_k \varphi_k u = T_{\min} \varphi_k u.$$

Proof. Let $u \in D(H_k)$. In view of (4.4) and the trivial relations

$$\varphi_k u \in \mathfrak{H}, \quad \operatorname{supp} \varphi_k u \quad \text{is compact in} \quad \Omega,$$

$$q \varphi_k u = q_k \varphi_k u \in L^1_{\mathrm{loc}}(\Omega),$$

it is only the statement $\tau \varphi_k u \in \mathfrak{H}$ that remains to be checked. Its validity, however,

7) $H_0^1(\Omega)$ is the closure of $C_0^\infty(\Omega)$ in the Sobolev norm $(\|\cdot\|^2 + \|\nabla \cdot\|^2)^{1/2}$.

results immediately from

$$\tau\varphi_k u = \varphi_k \tau u - u\Delta\varphi_k - 2\nabla u \nabla\varphi_k, \tag{4.5}$$

which holds in the sense of distributions on Ω, together with (4.2). ∎

After these preparations we are in a position to prove

Lemma 4. *$T_{\min}$ is a symmetric operator.*

Proof. Let $u\in\mathfrak{H}$ and $\varepsilon>0$. Now pick a number $j\geqq t_0$ such that $\|\varphi_j u-u\|<\frac{\varepsilon}{2}$. Since H_j is, of course, densely defined, there exists a $v\in D(H_j)$ with $\|v-u\|<\frac{\varepsilon}{2}$. By Lemma 3, $\varphi_j v$ is an element in $D(T_{\min})$ with $\|\varphi_j v-u\|<\varepsilon$. Hence $\overline{D(T_{\min})}=\mathfrak{H}$. That

$$(T_{\min}u, v) = (u, T_{\min}v) \quad \big(u, v\in D(T_{\min})\big)$$

holds, follows from Theorem 2. ∎

Let k and H_k be again as before.

Lemma 5. *Let $v\in\mathfrak{H}$ and suppose that there exists a number $K>0$ such that*

$$|(H_k u, v)| \leqq K(\|u\|+\|\nabla u\|) \quad \big(u\in D(H_k)\big). \tag{4.6}$$

Then ∇v exists in the sense of distributions on Ω and belongs to $\mathfrak{H}$.

Proof. Let $j\in\{1, \dots, n\}$ and $v\in\mathfrak{H}$. If we can show the existence of a number $M>0$ such that

$$|(v, \partial_j\varphi)| \leqq M\|\varphi\| \quad \big(\varphi\in C_0^\infty(\Omega)\big), \tag{4.7}$$

then the assertion follows by means of the Riesz representation theorem as in the last part of the proof of Theorem 1.

Let $a>\frac{1}{2}-\inf q_k$ where q_k is given by (4.1), and let $\varphi\in C_0^\infty(\Omega)$. Since H_k+a is self-adjoint and strictly positive, there exists an element $w\in D(H_k)$ with

$$(H_k+a)w = \partial_j\varphi.$$

Taking (4.2) and (4.3) into account we conclude

$$\begin{aligned}\|\nabla w\|^2+\tfrac{1}{2}\|w\|^2 &\leqq \|\nabla w\|^2+\int_{\mathbf{R}^n}(q_k+a)|w|^2\\ &= \big((H_k+a)w, w\big)\\ &= (\partial_j\varphi, w) = -(\varphi, \partial_j w)\\ &\leqq \tfrac{1}{2}(\|\nabla w\|^2+\|\varphi\|^2)\end{aligned}$$

whence

$$(\|w\|^2+\|\nabla w\|^2)^{1/2} \leqq \|\varphi\|.$$

Using (4.6) we therefore arrive at

$$\begin{aligned}|(v, \partial_j \varphi)| &= |(v, (H_k+a)w)| \\ &\leqq (K+|a|\,\|v\|)(\|w\|+\|\nabla w\|) \\ &\leqq \sqrt{2}(K+|a|\,\|v\|)(\|w\|^2+\|\nabla w\|^2)^{1/2} \\ &\leqq \sqrt{2}(K+|a|\,\|v\|)\|\varphi\|,\end{aligned}$$

which is inequality (4.7) we set out to prove. ▮

Theorem 4. $(T_{\min})^* = T_{\max}$.

Proof of $T_{\max} \subset (T_{\min})^*$. Let $v \in D(T_{\max})$ and $f := T_{\max} v$. Then it follows from Theorem 2 that

$$(T_{\min} u, v) = (u, f)$$

for all $u \in D(T_{\min})$. Hence $v \in D((T_{\min})^*)$ and $(T_{\min})^* v = \mathrm{f}$.

