

ON THE VIRIAL THEOREM IN QUANTUM MECHANICS

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For a class of potentials including Δ -form small potentials q , virial theorems of the type

$$2(u, -\Delta u) = (u, x \cdot \nabla qu)$$

are shown to hold, u being an eigenfunction of the Schrödinger operator $S = -\Delta + q$ and S satisfying certain conditions, e.g. $Q(S) \subset Q(-\Delta) \cap Q(q)$. The proof given here is based strictly on a canonical approximation of the formally valid commutator identity

$$[S, \frac{1}{2}(x \cdot \nabla + \nabla \cdot x)] = 2(-\Delta) - x \cdot \nabla q$$

employed in physical literature. In addition we show the validity of the "generalized" virial theorem

$$2(u, -\Delta u) = \lim_{\substack{n \rightarrow \infty \\ \epsilon \rightarrow 0}} (x \cdot \nabla q, (|u_\epsilon|^2 \Phi_n)^2)_{\text{dist}},$$

if e.g. q is a perturbation small relative to $-\Delta$, and we conclude the absence of certain energy bound states. Finally we prove a relativistic virial theorem.

1. Introduction and Notations

In the physical literature there exist basically two proofs for the quantum mechanical virial theorem which, roughly speaking, connects the kinetic and potential energies of a particle in a stationary, pure state. The first one, due to Finkelstein [2], makes use implicitly of the infinitesimal generator $\frac{i}{2}(x \cdot \nabla + \nabla \cdot x)$ of scale transformations, whereas the second, going back to Fock [3], employs the group of dilations itself. Both are not quite correct from the mathematical point of view, but they are heuristically of great value.

Weidmann [14] was the first one to give a correct proof for the virial theorem making use of scale transformations. In principle his assumptions admit Δ -small potentials q such as e.g. $r^{-\gamma}$ with $0 < \gamma < \min\{2, \frac{m}{2}\}$. In the sequel Kalf [6] extended Weidmann's result allowing potentials q as singular as r^{-2} at the origin. At the same time Müller-Pfeiffer [10] proved a

virial theorem for potentials satisfying the condition

$$\lim_{r \rightarrow 0} \sup_{x \in \mathbb{R}^m} \int_{|x-y|< r} |q(y)|^{m/2} dy = 0.$$

Hitherto further generalizations of Weidmann's result (partially in other directions) have been done by Albeverio [1], Kalf [7,8], Herbst [5].

In this paper, on one hand we like to enlargen the class of admissible potentials in order to include Schrödinger operators (and also Dirac operators) defined by quadratic forms. The only condition (of course restrictive) we need is a Δ -form bounded, dominating majorant W for the radial difference quotients

$$\frac{q_a - q}{a - 1}, \text{ that is } \left| \frac{q(ax) - q(x)}{a - 1} \right| \leq W(x) \text{ a.e. in } \mathbb{R}^m.$$

On the other hand we are able to prove "generalized" virial theorems of the type

$$(I) \quad 2(u, -\Delta u) = \lim_{\substack{n \rightarrow \infty \\ \varepsilon \rightarrow 0}} (u, |\psi_n|^2)_{\text{dist}}$$

(see Theorems 2.2, 2.3 for precise statements).

It turns out that e.g. the condition

$$\|q u\| \leq a \|\Delta u\| + \|u\|, \quad a < 1$$

is sufficient for the virial theorem (I) to hold (see Theorem 2.2). A similar result holds in the case of strongly singular potentials as considered in the paper [6] by Kalf (see Theorem 2.3).

We think that the two methods of proof we use below are extremely simple. The first one only makes precise the formally valid commutator identity

$$(II) \quad i[D, S] = 2(-\Delta) - x \cdot \nabla q$$

by showing that

$$\lim_{a \rightarrow 1} (u, [S, D_a] u) = 2(u, -\Delta u) - (u, x \cdot \nabla qu) \quad (u \in Q(S))$$

where now the domain problems in (II) are avoided.

Here $D_a = (a-1)^{-1}(U_a - id)$ denotes an obvious approximation of

$-iD = \frac{1}{2}(x \cdot \nabla + \nabla \cdot x)$ motivated by Stone's theorem (applied to the dilation group $(U_a)_{a>0}$). The second one is based on the observation that for every eigenfunction u of S we have

$$(III) \quad \lim_{n \rightarrow \infty} \left(\frac{i}{2} \Phi_n^2(x \cdot \nabla + \nabla \cdot x) u, Su \right) = 0$$

(Φ_n) being a suitable sequence of C_0^∞ -functions cutting off the "badly behaved" operator $\frac{i}{2}(x \cdot \nabla + \nabla \cdot x)$. We like to remark, that equation (III) is closely connected with Finkelstein's original proof.

Next we shall introduce some notations. For any real number $a > 0$ we define a unitary transformation on $L^2(\mathbb{R}^m)$ (equipped with the scalar product (\cdot, \cdot)) by setting

$$U_a \psi(x) = a^{m/2} \psi(ax).$$

One easily shows that $U_{aa'} = U_a \circ U_{a'}$, $U_a^* = U_{a-1}$,

$$U_a(H^s(\mathbb{R}^m)) = H^s(\mathbb{R}^m) \text{ and } \lim_{a \rightarrow 1} \|\psi - U_a \psi\|_{H^s(\mathbb{R}^m)} = 0,$$

where $H^s(\mathbb{R}^m)$ denotes the Sobolev space of order $s \geq 0$

(actually $s = 0, 1/2, 1, 2$ will be needed). We use the notation

$Q(T) = D(|T|^{1/2})$ for any self-adjoint operator T and denote by $(\varphi, T\psi)$ the quadratic form corresponding to T with domain $Q(T) \times Q(T)$. Every measurable, a.e. finite function $q: \mathbb{R}^m \rightarrow \mathbb{R} \cup \{\pm\infty\}$ defines a unique self-adjoint multiplication operator, also denoted by q , so that $(\varphi, q\psi) = \int q\bar{\varphi}\psi dx$ for all $\varphi, \psi \in Q(q) = \{u | u, |q|^{1/2}u \in L^2(\mathbb{R}^m)\}$. Finally we set (if $a \neq 1$) $D_a = (a-1)^{-1}(U_a - id)$ and $(\varphi, [T, D_a]\psi) = (\varphi, TD_a\psi) - (D_a^*\varphi, T\psi)$ for all $\varphi \in Q(T)$ if $Q(T)$ is invariant under the dilations U_a . Otherwise we shall use notations and definitions in the same way as in the books of Reed-Simon [12].

