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On the Weyl Quantized Relativistic Hamiltonian
- Kato's inequality and essential selfadjointness -

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1. Introduction.

The classical relativistic Hamilonian of a spinless particle with mass $m\geq 0$ in an electromagnetic field is given by

$$(1.1)\qquad h(p,x) = h_A(p,x) + \Phi(x) \equiv \sqrt{(p-A(x))^2+m^2} + \Phi(x), \qquad (p,x)\in R^d\times R^d.$$

Here measurable functions $A: R^d \to R^d$ and $\Phi: R^d \to R$ are respectively the vector and scalar potentials of the field. For $A(x)$ and $\Phi(x)$ as general as possible, we want to define the Weyl quantized relativistic Hamiltonian $H = H_A+\Phi$ corresponding to (1.1). Φ may be defined as the multiplication operator $\Phi(x)\times$ by the function $\Phi(x)$. But how does one define H_A corresponding to the symbol $h_A(p,x)$? Indeed, if $A \in \mathscr{B}^\infty$, H_A may be defined as the Weyl pseudo-differential operator H_A^w :

$$(1.2)\qquad (H_A^w u)(x) = (2\pi)^{-d}\iint e^{i(x-y)p} \sqrt{(p-A(\tfrac{x+y}{2}))^2+m^2}\, u(y)dydp, \qquad u\in\mathscr{S}(R^d).$$

The right-hand side of (1.2) exists as an oscillatory integral, so that H_A^w defines a symmetric operator in $L^2(\mathbf{R}^d)$ with domain $C_0^\infty(\mathbf{R}^d)$. It can be shown [4] with the general theory of Shubin [12] that H_A^w is essentially selfadjoint on $C_0^\infty(\mathbf{R}^d)$. How about the case for a more general A(x) which is not necessarily smooth and bounded ? This question is motivated by an inspection of the path integral representation, obtained in [4], for the semi-group $\exp[-tH_A^w]$: for $g \in L^2(\mathbf{R}^d)$,

$$(1.3) \qquad \Big(\exp[-t(H_A^w-m)]g\Big)(x) = \int e^{-iS(t,X)} g(X(t))\,d\lambda_x(X) ,$$

$$\text{with} \qquad S(t,X) = \int_0^{t+}\int_{|y|>0} A(X(s-)+y/2)\cdot y \ \tilde{N}_X(dsdy)$$

$$+ \int_0^t\int_{|y|>0} [A(X(s)+y/2)-A(X(s))]\cdot y \ dsn(dy).$$

Here $n(dy)$ is a σ-finite measure on $\mathbf{R}^d\setminus\{0\}$, called the Lévy measure, which behaves as $O(|y|^{-(d+1)})dy$ near $y=0$, and is, on $\{|y|\geq 1\}$, a bounded measure. Hence the right-hand side of (1.3) makes sense, at least, if A(x) is locally Hölder continuous. This suggests that there may be an alternative definition of the Weyl quantized relativistic Hamiltonian H_A corresponding to the classical symbol $h_A(p,x)$ which is still valid for general A(x). In the present lecture we shall give a survey of our recent results [2], [3] on this matter. Finally we quickly explain here the other notations in (1.3). λ_x is a probability measure on the space $D_x([0,\infty)\to\mathbf{R}^d)$ of the right-continuous paths $X : [0,\infty)\to\mathbf{R}^d$ having left-hand limits with $X(0)=x$. $\tilde{N}_X(dsdy)$ is a measure, depending on each path X, on $(0,\infty)\times(\mathbf{R}^d\setminus\{0\})$ defined by $\tilde{N}_X(dsdy) \equiv N_X(dsdy) - dsn(dy)$ with a counting measure

$$N_X((t,t']\times B) = \#\{\ s\in(t,t'];\ X(s)-X(s-)\in B\ \},$$

where $0<t<t'$ and B is a Borel set in $\mathbf{R}^d\setminus\{0\}$.