Proof of $(T_{\min})^* \subset T_{\max}$. Let $v \in D((T_{\min})^*)$. Furthermore, let k, φ_k, and H_k be as before. From (4.5) and Lemma 3 we deduce

$$\begin{aligned}(H_k u, \varphi_k v) &= (T_{\min} \varphi_k u, v) + (u \Delta \varphi_k, v) + 2(\nabla u \cdot \nabla \varphi_k, v) \\ &= (u, \varphi_k (T_{\min})^* v + \Delta \varphi_k \cdot v) + 2(\nabla u, v \nabla \varphi_k)\end{aligned} \tag{4.8}$$

for all $u \in D(H_k)$. Thus

$$|(H_k u, \varphi_k v)| \leqq K(\|u\|+\|\nabla u\|) \quad (u \in D(H_k))$$

where

$$K := \max\{\|\varphi_k (T_{\min})^* v\| + \|\Delta \varphi_k \cdot v\|,\ 2\|v \nabla \varphi_k\|\}.$$

Hence $\nabla(\varphi_k v) \in \mathfrak{H}$ by Lemma 5. Since $k \geqq t_0$ was arbitrary, we obtain $\nabla v \in L^2_{\mathrm{loc}}(\Omega)$.

This information together with Remark 4 enables us to carry out a partial integration in the second term on the r.h.s. of (4.8). Writing

$$g := \varphi_k (T_{\min})^* v - \Delta \varphi_k \cdot v - 2 \nabla \varphi_k \cdot \nabla v \in \mathfrak{H},$$

we have

$$(H_k u, \varphi_k v) = (u, g)$$

for all $u \in D(H_k)$. Thus

$$\varphi_k v \in D((H_k)^*) = D(H_k) \tag{4.9}$$

and

$$H_k \varphi_k v = g. \tag{4.10}$$

Because of (4.2), (4.9) implies in particular $qv \in L^1_{\mathrm{loc}}(\Omega)$. (4.10) yields

$$g(x) = ((T_{\min})^* v)(x) = (\tau v)(x)$$

for almost all $x \in \Omega_k$, which means $\tau v \in \mathfrak{H}$. Hence $v \in D(T_{\max})$. ▮

5. The Friedrichs extension of $T_{\min}$

Many proofs of the essential self-adjointness of *semibounded* Schrödinger operators ([3, 17, 18, 36, 42] for $n=1$, [6; 31, see Theorem 7 below] for $n\geqq 1$; cf. also [22, 25, 50] and [26, p. 190]) rest (sometimes in disguised form) on the existence of a comparison potential $Q\leqq q$ such that

$$-\Delta u+Qu = 0 \tag{5.1}$$

has positive solutions which are not square integrable near the boundary. In one dimension the existence of such solutions is in fact equivalent to the essential self-adjointness of the (semibounded) minimal operator, and it is apparently an open question to what extent this is also true in higher dimensions. It is Rellich's fundamental paper [42] that exhibits for $n=1$ most clearly the role positive solutions of (5.1) play both in the characterization of the Friedrichs extension of the minimal operator and in proving its essential self-adjointness.

In [24] we gave a version of Rellich's result that is amenable to multi-dimensional generalizations, as we mentioned loc. cit., p. 513. With Theorem 4 and the information from Section 2 that we can perform all partial integrations we wish with the elements of $D(T_{\max})$, we have now paved the way for actually carrying out this generalization. We consider the case (1.14). Employing the notation

$$B_{st} := \{x|x\in\mathbf{R}^n,\ s<|x|<t\} \quad (0\leqq s<t<\infty)$$

we assume without further repetition in this section that the following conditions are satisfied:

(5.i) $q\in L^1_{\mathrm{loc}}(\mathbf{R}^n_+)$;

(5.ii) there exist numbers $c, c_1, c_2\in\mathbf{R}$, $r_2>r_1>0$, and functions $0<f_1\in C^2((0,r_1])$, $0<f_2\in C^2([r_2,\infty))$ such that

$$q\geqq Q:=\begin{cases}(r^{n-1}f_1)^{-1}(r^{n-1}f_1')'+c_1 & \text{on } B_{0r_1}\\ c & \text{on } B_{r_1r_2}\\ (r^{n-1}f_2)^{-1}(r^{n-1}f_2')'+c_2 & \text{on } B_{r_2\infty}.\end{cases}$$

Lemma 6. *$T_{\min}$ is bounded from below.*

Proof. Because of Lemma 4 it suffices to prove

$$(T_{\min}u, u)\geqq \gamma\|u\|^2 \quad (u\in D(T_{\min}))$$

for some $\gamma\in\mathbf{R}$. Let $0<\eta\in C^2(\mathbf{R}^n_+)$, $u\in D(T_{\max})$, and write

$$S_t := \{x|x\in\mathbf{R}^n,\ |x|=t\} \quad (t>0).$$

By virtue of Theorem 1 and Fubini's theorem

$$\chi(t) := \int_{S_t} \eta^2 \frac{\bar{u}}{\eta}\left(\frac{u}{\eta}\right)'$$ [8]

exists for almost all $t>0$.