2. Virial Theorems

In this section we state and prove virial theorems concerning Schrödinger operators as well as Dirac equations.

THEOREM 2.1. Let S be a self-adjoint Schrödinger operator in $L^2(\mathbb{R}^m)$ satisfying

$$(1) \quad U_a(Q(S)) \subset Q(S) \subset Q(-\Delta) \cap Q(q), \quad a \text{ near } 1$$

$$(\varphi, S\varphi) = (\varphi, -\Delta\varphi) + (\varphi, q\varphi), \quad \varphi \in Q(S)$$

$$(2) \quad \begin{aligned} &\text{Suppose the potential } q \text{ possesses a.e. a radial derivative } x \cdot \nabla q \text{ and assume there exists a } \Delta\text{-form bounded} \\ &\text{function } W \geq 0 \text{ such that for a near } 1, a \neq 1, \text{ we have} \\ &\left| \frac{q(ax - q(x))}{a-1} \right| \leq W(x) \text{ a.e. in } \mathbb{R}^m. \end{aligned}$$

Then every $\varphi \in Q(S)$ satisfies

$$(3) \quad (\varphi, i[D, S]\varphi) = 2(\varphi, -\Delta\varphi) - (\varphi, x \cdot \nabla q\varphi)$$

where $(\varphi, i[D, S]\varphi) := \lim_{a \rightarrow 1} (\varphi, [S, D_a]\varphi)$. In particular the virial theorem

$$(4) \quad 2(\varphi, -\Delta\varphi) = (\varphi, x \cdot \nabla q\varphi)$$

holds true, if u is an eigenfunction of S . Moreover if $D(S) \subset D(-\Delta)$ is valid it suffices only to assume the Δ^2 -form boundedness of W in order to have equations (3) and (4) for all $\varphi \in D(S)$.

REMARKS. Denoting by $D = \frac{i}{2}(x \cdot \nabla + \nabla \cdot x)$ the infinitesimal generator of the dilation group, formula (3) indicates the close connection to the well known commutator formula

$$(5) \quad i[D, S] = 2(-\Delta) - x \cdot \nabla q.$$

Of course, identity (5) is valid only formally. In general there exist eigenfunctions φ of S not belonging to the domain of D (see [6,p.58], [1,p.173ff]). To avoid such difficulties we substitute $-iD$ by its natural approximation $D_a = (a-1)^{-1}(U_a - id)$ and put $(\varphi, i[D, S]\varphi) := \lim_{a \rightarrow 1} (\varphi, [S, D_a]\varphi)$, which is motivated by the fact that $D_a \rightarrow -iD$ strongly on $D(D)$. The existence of the limit is guaranteed by Theorem 2.1.

PROOF: Choose a near 1, $a \neq 1$, such that (1), (2) are valid.
Take $\varphi \in Q(S)$ then

$$\begin{aligned} (\varphi, [S, D_a] \varphi) &= (\varphi, S D_a \varphi) - (D_a^* \varphi, S \varphi) \\ &= (a-1)^{-1} \{ (\varphi, S U_a \varphi) - (U_a^* \varphi, S \varphi) \} \\ &= (a-1)^{-1} \{ (\varphi, -\Delta U_a \varphi) - (U_a^* \varphi, -\Delta \varphi) + \\ &\quad + (\varphi, q U_a \varphi) - (U_a^* \varphi, q \varphi) \} \end{aligned}$$

With the notation $q_a(x) = q(ax)$ one has

$$\begin{aligned} (\varphi, -\Delta U_a \varphi) &= a^2 (U_a^* \varphi, -\Delta \varphi) \quad \text{and} \\ (U_a^* \varphi, q \varphi) &= (\varphi, q_a U_a \varphi) \end{aligned}$$

Thus (use (2))

$$(\varphi, [S, D_a] \varphi) = (a+1) \cdot (U_a^* \varphi, -\Delta \varphi) - (\varphi, \frac{q_a - q}{a-1} U_a \varphi)$$

immediately follows. Since $(U_a^* \varphi, -\Delta \varphi) \rightarrow (\varphi, -\Delta \varphi)$ as $a \rightarrow 1$, it remains to consider the term $(\varphi, \frac{q_a - q}{a-1} U_a \varphi)$. First we have

the estimate

$$\begin{aligned} \|W|\varphi||U_a \varphi| - W|\varphi|^2\|_{L^1} &\leq \|W|\varphi||\varphi - U_a \varphi|\|_{L^1} \\ &\leq \|W^{1/2}\varphi\|_{L^2} \cdot \|W^{1/2}(\varphi - U_a \varphi)\|_{L^2} \\ &\leq (W|\varphi|)^{1/2} \cdot (\varphi - U_a \varphi, W(\varphi - U_a \varphi))^{1/2} \end{aligned}$$

from which $W|\varphi||U_a \varphi| \xrightarrow{L^1} W|\varphi|^2$ follows as $a \rightarrow 1$. Hence there exists a sequence $(a_n)_{n \in \mathbb{N}}$ tending to 1 and $w \in L^1(\mathbb{R}^m)$ such

that

$$W|\varphi||U_{a_n} \varphi| \leq w \quad \text{a.e. in } \mathbb{R}^m.$$

Now by Lebesgue's dominated convergence theorem and the estimate

(2) it follows

$$(\varphi, \frac{q_{a_n} - q}{a_n - 1} U_{a_n} \varphi) \rightarrow (\varphi, x \cdot \nabla q \varphi) \quad \text{as } n \rightarrow \infty .$$

Since we could have started with an arbitrary sequence $(a_n)_{n \in \mathbb{N}}$,

tending to 1, we conclude that

$$\lim_{a \rightarrow 1} (\varphi, \frac{q_a - q}{a - 1} U_a \varphi) = (\varphi, x \cdot \nabla q \varphi) .$$

Thus $(\varphi, i[D, S]\varphi) = 2(\varphi, -\Delta\varphi) - (\varphi, x \cdot \nabla q \varphi)$ is shown to hold true for all $\varphi \in Q(S)$. In the case $D(S) \subset D(-\Delta) = H^2(\mathbb{R}^m)$ one has

$$\lim_{a \rightarrow 1} (\varphi - U_a \varphi, W(\varphi - U_a \varphi)) = 0 ,$$

if W is Δ^2 -form bounded, and the just demonstrated method of concluding can be applied. \square

Now let us make some concrete applications.