In Section 2 we give our definition of the Weyl quantized relativistic Hamiltonian H_A for general A(x) and discuss the problem of its essential selfadjointness. The solution is reduced to establishing of an analogue of Kato's inequality between H_A and $\sqrt{-\Delta+m^2}$. Section 3 is devoted to an outline of proofs of the theorems. In Section 4 some remarks are given.

2. Definition of the Weyl Quantized Relativistic Hamiltonian and Theorems.

Unless otherwise specified, we assume that $A: \mathbf{R}^d \to \mathbf{R}^d$ is measurable and satisfies that

$$(2.1) \qquad A(x) \text{ and } \int_{0<|y|<1} |A(x-y/2)-A(x)|\,|y|^{-d}\,dy \quad \textit{are locally bounded.}$$

In particular, a locally Hölder continuous A(x) satisfies (2.1).

We shall define the *Weyl quantized relativistic Hamiltonian* H_A corresponding to the classical symbol $h_A(p,x)$ as follows.

Definition.

$$(2.2) \qquad (H_A u)(x) = mu(x) - \int_{|y|>0} [e^{-iyA(x+y/2)}u(x+y)-u(x) - I_{\{|y|<1\}}\, y(\partial_x - iA(x))u(x)]\,n(dy), \quad u \in \mathcal{S}(\mathbf{R}^d).$$

Here $I_{\{|y|<1\}}$ is the characteristic function of the set $\{|y|<1\}$. The Lévy measure n(dy) is given by

$$(2.3) \qquad n(dy) = \begin{cases} C(d)m^{(d+1)/2}|y|^{-(d+1)/2}K_{(d+1)/2}(m|y|)dy, & m>0, \\ C'(d)|y|^{-(d+1)}dy, & m=0, \end{cases}$$

where C(d) and C'(d) are constants depending on the dimension d, and $K_\nu(z)$ is the modified Bessel function of the third kind of order ν. One can directly calculate (2.3), using the fact [7] that $t^{-1}k_o(t,y)dy \to n(dy)$ as $t\downarrow 0$, where $k_o(t,x-y)$ is the kernel of the operator $\exp[-t(\sqrt{-\Delta+m^2}-m)]$.

Lemma 1. H_A is a symmetric operator in $L^2(\mathbf{R}^d)$ with domain $C_o^\infty(\mathbf{R}^d)$.

Proof. Let $u \in C_o^\infty(\mathbf{R}^d)$, and write

$$(2.4)\quad (H_Au)(x) = mu(x) - \int_{|y|\geq 1}[e^{-iyA(x+y/2)}u(x+y)-u(x)]n(dy)$$
$$- \int_{0<|y|<1}[e^{-iyA(x+y/2)}u(x+y)-u(x)-y(\partial_x-iA(x))u(x)]n(dy)$$
$$\equiv mu + I_1u + I_2u.$$

Noting (2.3), we can show that I_1 is a bounded linear operator on $L^2(\mathbf{R}^d)$ and that I_2u is a continuous function with compact support, and for every compact $K_4 \subseteq \mathbf{R}^d$ there exists a constant C_K such that, for $u \in C_o^\infty(\mathbf{R}^d)$ with supp $u \subseteq K$,

$$(2.5)\qquad \|I_2u\|_2 \leq C_K[\|u\|_\infty+\|\partial u\|_\infty+\|\partial\partial u\|_\infty].$$

To show H_A is symmetric we have to show that for I_1 and I_2. It is seen that $(I_1u,v) = (u,I_1v)$, $u,v \in C_o^\infty(\mathbf{R}^d)$, by change of variables and by invariance of $n(dy)$ under the transformation $y \to -y$. Similarly, I_2 is symmetric, if we note

$$(I_2u)(x) = -\lim_{\varepsilon\downarrow 0}\int_{\varepsilon\leq|y|<1}[e^{-iyA(x+y/2)}u(x+y)-u(x)]n(dy). \quad \square$$