It follows from the factorization identity

$$\eta\tau u = u\tau\eta - \nabla\left(\eta^2 \nabla \frac{u}{\eta}\right)$$

and Theorem 3 that

$$\int_{B_{st}} \tau u \cdot \bar{u} = -\chi|_t^s + \int_{B_{st}} \left(\eta^2 \left|\nabla \frac{u}{\eta}\right|^2 + \frac{\tau\eta}{\eta}|u|^2\right) \tag{5.2}$$

for almost all $0<s<t<\infty$. Now, if $u \in D(T_{\min})$ we can immediately let $s \to 0$, $t \to \infty$ to obtain

$$(T_{\min} u, u) = \left\|\eta\nabla\frac{u}{\eta}\right\|^2 + \int_{\mathbf{R}^n} \frac{\tau\eta}{\eta}|u|^2.$$

If we choose η such that

$$\eta = \begin{cases} f_1 & \text{on} \quad B_{0r_1} \\ f_2 & \text{on} \quad B_{r_2\infty} \end{cases} \tag{5.3}$$

and use (5.ii), we get

$$(T_{\min} u, u) \geqq \int_{B_{0r_1}} f_1^2 \left|\nabla \frac{u}{f_1}\right|^2 + \int_{B_{r_2\infty}} f_2^2 \left|\nabla \frac{u}{f_2}\right|^2 - \gamma\|u\|^2 \tag{5.4}$$

where $\gamma := \max\{|c|, |c_1|, |c_2|\}$. ∎

Let us introduce the following function,

$$h_\gamma^{(j)}(r) := \left|\int_\gamma^r \frac{dt}{t^{n-1} f_j^2(t)}\right|$$

$$(\gamma, r \in [0, r_1] \text{ if } j = 1; \quad \gamma, r \in [r_2, \infty] \text{ if } j = 2).$$

As far as the behaviour of the functions f_1, f_2 from (5.ii) near the endpoints 0 or ∞ is concerned, the following four cases are possible,

case a: $h_0^{(1)}(r_1) < \infty, \quad h_\infty^{(2)}(r_2) < \infty;$

case b: $h_0^{(1)}(r_1) < \infty, \quad h_\infty^{(2)}(r_2) = \infty;$

case c: $h_0^{(1)}(r_1) = \infty, \quad h_\infty^{(2)}(r_2) < \infty;$

case d: $h_0^{(1)}(r_1) = \infty, \quad h_\infty^{(2)}(r_2) = \infty.$

Writing

$$\psi_u(t) := \int_{S_t} |u|^2 \quad (u \in D(T_{\max});\ t > 0) \tag{5.5}$$

[8] A dash on a function of several variables denotes the radial derivative.

(we shall not distinguish notationally between equivalence classes of functions belonging to $D(T_{\max})$ and particular representatives of these classes for which (5.5) is meaningful owing to Theorem 1 and Lemma 2) and

$$\mathfrak{F} := \left\{u \,|\, u \in D(T_{\max}),\, f_1 \nabla \frac{u}{f_1} \in L^2(B_{0r_1}),\, f_2 \nabla \frac{u}{f_2} \in L^2(B_{r_2\infty})\right\},$$

we define a restriction S of $T_{\max}$ by considering (1.1) on one of the following subspaces of $\mathfrak{H} := L^2(\mathbf{R}^n_+) = L^2(\mathbf{R}^n)$ according to the distinction just made:

$$\left\{u \,|\, u \in \mathfrak{F},\, \lim_{r \to 0} \frac{\psi_u(r)}{r^{n-1} f_1^2(r)} = 0 = \lim_{r \to \infty} \frac{\psi_u(r)}{r^{n-1} f_2^2(r)}\right\}, \tag{5.6a}$$

$$\left\{u \,|\, u \in \mathfrak{F},\, \lim_{r \to 0} \frac{\psi_u(r)}{r^{n-1} f_1^2(r)} = 0\right\}, \tag{5.6b}$$

$$\left\{u \,|\, u \in \mathfrak{F},\, \lim_{r \to \infty} \frac{\psi_u(r)}{r^{n-1} f_2^2(r)} = 0\right\}, \tag{5.6c}$$

$$\mathfrak{F}. \tag{5.6d}$$

An analogous distinction arises in [21] in connection with the main part of the general Schrödinger expression

$$\left(\frac{1}{i}\partial_j - b_j\right) a_{jk} \left(\frac{1}{i}\partial_k - b_k\right).$$