COROLLARY 2.1. Let q be a measurable, a.e. finite function on \mathbb{R}^m bounded from below. Assume $Q(-\Delta) \cap Q(q)$ is dense in $L^2(\mathbb{R}^m)$ and (2) is valid. Then the virial theorem holds true for the form sum $S = -\Delta + q$.

PROOF: Clearly $Q(S) = Q(-\Delta) \cap Q(q)$ and $(\varphi, S\varphi) = (\varphi, -\Delta\varphi) + (\varphi, q\varphi)$ for each $\varphi \in Q(S)$. So it remains to show $U_a(Q(S)) \subset Q(S)$, but due to

$$(U_a \varphi, |q| U_a \varphi) = (\varphi, |q_{a-1}| \varphi) \\ |q_{a-1}| \leq |a^{-1}| W + |q|$$

this is obvious. \square

COROLLARY 2.2. Let the potential q be Δ -form bounded with relative bound smaller than 1 and assume (2). Then the virial theorem is valid for the Schrödinger operator $S = -\Delta + q$ (defined by the KLMN-theorem).

REMARK. The result above generalizes papers of Weidmann [14], Albeverio [1] (partially) and Müller-Pfeiffer [10] (the condition III there turns out to be superfluous). We like to mention that now Röllnik potentials are included.

In the case of strongly singular potentials we have the following result.

COROLLARY 2.3. Suppose $m \geq 3$, $q \in L^2_{loc}(\mathbb{R}^m \setminus \{0\})$ and there exist numbers $\beta > -[\frac{m-2}{2}]^2$, $\gamma \geq 0$ such that

$$q(x) \geq \frac{\beta}{|x|^2} - \gamma \quad (x \in \mathbb{R}^m \setminus \{0\})$$

and assume (2). Then the virial theorem holds true for the Friedrichs extension S of $(-\Delta + q)|C_0^\infty(\mathbb{R}^m \setminus \{0\})$.

REMARKS. Corollary 2.3 generalizes a result of Kalf [6], where $W = c(1 + \frac{1}{|x|^2})$ and additionally $q \in Q_{\alpha, loc}(\mathbb{R}^m \setminus \{0\})$ is assumed.

It should be remarked that $W = c(\frac{1}{|x|^2} + 1)$ is Δ -form bounded due to an inequality of Hardy [1, p. 262ff.],

$$(6) \quad [\frac{m-2}{2}]^2 (\varphi, \frac{1}{|x|^2} \varphi) \leq (\varphi, -\Delta \varphi) \quad (\varphi \in Q(-\Delta)).$$

PROOF. Let $\varphi \in C_0^\infty(\mathbb{R}^m \setminus \{0\})$, $\beta_0 := -[\frac{m-2}{2}]^2$ and $0 < \lambda < 1$

such that $\frac{\beta}{\lambda} - \beta_0 > 0$. Then with the notations $q_\pm = \frac{1}{2}(|q| \pm q)$

we have

$$(7) \quad (1-\lambda)(\varphi, -\Delta \varphi) + \lambda(\frac{\beta}{\lambda} - \beta_0)(\varphi, \frac{1}{|x|^2} \varphi) \leq \gamma(\varphi, \varphi) + (\varphi, S\varphi)$$

$$(8) \quad (\varphi, q_- \varphi) \leq |\beta|(\varphi, \frac{1}{|x|^2} \varphi) + \gamma(\varphi, \varphi)$$

$$(9) \quad (\varphi, q_+ \varphi) \leq (\varphi, S\varphi) + (\varphi, q_- \varphi)$$

From (7) - (9) it follows $Q(S) \subset Q(-\Delta) \cap Q(\frac{1}{|x|^2}) \cap Q(q_-) \cap Q(q_+)$

hence $Q(S) \subset Q(-\Delta) \cap Q(q)$ and

$$(\psi, S\psi) = (\psi, -\Delta \psi) + (\psi, q\psi) \quad (\psi \in Q(S))$$

It remains to show that $Q(S)$ is invariant under dilations.

First let be $\varphi \in C_0^\infty(\mathbb{R}^m \setminus \{0\})$ then $U_a \varphi \in C_0^\infty(\mathbb{R}^m \setminus \{0\})$ and

$$\begin{aligned} (U_a \varphi, S U_a \varphi) &= a^2 (\varphi, -\Delta \varphi) + (\varphi, q_a^{-1} \varphi) \\ &\leq a^2 (\varphi, -\Delta \varphi) + |a^{-1}-1| (\varphi, W\varphi) + (\varphi, |q| \varphi) \\ (10) \quad &\leq a^2 (\varphi, -\Delta \varphi) + |a^{-1}-1| (\varphi, W\varphi) + c[(\varphi, \varphi) + (\varphi, S\varphi)] \end{aligned}$$

Suppose $\varphi \in Q(S)$, then there exists a sequence $(\varphi_n)_{n \in \mathbb{N}}$

$\in C_0^\infty(\mathbb{R}^m \setminus \{0\})$ with $\varphi_n \rightarrow \varphi$ in $Q(S)$. Thus $U_a \varphi_n \rightarrow U_a \varphi$

in $L^2(\mathbb{R}^m)$ and $\sup_{n \in \mathbb{N}} (\varphi_n, S\varphi_n) < \infty$. Due to (10) we have

$\sup_{n \in \mathbb{N}} (U_a \varphi_n, S U_a \varphi_n) < \infty$, hence $U_a \varphi \in Q(S)$ and the corollary

is proven. \square

Up till now strongly singular potentials were allowed as long as $Q(S) \subset Q(-\Delta)$ was guaranteed. Now we deal with potentials q which are not so badly behaving in order to insure $D(S) \subset H^2_{loc}$. Without any further assumptions on q we are able to prove virial theorems using the distribution $x \cdot \nabla q$ instead of the corresponding form. With the notations $u_\varepsilon = u * j_\varepsilon$ (where j_ε is a mollifying function), $(x \cdot \nabla q, \varphi)_{dist} = - \int q \operatorname{div}[x \varphi] dx$ and $\Phi_n = \Phi(\frac{\cdot}{n})$ ($\Phi \in C_0^\infty(\mathbb{R}^m)$ satisfying $0 \leq \Phi \leq 1$, $\Phi(x) = 1$ if $|x| \leq 1$ and $\Phi(x) = 0$ if $|x| \geq 2$) we have the following theorem.