Next, we shall explain where the definition (2.2) of H_A comes from and see that H_A coincides with the Weyl pseudo-differential operator H_A^W, (1.2), if $A(x)$ satisfies, for instance,

$$(2.6)\qquad A \in C^\infty,\quad |\partial^\alpha A(x)| \leq C_\alpha,\quad |\alpha| \geq 1.$$

Notice that the condition (2.6), which is a little more general than $A \in B^{\infty}$, includes the physically important case of constant magnetic fields : $A(x) = A\cdot x$ with A a real constant matrix.

Our starting point is the Lévy-Khinchin formula ([6],[11])

$$\sqrt{p^2+m^2} = m - \int_{|y|>0} [e^{ipy}-1-I_{\{|y|<1\}}ipy]n(dy). \tag{2.7}$$

Let $u \in \mathcal{S}(\mathbf{R}^d)$. Multiply both sides of (2.7) by the Fourier transform $\hat{u}(p)$ of u and make the inverse Fourier transform. Then

$$\left(\sqrt{-\Delta+m^2}\, u\right)(x) = mu(x) - \int_{|y|>0} [u(x+y)-u(x)-I_{\{|y|<1\}}y\partial_x u(x)]n(dy). \tag{2.8}$$

First note with $H_o \equiv \sqrt{-\Delta+m^2}$ that when $A(x)\equiv 0$, (2.8) is consistent with (2.2). On the other hand, if A(x) satisfies (2.6), we can rewrite (1.2) as oscillatory integrals, by changing the variables $p-A\left(\frac{x+y}{2}\right) = p'$ (writing p again instead of p'), to get

$$\begin{aligned}(H_A^W u)(x) &= (2\pi)^{-d}\iint \exp\left[i(x-y)\cdot\left(p+A\left(\frac{x+y}{2}\right)\right)\right]\sqrt{p^2+m^2}\, u(y)dydp \\ &= \left(\sqrt{-\Delta+m^2}\left(\exp\left[i(x-\cdot)\cdot A\left(\frac{x+\cdot}{2}\right)\right]u(\cdot)\right)\right)(x).\end{aligned}$$

Since, for x fixed, the function $y \to \exp\left[i(x-y)\cdot A\left(\frac{x+y}{2}\right)\right]u(y)$ belongs to $\mathcal{S}(\mathbf{R}^d)$, we see in virtue of (2.8) that the above last formula equals $H_A u$, concluding that $H_A^W = H_A$ on $\mathcal{S}(\mathbf{R}^d)$. Thus we have shown

<u>Lemma 2</u>. If A(x) satisfies (2.6), then, for $u \in \mathcal{S}(\mathbf{R}^d)$,

$$(H_A u)(x) = (H_A^W u)(x) = \left(\sqrt{-\Delta+m^2}\left(\exp\left[i(x-\cdot)\cdot A\left(\frac{x+\cdot}{2}\right)\right]u(\cdot)\right)\right)(x). \tag{2.9}$$

Remarks 1°. The relation (2.9) says that apply H_A or H_A^W to u amounts to the same thing as apply the free quantum Hamiltonian $\sqrt{-\Delta+m^2}$ to the appropriately "gauge transformed" u. Of course, the same is valid for the Schrödinger operator with magnetic fields:

$$(-i\partial-A(x))^2u(x) = \left(-\Delta\left(\exp\left[i(x-\cdot)\cdot A\left(\frac{x+\cdot}{2}\right)\right]u(\cdot)\right)\right)(x), \quad u \in \mathcal{S}(\mathbf{R}^d).$$

2^o. The expression (2.2) of H_A can also be obtained by calculating, through Itô's formula (e.g. [6]), the generator of the semigroup represented by path integral (1.3).

The main results are the following two theorems.