Theorem 5. *S is equal to the Friedrichs extension $(T_{\min})_F$ of $T_{\min}$.*

Proof. The assertion follows if we can prove

$$1.\quad S \subset S^* \quad \text{and} \quad 1.\quad (T_{\min})_F \subset S.$$

1. S is densely defined since $T_{\min}$ is (note Lemma 3 and $T_{\min} \subset S$ by virtue of Theorem 1). If therefore suffices to show that given $u \in D(S)$ there exist sequences $s_j \to 0$, $t_j \to \infty$ such that

$$\operatorname{Im} \int_{B_{s_j t_j}} Su \cdot \bar{u} \to 0 \quad \text{as} \quad j \to \infty. \tag{5.7}$$

To this end we regard (5.2) with $u \in D(S)$ and η as in (5.3). Putting $v := \frac{u}{f_1}$ and using Lemma 1 of [21] one can conclude exactly as in [24] that (it is this step which requires distinction between Cases a to d)

$$\int_{B_{0r_1}} \frac{|v|^2}{f_1^2 (r^{n-1} h_j^{(1)})^2} < \infty. \tag{5.8}$$

Here (and in the sequel) $\gamma = 0$ in Cases a or b and $\gamma \in (0, r_1]$ in Cases c or d. Hence

$$\int_{B_{0r_1}} \frac{f_1^2 |vv'|}{r^{n-1} f_1^2 h_j^{(1)}} < \infty. \tag{5.9}$$

In view of

$$\int_0^{r_1} \frac{1}{r^{n-1} f_1^2 h_j^{(1)}} = \infty,$$

(5.9) implies the existence of a null sequence $\{s_j\}$ on which χ is defined and which is such that

$$\lim_{j\to\infty} \int_{S_{s_j}} f_1^2 |vv'| = 0.$$

Thus

$$\lim_{j\to\infty} |\chi(s_j)| = 0. \tag{5.10}$$

The conclusion

$$\lim_{j\to\infty} |\chi(t_j)| = 0 \tag{5.11}$$

on an appropriate sequence $\{t_j\}$ tending to ∞ can be drawn in the same way. This proves (5.7).

2. We employ a well-known abstract characterization of $(T_{\min})_F$ [56, p. 317 f.]. Let $u \in D((T_{\min})_F)$. Then $u \in D((T_{\min})^*)$. Moreover, there exists a sequence $\{u_j\}$ in $D(T_{\min})$ such that

$$u_j \to u, \quad (T_{\min}(u_j - u_k), u_j - u_k) \to 0 \quad \text{as} \quad j, k \to \infty.$$

Owing to Theorem 4 all that remains to be proved is

$$f_1 \nabla \frac{u}{f_1} \in L^2(B_{0r_1}), \quad f_2 \nabla \frac{u}{f_2} \in L^2(B_{r_2\infty}) \tag{5.12}$$

and possibly

$$\lim_{r\to 0} \frac{\psi_u(r)}{r^{n-1} f_1^2(r)} = 0 \quad \text{or} \quad \lim_{r\to\infty} \frac{\psi_u(r)}{r^{n-1} f_2^2(r)} = 0. \tag{5.13}$$

(5.12) follows from the fact that (5.4) holds good with "u" replaced by "$u_j - u_k$" (cf. [21, p. 244]). (5.13) is a consequence of the inequality

$$\left| \frac{[\psi_v(t)]^{1/2}}{t^{\frac{n-1}{2}} f_l(t)} - \frac{[\psi_v(s)]^{1/2}}{s^{\frac{n-1}{2}} f_l(s)} \right|^2 \tag{5.14}$$

$$\leqq \int_s^t \frac{d\tau}{\tau^{n-1} f_l^2(\tau)} \int_{B_{st}} f_l^2 \left| \nabla \frac{v}{f_l} \right|^2 \quad (l \in \{1, 2\})$$

which holds for all $v \in H^1_{\mathrm{loc}}(\mathbf{R}^n_+)$ with $0 < s < t$ suitably restricted. In order to convince ourselves of its validity[9] we mollify $w = \frac{v}{f_l}$ and observe

$$|[t^{1-n} \psi_{J_\varrho w}(t)]^{1/2} - [s^{1-n} \psi_{J_\varrho w}(s)]^{1/2}|^2 \leqq \int_{S_1} |(J_\varrho w)(t\cdot) - (J_\varrho w)(s\cdot)|^2$$