THEOREM 2.2. Assume $q \in L^2_{loc}(\mathbb{R}^m, \mathbb{R})$ is Δ -bounded with relativ bound smaller than 1. Let u be an eigenfunction of the self-adjoint Schrödinger operator $S = (-\Delta + q)|C_0^\infty(\mathbb{R}^m)$. Then

$$(11) \quad \begin{aligned} 2(u, -\Delta u) &= \lim_{n \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} (x \cdot \nabla q, (|u_\varepsilon| \Phi_n)^2)_{dist} \\ &= - \lim_{n \rightarrow \infty} \int q \operatorname{div}[x(|u| \Phi_n)^2] \end{aligned}$$

We first make some conclusions (hence we suppose the assumptions of Theorem 2.2) and then prove the theorem.

COROLLARY 2.4. Assume $x \cdot \nabla q \leq -\gamma q$ in the distributional sense with $0 \leq \gamma \leq 2$. Then

- i) S has no eigenvalues, if $\gamma = 0$ (repulsive potential)
- ii) S has no nonnegative eigenvalues, if $0 < \gamma < 2$
- iii) S has no positive eigenvalues, if $\gamma = 2$

PROOF OF COROLLARY 2.4. Let u be an eigenfunction of S with eigenvalue λ . Then $0 \leq (|u_\varepsilon| \Phi_n)^2 \in C_0^\infty(\mathbb{R}^m)$ and $(x \cdot \nabla q, (|u_\varepsilon| \Phi_n)^2)_{dist} \leq -\gamma (u_\varepsilon \Phi_n, qu_\varepsilon \Phi_n)$

From this inequality and Theorem 2.2 we get

$$2(u, -\Delta u) = \lim_{n \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} (x \cdot \nabla q, (|u_\varepsilon| \Phi_n)^2)_{\text{dist}} \leq -\gamma(u, qu)$$

Since $Su = \lambda u$ we see $(2-\gamma)(u, -\Delta u) \leq -\gamma \cdot \lambda(u, u)$ hence i)-iii) follows. \square

COROLLARY 2.5. Assume $x \cdot \nabla q \in L^1_{\text{loc}}(\mathbb{R}^m)$ and suppose $(x \cdot \nabla q)_+$ or $(x \cdot \nabla q)_-$ is Δ -form bounded. Let u be an eigenfunction of $S = (-\Delta + q) | C_0^\infty(\mathbb{R}^m)$. Then $u \in Q(x \cdot \nabla q)$ and the virial theorem

$$2(u, -\Delta u) = (u, x \cdot \nabla qu)$$

holds true.

PROOF OF COROLLARY 2.5. First we remark that u may be chosen real-valued. For any $n \in \mathbb{N} \cup \{\infty\}$ consider the real function

$$\varphi_n(t) = \begin{cases} t & , |t| \leq n \\ \text{sgn}t \cdot n & , |t| \geq n \end{cases}$$

It is well known [4,p.146] that $\varphi_n \circ u \in H^1(\mathbb{R}^m)$ and

$\nabla(\varphi_n \circ u) = (\varphi'_n \circ u) \nabla u$. Clearly $x(\varphi_n \circ u)^2 \in H^{1,1}_{\text{loc}}(\mathbb{R}^m)^m$ and in the distributional sense we have with $\Phi \in C_0^\infty(\mathbb{R}^m)$

$$(12) \quad \text{div}[x(\varphi_n \circ u)^2 \Phi^2] = m(\varphi_n \circ u)^2 \Phi^2 + 2(\varphi_n \circ u) x \cdot \nabla(\varphi_n \circ u) \Phi^2 + 2 \Phi x \cdot \nabla \Phi (\varphi_n \circ u)^2$$

$$\text{Now } |\varphi(\varphi_n \circ u)^2 \Phi^2| \leq |\varphi| |u|^2 \Phi^2 \in L^1(\mathbb{R}^m)$$

$$|\varphi \Phi x \cdot \nabla \Phi (\varphi_n \circ u)^2| \leq C_\Phi |\varphi| |u|^2 |\Phi| \in L^1(\mathbb{R}^m)$$

$$|\varphi(\varphi_n \circ u) x \cdot \nabla(\varphi_n \circ u) \Phi^2| \leq C_\Phi |\varphi| |u| |\nabla u| |\Phi|^2$$

$$\begin{aligned} \||\varphi| |u| |\nabla u|\| &\leq c \||\varphi|^{1/2} u\|_{L^2} \cdot \sum_{k=1}^m \||\varphi|^{1/2} \partial_k u\|_{L^2} \\ &\leq c' \|u\|_{H^1} \sum_{k=1}^m \|\partial_k u\|_{H^1} \leq c'' \|u\|_{H^2}^2 \end{aligned}$$

since $u \in D(-\Delta) = H^2(\mathbb{R}^m)$ and we get

$$\int q \text{ div}[x(u\Phi)^2] dx = \lim_{n \rightarrow \infty} \int q \text{ div}[x(\varphi_n \circ u)^2 \Phi^2] dx$$

On the other hand

$$\begin{aligned} \int q \operatorname{div}[x(\varphi_n \circ u)^2 \Phi^2] dx &= \lim_{\varepsilon \rightarrow 0} \int q \operatorname{div}[x(\varphi_n \circ u)_\varepsilon^2 \Phi^2] dx \\ &= - \lim_{\varepsilon \rightarrow 0} (x \cdot \nabla q, (\varphi_n \circ u)_\varepsilon^2 \Phi^2)_{\text{dist}} \\ &= - \int x \cdot \nabla q (\varphi_n \circ u)^2 \Phi^2 dx \quad (\text{note } x \cdot \nabla q \in L^1_{\text{loc}}(\mathbb{R}^m)) \end{aligned}$$