[9] The hint given in [21, p. 244] is erroreous.

and insert

$$|(J_\varrho w)(t\xi)-(J_\varrho w)(s\xi)|^2 = \left|\int_s^t (J_\varrho w)'(\tau\xi)\,d\tau\right|^2$$

$$\leq \int_s^t \frac{d\tau}{\tau^{n-1}f_l^2(\tau)} \int_s^t \tau^{n-1}f_l^2(\tau)\,|\nabla J_\varrho w|^2(\tau\xi)\,d\tau$$

($\xi\in S_1$). (5.14) now follows once we let $\varrho\to 0$. ▮

Example 2 (Cf. [6]). Let $c\geqq 0$, $r_1>0$, and suppose that $q\in L^1_{\mathrm{loc}}(\mathbf{R}^n_+)$ satisfies

(5.15) $$q \geqq -\left(\frac{n-2}{2}\right)^2 r^{-2}-c.$$

Then

(5.16) $$D((T_{\min})_F) = \{u\,|\,u\in D(T_{\max}),$$

$$\int_{B_{0r_1}} \left|\nabla u+\frac{n-2}{2}\frac{u}{r}\frac{x}{r}\right|^2 < \infty,\quad \int_{B_{r_1\infty}} |\nabla u|^2 < \infty.\}.$$

Indeed, (5.ii) holds with

$$f_1(r) := r^{-\frac{n-2}{2}},\quad f_2(r) := \text{const} > 0 \quad (r>0).$$

We are in Case d if $n\in\{1,2\}$ and in Case c if $n\geqq 3$. The additional information $\lim_{r\to\infty} r^{1-n}\psi_u(r)=0$ given by Theorem 5 in the latter case is, of course, a trivial consequence of u, $\nabla u\in L^2(B_{r_1\infty})$ and therefore left out of account in (5.16).

Condition (5.15) does not admit of negative singularities if $n=2$. This is remedied in

Example 3. Let $c\geqq 0$, and assume that $q\in L^1_{\mathrm{loc}}(\mathbf{R}^2_+)$ satisfies

$$q(x) \geqq -\begin{cases} -\frac{1}{4}(|x|\log|x|)^{-2} & \text{if } \ 0<|x|<\frac{1}{2} \\ -c & \text{if } \ |x|\geqq\frac{1}{2}. \end{cases}$$

Then

$$D((T_{\min})_F) = \left\{u\,|\,u\in D(T_{\max}),\ \int_{B_{0\frac{1}{2}}} \left|\nabla u-\frac{u}{2r\log r}\frac{x}{r}\right|^2 < \infty,\ \int_{B_{\frac{1}{2}\infty}} |\nabla u| < \infty\right\}$$

because (5.ii) holds with

$$f_1(r) := (-\log r)^{1/2},\quad f_2(r) := \text{const} > 0 \quad (r>0).$$

Remark 5. The $\frac{1}{r^2}$-potential itself shows that $T_{\min}$ in Example 2 need not have a unique self-adjoint extension. Furthermore, $T_{\min}$ may fail to be bounded from below if the constant $-\left(\frac{n-2}{2}\right)^2$ is a replaced by a smaller number. Similar remarks apply to Example 3.

It should be noted that there may be functions in $D((T_{\min})_F)$ whose gradient is not in $\mathfrak{H}$ (assume equality in (5.15) and take a function $v \in C^2(\mathbf{R}^n_+)$ which vanishes outside some ball and which behaves like $|x|^{-\frac{n-2}{2}}$ as $|x| \to 0$). So there may be cancellations between the singularities of the summands of the first integral in (5.16). We give a criterion which tells us when such pathologies do not occur.

Remark 6. Assume that the function f_1 from (5.ii) has the additional property that

$$f_1(r)|f_1'(r)| = 0\left(\frac{1}{r^{n-1}h_\gamma^{(1)}(r)}\right) \quad \text{as} \quad r \to 0 \tag{5.17}$$

where γ is zero in Cases a and b and a suitable number belonging to $(0, r_1]$ in Cases c and d. Then

$$D((T_{\min})_F) = \left\{u \,|\, u \in D(T_{\max});\ \frac{f_1'}{f_1}u,\ \nabla u \in L^2(B_{0r_1});\ f_2 \nabla \frac{u}{f_2} \in L^2(B_{r_2\infty})\right\},$$

and every element $v \in D((T_{\min})_F)$ has the property $|q|^{1/2} v \in L^2(B_{0r_1})$. This can be proved in entirely the same manner as the corresponding one-dimensional result [24]. (For $n=1$ condition (5.17) was first introduced by Hinton [18].)

It is clear that Remark 6 applies mutatis mutandis to the function f_2 occurring in (5.ii).

Examples 2 and 3 Revisited. Suppose in addition to (5.i) that there exist numbers

$$c \geqq 0, \quad \beta_1 > -\left(\frac{n-2}{2}\right)^2, \quad \text{and} \quad \beta_2 > -\frac{1}{4} \quad \text{such that}$$

$$q \geqq \beta_1 r^{-2} - c \tag{5.18}$$

or (in case $n=2$)

$$q \geqq \begin{cases} \beta_2 (r \log r)^{-2} & \text{on} \quad B_{0\frac{1}{2}} \\ -c & \text{on} \quad B_{\frac{1}{2}\infty}. \end{cases} \tag{5.19}$$

Then

$$D((T_{\min})_F) = \{u \,|\, u \in D(T_{\max});\ r^{-1}u,\ \nabla u \in \mathfrak{H}\}. \tag{5.20}$$

In fact, put $\nu := 2\left[\beta_1 + \left(\frac{n-2}{2}\right)^2\right]^{1/2}$. Then (5.18) results from (5.ii) when

$$f_1(r) := r^{\frac{\nu-(n-2)}{2}}$$

is taken. Now,

$$f_1(r)f_1'(r) = \frac{\nu-(n-2)}{2}\, r^{\nu-(n-1)} \quad \text{and}$$

$$[h_\gamma^{(1)}(r)]^{-1} = \frac{\nu(r\gamma)^\nu}{|\gamma^\nu - r^\nu|},$$

so that (5.17) is indeed satisfied. Similarly one can take care of (5.19) by setting $f_1(r) := (-\log r)^{\frac{1-\nu}{2}}$ with $\nu := 2(\beta_2+\frac{1}{4})^{1/2}$. — It is not difficult to derive from (5.20) the familiar characterization

$$(5.21)\quad D((T_{\min})_F) = \begin{matrix} \{u | u \in D(T_{\max});\ \nabla u,\ \sqrt{|q|}\, u \in \mathfrak{H}\} & \text{if} \quad n \geqq 2 \\ \{u | u \in D(T_{\max});\ u', \sqrt{|q|}\, u \in \mathfrak{H};\ \lim\limits_{x\to 0} |u(x)| = 0\} & \text{if} \quad n = 1 \end{matrix}$$

given by Friedrichs [14, 15] for the case that q is smooth outside the origin (cf. [29, pp. 344 ff., 349 ff.]).

Note that any u in (5.20) has the property $\liminf_{r\to 0} \psi_u(r) = 0$. By means of (5.14) (replacing f_l by a constant) we can then even conclude $\lim_{r\to 0} \frac{\psi_u(r)}{r} = 0$ if $n=1$. This accounts for the difference between $n=1$ and $n>1$ in (5.21).

6. The essential self-adjointness of $T_{\min}$

While hypotheses (5.i), (5.ii) are strong enough to secure the existence of a physically as well as mathematically distinguished self-adjoint restriction of $T_{\max}$ (or extension of $T_{\min}$), they are too weak to guarantee that $T_{\max}$ itself is self-adjoint (see Remark 5). We now give a sufficient condition under which this is the case. As before, our tool will be nothing but partial integration. As a matter of fact we shall indicate two proofs of the following Theorem 6 with partial integration in extreme situations as their common feature. The first, which may be labelled a "Friedrichs-type proof", relies on Theorem 5 and establishes $T_{\max} = (T_{\min})_F$. The second, which may be called a "Carleman-type proof", is independent of the notion of the Friedrichs extension and shows that $T_{\max}$ is a symmetric operator. In each case substantial information about the elements of $D(T_{\max})$ is obtained, from which the physically relevant proposition

$$(6.1)\qquad \nabla u,\ \sqrt{|q|}\, u \in \mathfrak{H} \quad (u \in D(T_{\max}))$$

can be derived as soon as (5.17) and its counterpart at ∞ are available.