Suppose now $(x \cdot \nabla q)_-$ is Δ -form bounded (we may consider only this case). Then $u\Phi, (\varphi_n \circ u)\Phi \in H^1(\mathbb{R}^m) = Q(-\Delta) \subset Q((x \cdot \nabla q)_-)$

and since $(\varphi_n \circ u)\Phi \rightarrow u\Phi$ in $H^1(\mathbb{R}^m)$ we get

$$(u\Phi, (x \cdot \nabla q)_- u\Phi) = \lim_{n \rightarrow \infty} ((\varphi_n \circ u)\Phi, (x \cdot \nabla q)_- (\varphi_n \circ u)\Phi)$$

Hence $\lim_{n \rightarrow \infty} \int (x \cdot \nabla q)_+ (\varphi_n \circ u)^2 \Phi^2 dx = - \int q \operatorname{div}[xu^2 \Phi^2] dx + (u\Phi, (x \cdot \nabla q)_- u\Phi)$.

Thus by Fatou $u\Phi \in Q(x \cdot \nabla q)$ and then by Lebesgue

$$\int (x \cdot \nabla q)_+ u^2 \Phi^2 dx = - \int q \operatorname{div}[xu^2 \Phi^2] dx + (u\Phi, (x \cdot \nabla q)_- u\Phi)$$

Putting $\Phi = \Phi_1$, using Theorem 2.2, the Δ -form boundedness of $(x \cdot \nabla q)_-$ and Fatou one gets $u \in Q(x \cdot \nabla q)$ (notice that $\int q \operatorname{div}[xu^2 \Phi_1^2] dx = \lim_{\varepsilon \rightarrow 0} \int q \operatorname{div}[xu_\varepsilon^2 \Phi_1] dx$ as is shown at the end of the proof of Theorem 2.2).

Thus by Lebesgue

$$\int (x \cdot \nabla q)_+ u^2 dx = 2(u, -\Delta u) + (u, (x \cdot \nabla q)_- u)$$

hence $2(u, -\Delta u) = (u, x \cdot \nabla qu)$. \square

PROOF OF THEOREM 2.2. Let be $Su = \lambda u$. We may assume that u is realvalued. Denote by D_{Φ_n} the truncated infinitesimal generator of the dilation group, that is

$$D_{\Phi_n} = \frac{i}{2} \Phi_n^2 (x \cdot \nabla + \nabla \cdot x)$$

Multiplying the equation $Su = \lambda u$ with $iD_{\Phi_n} u$ one obtains

$$(iD_{\Phi_n} u, Su) = \lambda (iD_{\Phi_n} u, u)$$

Due to (A1) we have

$$\begin{aligned} |(iD_{\Phi_n} u, Su)| &= |\lambda| (ux \cdot \nabla \Phi_n, u \Phi_n) \\ &\leq \frac{2|\lambda|}{n} \|\nabla \Phi\|_\infty \cdot \|u\|_{L^2}^2. \end{aligned}$$

Hence

$$(13) \quad \lim_{n \rightarrow \infty} (iD_{\Phi_n} u, Su) = 0$$

$$\text{Since } (14) \quad (iD_{\Phi_n} u, Su) = (iD_{\Phi_n} u, -\Delta u) + (iD_{\Phi_n} u, qu)$$

$$(iD_{\Phi_n} u, -\Delta u) = -\|\Phi_n \nabla u\|^2 + (x \cdot \nabla \Phi_n, \Phi_n \nabla u, \nabla u) -$$

$$- 2(\Phi_n \nabla u \cdot \nabla \Phi_n, x \cdot \nabla u) - m(\nabla \Phi_n \cdot \nabla u, \Phi_n u)$$

$$(iD_{\Phi_n} u, qu) = (\Phi_n ux \cdot \nabla \Phi_n, qu) + \frac{1}{2} \lim_{\varepsilon \rightarrow 0} (x \cdot \nabla q, u_\varepsilon^2 \Phi_n^2) \text{ dist} \quad ((A3))$$

as $n \rightarrow \infty$ we get (remind $u, \nabla u \in L^2(\mathbb{R}^m)$)

$$(15) \quad \lim_{n \rightarrow \infty} (iD_{\Phi_n} u, -\Delta u) = -\|\nabla u\|^2 = -(u, -\Delta u)$$

$$(16) \quad \lim_{n \rightarrow \infty} (\Phi_n ux \cdot \nabla \Phi_n, qu) = 0 \quad \text{since } u \in Q(q).$$

Now (13)-(16) shows

$$0 = -(u, -\Delta u) + \frac{1}{2} \lim_{n \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} (x \cdot \nabla q, (u_\varepsilon \Phi_n)^2) \text{ dist}$$

and the first part of formula (11) is proven. To justify the second part of (11) one only has to state that in the distributional sense

$$\operatorname{div}[x(u\Phi_n)^2] = m(u\Phi_n)^2 + 2ux \cdot \nabla u \Phi_n^2 + 2\Phi_n x \cdot \nabla \Phi_n u^2$$

hence

$$\int q \operatorname{div}[x(u\Phi_n)^2] dx = \lim_{\varepsilon \rightarrow 0} \int q [\operatorname{div} x(u_\varepsilon \Phi_n)^2] dx. \quad \square$$

Similar results can be obtained for strongly singular potentials. We denote by φ a C^∞ -function with the properties

$$0 \leq \varphi \leq 1, \quad \varphi(x) = 1 \quad \text{if } |x| \leq 1 \quad \text{and} \quad \varphi(x) = 0 \quad \text{if } |x| \geq 2$$

and put $\Phi_n = \varphi(\frac{\cdot}{n})[1-\varphi(n\cdot)]$, $\mathbb{R}_+^m = \mathbb{R}^m \setminus \{0\}$.