Theorem 6. *Assume that* (5.i), (5.ii) *hold and that the functions* f_1 *and* f_2 *occuring in* (5.ii) *additionally satisfy*

$$\int_0^{r_1} r^{n-1} f_1^2(r)\,dr = \infty = \int_{r_2}^{\infty} r^{n-1} f_2^2(r)\,dr. \tag{6.2}$$

Then $T_{\min}$ *is bounded from below (by Lemma 6) and essentially self-adjoint.*

Proof. Let $u \in D(T_{\max})$. We claim that (5.12) holds good. Put $v := \frac{u}{f_1}$ and $\varphi_v := r^{1-n}\psi_v$, ψ_v being given by (5.5). From Lemma 2 (whose assumptions are satisfied owing to Theorem 1) and (5.2), (5.3) we get

$$\begin{aligned}\operatorname{Re}\int_{B_{st}} T_{\max} u\cdot\bar{u} &= -\tfrac{1}{2} r^{n-1} f_1^2 \varphi_v'|_s^t \\ &+ \int_{B_{st}} \{f_1^2|\nabla v|^2 + [q - (r^{n-1}f_1)^{-1}(r^{n-1}f_1')']|v|^2\}\end{aligned} \tag{6.3}$$

for almost all $0<s<t<r_1$. Now we take advantage of (6.2). Together with

$$\int_0^{r_1} r^{n-1} f_1^2(r)\varphi_v(r)\,dr = \int_{B_{0r_1}} |u|^2 < \infty \tag{6.4}$$

this assumption shows that there exists a null sequence $\{s_n\}$ with

$$\varphi_v'(s_n) \geqq 0 \quad (n \in \mathbf{N}).$$

Using (5.ii), this information enables us to infer the first statement of (5.12) from (6.3). It is clear that the other relation can be derived similarly. We also note

$$0 = \liminf_{s\to 0} \varphi_v(s) = \liminf_{s\to 0} \frac{\psi_u(s)}{s^{n-1} f_1^2(s)} \tag{6.5}$$

(exploit (6.2) and (6.4) again).

We are now at a fork. We may continue to show (5.13) for our element $u \in D(T_{\max})$ in case $h_0^{(1)}(r_1) < \infty$ or $h_\infty^{(2)}(r_2) < \infty$ holds. As a matter of fact this relation follows immediately from (6.5), (5.12) and (5.14). u therefore belongs to the domain of the operator S defined by (5.6). Hence $T_{\max} = (T_{\min})_F$ by Theorem 5.

We can, however, also do without the Friedrichs extension if we repeat the first part of the proof of Theorem 5. Indeed, Lemma 1 of [21] allows us to deduce (5.8) from (5.12) and (6.5). We therefore also arrive at relations (5.10) and (5.11) again which accomplish the proof that $T_{\max}$ is a symmetric operator. ∎

Example 2 Rerevisited (Cf. [6, 25, 50]). Suppose in addition to (5.i) that there is a $c \geqq 0$ such that

$$q \geqq \left[1 - \left(\frac{n-2}{2}\right)^2\right] r^{-2} - c.$$

Then $T_{\min}$ is essentially self-adjoint. This follows from Theorem 6 when we put

$f_1(r):=r^{-n/2}$, $f_2(r):=\text{const}>0$ $(r>0)$. With this choice, (5.17) holds good also, so that (6.1) is valid. The constant $1-\left(\frac{n-2}{2}\right)^2$ is again best possible.

That an essentially self-adjoint Schrödinger operator albeit bounded from below can be rather weird is testified by

Example 4. Any $q\in L^1_{\text{loc}}(\mathbf{R}^n_+)$ with

$$q \geqq \left[2-\frac{(n-1)(n-3)}{4}\right] r^{-2}-4\left[r^6\left(2+\sin\frac{1}{r^4}\right)\right]^{-1}\cdot \left[(n-2)\cos\frac{1}{r^4}+\frac{4}{r^4}\sin\frac{1}{r^4}\right] \tag{6.6}$$

satisfies the assumptions of Theorem 6. Choose

$$f(r):=r^{-\frac{n-1}{2}+2}\left(2+\sin\frac{1}{r^4}\right),\quad g(r):=f(r)\int_r^1\frac{dt}{t^{n-1}f^2(t)}\quad (r>0)$$

in which case

$$q\geqq (r^{n-1}f)^{-1}(r^{n-1}f')' = (r^{n-1}g)^{-1}(r^{n-1}g')'.$$

The conditions of Theorem 6 can therefore be fulfilled by restricting g and f to say $(0, \frac{1}{2}]$ and $[\frac{1}{2}, \infty)$, respectively.

The remarkable thing about this example is the following. Let $u\in C^2(\mathbf{R}^n_+)$ be a function which vanishes outside some ball and which behaves like $f(|x|)$ as $|x|\to 0$. When we choose equality in (4.6), it is clear from (6.7) that $u\in D(T_{\max})$. An easy calculation shows that $\nabla u\notin \mathfrak{H}$. Furthermore, one can convince oneself that even

$$\lim_{s\to 0}\int_{B_{s\infty}}(|\nabla u|^2+q|u|^2)$$

does not exist, since

$$\lim_{t\to 0}\int_{S_t}\bar{u}u'$$

does not exist. For $n=1$ a similar example (with heavy oscillations at infinity rather than at zero) was given by Moser in [42].

Theorem 6 is basically the L^1_{loc}-version of the following unpublished result of Kato [31].

Theorem 7. *Let* $q\in L^2_{\text{loc}}(\mathbf{R}^n_+)$ *and*

$$q(x)\geqq -q^*(|x|)\quad (x\in\mathbf{R}^n_+)$$

for some $q^*\in L^2_{\text{loc}}((0,\infty))$. *Suppose, there exist a* $K\in\mathbf{R}$ *and a function* $0<w\in L^2_{\text{loc}}((0,\infty))$ *with*

$$\int_0^1 r^{n-1}w^2(r)\,dr=\infty=\int_1^\infty r^{n-1}w^2(r)\,dr \tag{6.8}$$

such that

$$r^{1-n}(r^{n-1}w')' + q^* w \leqq Kw \tag{6.9}$$

holds in the sense of distributions on $(0, \infty)$. *Then*

$$T_{\min} := (-\Delta + q) \upharpoonright C_0^\infty(\mathbf{R}_+^n)$$

is bounded from below with $-K$ *as a lower bound (by Lemma 6) and essentially self-adjoint.*

Proof (Kato). Let $u \in [R(T_{\min}+K+1)]^\perp = N((T_{\min}+K+1)^*)$. By (1.5) and Lemma 1 we have

$$0 = (-\Delta + q + K + 1)u \geqq (-\Delta - q^* + K + 1)\,|u| \tag{6.10}$$

in the sense of distributions on $\mathbf{R}_+^n$.

$$U(t) := t^{1-n} \int_{S_t} |u|$$

clearly exists for almost all $t > 0$ and has the property

$$\int_0^\infty r^{n-1} U^2(r)\, dr < \infty. \tag{6.11}$$

It follows from (6.10) that

$$\int_0^\infty [-r^{1-n}(r^{n-1}\varphi')' + (-q^* + K + 1)\varphi] U r^{n-1} \leqq 0$$

for all $0 \leqq \varphi \in C_0^\infty((0, \infty))$ so that

$$r^{1-n}(r^{n-1}U')' + (q^* - K - 1)U \geqq 0 \tag{6.12}$$

holds in the sense of distributions on $(0, \infty)$. Since a nonnegative distribution is a measure [46, p. 29] and since q^* and U are functions, (6.12) implies that $(r^{n-1}U')'$ is a measure. $r^{n-1}U'$ is therefore locally of bounded variation [46, p. 53]. The same concludion holds for $r^{n-1}w'$. Thus U' and w' are of bounded variation and so U'' and w'' are measures [46, p. 53]. Since U' and w' are functions, U and w are (equivalent to) locally absolutely continuous functions [46, p. 54].

From (6.9) and (6.12) we see that

$$r^{1-n}(r^{n-1}U')' \geqq (K + 1 - q^*)\frac{U}{w} w \geqq r^{1-n}(r^{n-1}w')' \frac{U}{w}.$$

Thus $(r^{n-1}(U'w - Uw'))'$ is a nonnegative measure and therefore

$$f := r^{n-1}(U'w - Uw') = r^{n-1}w^2 \left(\frac{U}{w}\right)'$$

an increasing function [46, p. 54].

Unless $U=0$, there is a point $r_0>0$ with $U(r_0)>0$ and at which f is defined. As a consequence

$$r^{n-1}w^2(r)\left(\frac{U}{w}\right)'(r) \geqq f(r_0) \quad \text{for almost all} \quad r\in[r_0, \infty) \tag{6.13}$$

and

$$f(r_0) \geqq r^{n-1}w^2(r)\left(\frac{U}{w}\right)'(r) \quad \text{for almost all} \quad r\in(0, r_0]. \tag{6.14}$$

Integration of (6.13) or (6.14) gives (here we use that $U, w\in AC_{\mathrm{loc}}((0, \infty))$)

$$U(r) \geqq \frac{U}{w}(r_0)w(r)$$

for all $r\in[r_0, \infty)$ or for all $r\in(0, r_0]$ in case $f(r_0)\geqq 0$ or $f(r_0)<0$, respectively. In any case, this relation taken together with (6.11) contradicts (6.8). Hence $U=0$ and therefore $u=0$. ∎

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Received March 23, 1979

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