THEOREM 2.3. Suppose $m \geq 3$, $q \in L^2_{loc}(\mathbb{R}_+^m)$ and there exist numbers $\beta > -[\frac{m-2}{2}]^2$, $\gamma \geq 0$ such that

$$q(x) \geq \frac{\beta}{|x|^2} - \gamma$$

In addition we assume q to be locally Δ -bounded in \mathbb{R}_+^m with local relative bounds smaller than 1. Let u be an eigenfunction of the Friedrichs extension S of $(-\Delta+q)|C_0^\infty(\mathbb{R}_+^m)$

Then $2(u, -\Delta u) = \lim_{n \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} (x \cdot \nabla q, (|u_\varepsilon| \Phi_n)^2)_{\text{dist}}$

$$= - \lim_{n \rightarrow \infty} \int q \operatorname{div}[x(|u| \Phi_n)^2] dx$$

PROOF. Put $\mathbb{R}_+^m = \mathbb{R}^m \setminus \{0\}$, $S_0 = (-\Delta+q)|C_0^\infty(\mathbb{R}_+^m)$, then due to

$$(A4) \quad D(S) \subset D(S_0^*) \subset H^2_{loc}(\mathbb{R}_+^m)$$

In the proof of Corollary 2.3 we already showed

$$Q(S) \subset Q(-\Delta) \cap Q(q) \cap Q\left(\frac{1}{|\cdot|^2}\right)$$

Noticing $\Phi_n \rightarrow 1$, $x \cdot \nabla \Phi_n \rightarrow 0$ a.e. in \mathbb{R}_+^m and

$$\|\Phi_n\|_\infty \leq 1, \|x \cdot \nabla \Phi_n\|_\infty \leq 4 \|\nabla \varphi\|_\infty$$

one observes that the proof of Theorem 2.2 here is valid too. \square

Theorem 2.3 may be used to show the absence of certain energy bound states (compare [6])

COROLLARY 2.6. Assume the conditions of Theorem 2.3. Then

- i) S has no positive eigenvalue if $x \cdot \nabla q \leq -2q$
- ii) S has no eigenvalue if $x \cdot \nabla q \leq 2[\frac{m-2}{2}]^2 \frac{1}{|\cdot|^2}$

(Of course, the inequalities are to be understood in the distributional sense on \mathbb{R}_+^m).

PROOF. Let $Su = \lambda u$ and define

$$p = \begin{cases} -2q & \text{in case i)} \\ 2[\frac{m-2}{2}]^2 \frac{1}{|x|^2} & \text{in case ii)} \end{cases}$$

Then $0 \leq (|u_\varepsilon| \Phi_n)^2 \in C_0^\infty(\mathbb{R}_+^m)$ and

$$(x \cdot \nabla q, (|u_\varepsilon| \Phi_n)^2)_{\text{dist}} \leq (u_\varepsilon \Phi_n, p u_\varepsilon \Phi_n)$$

Due to Theorem 2.3, $u \in Q(q) \cap Q(\frac{1}{|x|^2})$ we have

$$(17) \quad 2(u, -\Delta u) = \lim_{n \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} (x \cdot \nabla q, (|u_\varepsilon| \Phi_n)^2)_{\text{dist}} \leq (u, pu)$$

In case i) we conclude $0 \leq -2\lambda(u, u)$, hence $u = 0$.

In case ii) Hardy's inequality

$$[\frac{m-2}{2}]^2 (\varphi, \frac{1}{|x|^2} \varphi) < (\varphi, -\Delta \varphi), \quad \varphi \in Q(-\Delta), \quad \varphi \neq 0$$

contradicts the relation (17) if $u \neq 0$. \square

COROLLARY 2.7. In addition to the assumptions of Theorem 2.3 we suppose $x \cdot \nabla q \in L_{\text{loc}}^1(\mathbb{R}_+^m)$ and $(x \cdot \nabla q)_+$ or $(x \cdot \nabla q)_-$ to be Δ -form bounded. Let u be an eigenfunction of S .

Then $u \in Q(x \cdot \nabla q)$ and $2(u, -\Delta u) = (u, x \cdot \nabla qu)$.

PROOF. By inspecting the proof of Corollary 2.5 one sees that Corollary 2.7 is valid. \square

Let us now consider relativistic quantum mechanics and look at the energy equation, which corresponds to the Schrödinger equation. In Hilbert space $L^2(\mathbb{R}^m)^4$ with scalar product

$$(\varphi, \psi) = \sum_{k=1}^4 \int \bar{\varphi}_k \psi_k dx \quad \text{the formal Dirac operator, which describes}$$

the behaviour of a spin 1/2 particle with non-zero rest mass under the influence of an electrostatic potential q , is given by $\tau = \alpha \cdot p + \beta + q$ where $p = \frac{1}{i}(\partial_1, \partial_2, \partial_3)$, $\alpha = (\alpha_1, \alpha_2, \alpha_3)$;

$\alpha_1, \alpha_2, \alpha_3, \alpha_4 = \beta$ are Hermitian 4x4 matrices satisfying the commutation relations $\alpha_j \alpha_k + \alpha_k \alpha_j = 2\delta_{jk} I$. It is well known

that $H_0 = \overline{(\tau - q) | C_0^\infty(\mathbb{R}^3)^4}$ is self-adjoint with $D(H_0) = H^1(\mathbb{R}^3)^4$

and $Q(H_0) = H^{1/2}(\mathbb{R}^3)^4$ [15, p. 306ff]. By $U_a \psi(x) = a^{3/2} \psi(ax)$ ($a > 0$) we define a unitary operator in $L^2(\mathbb{R}^3)^4$ mapping the space $H^s(\mathbb{R}^3)^4$ ($s \geq 0$) onto itself and put $D_a = (a-1)^{-1}[U_a - id]$ if $a > 0$, $a \neq 1$. If $\varphi, \psi \in Q(H_0)$ and $a: \mathbb{R}^3 \rightarrow \mathbb{R}$ measurable we define $(\varphi, \alpha \cdot p\psi) = (\varphi, H_0 \psi) - (\varphi, \beta\psi)$ and the self-adjoint operator q by $(q\psi)_k = q\psi_k$, $\psi \in D(q) = \{u \mid u, qu \in L^2(\mathbb{R}^3)^4\}$ with $Q(q) = \{u \mid u, |q|^{1/2}u \in L^2(\mathbb{R}^3)^4\}$.

THEOREM 2.4. Let H be a self-adjoint Dirac operator in $L^2(\mathbb{R}^3)^4$ satisfying $D(H) \subset Q(H_0) \cap Q(q)$ and

$$(\varphi, H\psi) = (\varphi, H_0\psi) + (\varphi, q\psi), \quad \varphi \in Q(H_0) \cap Q(q), \quad \psi \in D(H)$$

(18) Suppose the potential q possesses a.e. a radial derivative $x \cdot \nabla q$ and assume there exists a $|H_0|$ -form bounded function $W \geq 0$ such that for a near 1, $a \neq 1$, we have $\left| \frac{q(ax - q(x))}{a-1} \right| \leq W(x)$ a.e. in \mathbb{R}^3 .

Then every $\varphi \in D(H)$ satisfies

$$(19) \quad (\varphi, i[D, H]\varphi) = (\varphi, H_0\varphi) - (\varphi, x \cdot \nabla q\varphi)$$

where $(\varphi, i[D, H]\varphi) := \lim_{a \rightarrow 1} (\varphi, [H, D_a]\varphi)$.

In particular the virial theorem

$$(20) \quad (\varphi, \alpha \cdot p\varphi) = (\varphi, x \cdot \nabla q\varphi)$$

holds true, if φ is an eigenfunction of S . Moreover if $D(H) \subset D(H_0)$ is valid, it suffices to assume the H_0^2 -form boundedness of W in order to have equations (19), (20).

REMARKS. Theorem 2.4 extends results of Kalf [8] and Albeverio [1]. Albeverio assumes $D(H) = D(H_0)$ and $q, W \in Q_\alpha(\mathbb{R}^3)$ with $\alpha > 0$ suitable (hence W is H_0^2 -form bounded). We remark that in the special case $q(x) = \frac{\mu}{|x|}$, the condition $D(H) = D(H_0)$ implies $|\mu| \leq \frac{1}{2}\sqrt{3}$. In the paper of Kalf [8], $W = c(\frac{1}{|x|} + 1)$,

$q \in C^0(\mathbb{R}_+^3)$ and $|q(x)| \leq \frac{\mu}{|x|} + v$ with $0 \leq \mu < 1, v > 0$ are assumed. Notice that W is $|H_0|$ -form bounded, since $\frac{1}{|T|} \leq \frac{\pi}{2}|H_0|$ in the sense of forms. The self-adjoint realization H , considered there, satisfies the conditions of our Theorem 2.4 as may be seen e.g. by the papers of Klaus-Wüst [9] and Nenciu [11]. Too, the paper of Nenciu [11, Theorem 5.1] gives further examples of self-adjoint Dirac operators H satisfying the assumptions required on H in Theorem 2.4.

PROOF. Since the proof is very similar to that of Theorem 2.1 we will not go into details. Assume $\varphi \in D(H)$, then $U_a \varphi \in Q(H_0) \cap Q(q)$ and thus (use (18))

$$\begin{aligned} (\varphi, [H, D_a] \varphi) &= (a-1)^{-1} [\overline{(D_a \varphi, H\varphi)} - (D_a^* \varphi, H\varphi)] \\ &= (a-1)^{-1} [\overline{(U_a \varphi, H\varphi)} - (U_a^* \varphi, H\varphi)] \\ &= (a-1)^{-1} [\overline{(U_a \varphi, H_0 \varphi)} - (U_a^* \varphi, H_0 \varphi) + \overline{(U_a \varphi, q\varphi)} \\ &\quad - (U_a^* \varphi, q\varphi)] \end{aligned}$$

Since $\overline{(U_a \varphi, H_0 \varphi)} = a(U_a^* \varphi, H_0 \varphi) + (1-a) \cdot (U_a^* \varphi, \beta\varphi)$ and $(U_a^* \varphi, q\varphi) =$
 $= (\varphi, q_a U_a \varphi)$ we obtain

$$(\varphi, [H, D_a] \varphi) = (U_a^* \varphi, H_0 \varphi) - (U_a^* \varphi, \beta\varphi) - (\varphi, \frac{q_a - q}{a-1} U_a \varphi)$$

As in the proof of Theorem 2.1 we conclude

$$\begin{aligned} \lim_{a \rightarrow 1} (U_a^* \varphi, H_0 \varphi) &= (\varphi, H_0 \varphi) \\ \lim_{a \rightarrow 1} (\varphi, \frac{q_a - q}{a-1} U_a \varphi) &= (\varphi, x \cdot \nabla q \varphi) \end{aligned}$$

Thus $\lim_{a \rightarrow 1} (\varphi, [H, D_a] \varphi) = (\varphi, H_0 \varphi) - (\varphi, x \cdot \nabla q \varphi) . \square$

CONCLUDING REMARKS. 1) We like to mention, that Corollary 2.4. i) has been proven, using different methods, by R. Lavine (see [12], Theorem XIII 29) and C.G.Simader (private communication).
 2) We did not prove "generalized" virial theorems (in the sense of Theorem 2.2) for the Dirac operator, in order to keep the length of this paper bearable. We also have to mention, that new

difficulties appear if one likes to extend the method, used in Theorem 2.2 and Corollary 2.5, to the case of Dirac operators (see [8], Remark 2).

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Appendix

Let $\Omega \subset \mathbb{R}^m$ be an open set, $\Phi \in C_0^\infty(\Omega, \mathbb{R})$ and

$$D_\Phi = \frac{i}{2} \Phi^2 [x \cdot \nabla + \nabla \cdot x] = i\Phi^2 \left[\sum_{k=1}^m x_k \partial_k + \frac{m}{2} \right]$$

(A1). For $u \in H_{loc}^1(\Omega, \mathbb{R})$ we have

$$(iD_\Phi u, u) = (u\Phi, ux \cdot \nabla \Phi) .$$

PROOF. First suppose $u \in C^\infty(\Omega)$, then

$$\begin{aligned} (iD_\Phi u, u) &= -(x \cdot \nabla u, u\Phi^2) - \frac{m}{2}(u\Phi, u\Phi) \\ &= (u, \text{div}[xu\Phi^2]) - \frac{m}{2}(u\Phi, u\Phi) \\ &= \frac{m}{2}(u\Phi, u\Phi) + (u, \Phi^2 x \cdot \nabla u) + 2(u\Phi, ux \cdot \nabla \Phi) \\ &= -(iD_\Phi u, u) + 2(u\Phi, ux \cdot \nabla \Phi) . \end{aligned}$$

(A1) now follows by approximation. \square

(A2). Suppose $u \in H_{loc}^2(\Omega, \mathbb{R})$, then

$$\begin{aligned} (iD_\Phi u, -\Delta u) &= -||\Phi \nabla u||^2 + (x \cdot \nabla \Phi \Phi \nabla u, \nabla u) \\ &\quad - 2(\Phi \nabla u \cdot \nabla \Phi, x \cdot \nabla u) - m(\nabla \Phi \cdot \nabla u, \Phi u) . \end{aligned}$$

PROOF. It suffices to prove (A2) for $u \in C^\infty(\Omega)$. We have

$$\begin{aligned} (iD_\Phi u, -\Delta u) &= -(\nabla(\Phi^2 x \cdot \nabla u), \nabla u) - \frac{m}{2}(\nabla(\Phi^2 u), \nabla u) \\ &= -(1 + \frac{m}{2}) ||\Phi \nabla u||^2 + A - 2(\Phi \nabla u \cdot \nabla \Phi, x \cdot \nabla u) - m(\nabla \Phi \cdot \nabla u, \Phi u) \end{aligned}$$

$$\text{where } A = - \sum_{j,k=1}^m \int \partial_k \partial_j u [x_k \partial_j u \Phi^2] dx \\ = m \|\Phi \nabla u\|^2 - A + 2(x \cdot \nabla \Phi \Phi \nabla u, \nabla u) ,$$

so $A = \frac{m}{2} \|\Phi \nabla u\|^2 + (x \cdot \nabla \Phi \Phi \nabla u, \nabla u)$, hence the result. \square

(A3). Suppose q is locally Δ -bounded and $u \in H_{loc}^2(\Omega, \mathbb{R})$.

$$\text{Then } (iD_\phi u, qu) = (x \cdot \nabla \Phi u, qu \Phi) + \frac{1}{2} \lim_{\varepsilon \rightarrow 0} (x \cdot \nabla q, (u_\varepsilon \Phi)^2)_{dist}$$

$$\text{where } u_\varepsilon = u * j_\varepsilon \text{ and } (x \cdot \nabla q, \varphi)_{dist} = - \int q \operatorname{div}[x \varphi] dx$$

$$\text{for all } \varphi \in C_0^\infty(\Omega) .$$

PROOF. Put $u = u_\varepsilon$, $\operatorname{dist}(\operatorname{supp} \Phi, \bar{\Omega}) > \varepsilon > 0$ then

$$\operatorname{div}[x(u\Phi)^2] \in C_0^\infty(\Omega) \text{ and}$$

$$(x \cdot \nabla q, (u\Phi)^2)_{dist} = - \int q \operatorname{div}[xu^2\Phi^2] dx \\ = - m(u\Phi, qu\Phi) - 2(\Phi^2 x \cdot \nabla u, qu) - 2(x \cdot \nabla \Phi u, qu\Phi) .$$

From this identity we conclude (remind $u = u_\varepsilon$)

$$(iD_\phi u, qu) = (x \cdot \nabla \Phi u, qu\Phi) + \frac{1}{2}(x \cdot \nabla q, (u\Phi)^2)_{dist} .$$

Since q is locally Δ -bounded and the forms $(iD_\phi u, qu)$

resp. $(x \cdot \nabla \Phi u, qu\Phi)$ are continuous in H_{loc}^2 , the desired result follows if ε tends to 0. \square

(A4). Suppose q is locally Δ -bounded in Ω , where each local relative bound is smaller than 1. Let $S = -\Delta + q$,

$D(S) = C_0^\infty(\Omega)$ and S^* the adjoint of S in $L^2(\Omega)$. Then $D(S^*) \subset H_{loc}^2(\Omega)$.

PROOF. Let $\psi \in C_0^\infty(\Omega) \subset C_0^\infty(\mathbb{R}^m)$, $0 \leq \psi \leq 1$. Choose

$\Phi \in C_0^\infty(\Omega) \subset C_0^\infty(\mathbb{R}^m)$, $0 \leq \Phi \leq 1$ such that $\operatorname{supp} \psi \subset \Phi^{-1}(\{1\})$,

then $\Phi \psi = \psi$. Put $S_\Phi = -\Delta + q\Phi$ with $D(S_\Phi) = C_0^\infty(\mathbb{R}^m)$. It is

well known that S_Φ is essentially self-adjoint and $D(S_\Phi) = H^2(\mathbb{R}^m)$. Consider $u \in C_0^\infty(\mathbb{R}^m)$ and $v \in D(S^*) \subset L^2(\mathbb{R}^m)$

then $(S_\phi u, v\psi) = (-\Delta u + q\Phi u, v\psi)$
 $= (-\Delta(u\psi) + u\Delta\psi + 2\nabla u \cdot \nabla\psi + qu\Phi\psi, v)$.

Since $u\psi \in C_0^\infty(\Omega)$ and $\Phi\psi = \psi$ we have

$$(S_\phi u, v\psi) = (S(u\psi), v)_{L^2(\Omega)} + (u\Delta\psi + 2\nabla u \cdot \nabla\psi, v)$$
 $= (u\psi, S^*v)_{L^2(\Omega)} + (u\Delta\psi + 2\nabla u \cdot \nabla\psi, v)$

hence $|(S_\phi u, v\psi)| \leq c \|u\|_{H^1(\mathbb{R}^m)}$. Similarly as in [13] it

follows $v\psi \in H^1(\mathbb{R}^m)$. By partial integration we now get
 (with $S^*v \in L^2(\Omega) \subset L^2(\mathbb{R}^m)$)

$$(S_\phi u, v\psi) = (u, \psi S^*v + v\Delta\psi + 2\nabla\psi \cdot \nabla v)$$

Since $S^*v + v\Delta\psi + 2\nabla\psi \cdot \nabla v \in L^2(\mathbb{R}^m)$ it follows $v\psi \in D(S_\phi^*) =$
 $= D(S_\phi) = H^2(\mathbb{R}^m)$, hence $v \in H_{loc}^2(\Omega)$. \square

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