Theorem 1. Suppose that A(x) satisfies (2.1) and $\Phi \in L^2_{loc}(\mathbf{R}^d)$, $\Phi(x)\geq 0$ a.e. Then

(i) $H_A + \Phi$ is essentially selfadjoint on $C_o^\infty(\mathbf{R}^d)$.

(ii) The selfadjoint extension of H_A, denoted again by the same H_A, is bounded from below: $H_A \geq m$.

Remark. Nagase-Umeda [10] have shown that if A(x) satisfies (2.6), the Weyl pseudo-differential operator H_A^w is essentially selfadjoint.

Theorem 1-(i) can be shown in just the same way as in Kato [8], if an analogue of Kato's inequality (as in Theorem 2 below) is established. Notice that $\left(\sqrt{-\Delta+m^2}+1\right)^{-1}$ is positivity preserving. The proof of Theorem 2-(ii) follows from the proof of Theorem 2.

Now, for $u \in L^2(\mathbf{R}^d)$, define a distribution $H_Au \in \mathcal{D}'(\mathbf{R}^d)$ by

(2.10) $$(H_Au,\varphi) = (u,H_A\varphi), \quad \varphi \in C_o^\infty(\mathbf{R}^d).$$

Here note with (2.4) that $\|I_1\varphi\|_2 \le C\|\varphi\|_2$ and (2.5).

<u>Theorem 2</u> (Kato's inequality). Suppose A(x) satisfies (2.1). If $u \in L^2$ and $H_A u \in L^1_{loc}$, then the following distributional inequality holds:

$$\text{(2.11)} \qquad \mathrm{Re}[(\mathrm{sgn}\ u)H_A u] \ge \sqrt{-\Delta+m^2}\ |u|.$$

with
$$(\mathrm{sgn}\ u)(x) = \begin{cases} \overline{u(x)}/|u(x)|, & u(x)\ne 0 \\ 0 & , \quad u(x)= 0. \end{cases}$$

<u>3. Outline of Proofs of Theorem 2 and Theorem 1-(ii).</u>

In the proof it is crucial that H_A is represented as an integral operator (2.2).

(*First Step*) Let $u \in C^\infty \cap L^2$, and put $u_\varepsilon(x) = \sqrt{|u(x)|^2+\varepsilon^2}$, $\varepsilon>0$. Then u_ε is C^∞. Since $-|v(x)||v(x+y)|+|v(x)|^2 \ge -v_\varepsilon(x)v_\varepsilon(x+y)+v_\varepsilon(x)^2$, and $\partial|u(x)|^2 = \partial u_\varepsilon(x)^2$, we have (writing, for simplicity, $((H_A-m)u)(x)$ and $((H_o-m)u_\varepsilon)(x)$ as $(H_A-m)u(x)$, and $(H_o-m)u_\varepsilon(x)$, respectively)

$$\text{(3.1)} \quad \mathrm{Re}[\overline{u(x)}(H_A-m)u(x)] = 2^{-1}\{\overline{u(x)}(H_A-m)u(x)+u(x)\overline{(H_A-m)u(x)}\}$$

$$= \frac{1}{2}\int_{|y|>0} -\Big(\overline{u(x)}[e^{-iyA(x+y/2)}u(x+y)-u(x)-I_{\{|y|<1\}}y(\partial_x-iA(x))]u(x)$$

$$+ u(x)[e^{iyA(x+y/2)}\overline{u(x+y)}-\overline{u(x)}-I_{\{|y|<1\}}y(\partial_x+iA(x))\overline{u(x)})]\Big)n(dy)$$

$$\ge \int_{|y|>0}[-|u(x)||u(x+y)|+|u(x)|^2 + 2^{-1}I_{\{|y|<1\}}y\partial|u(x)|^2]n(dy).$$

$$\ge \int_{|y|>0}[-u_\varepsilon(x)u_\varepsilon(x+y)+u_\varepsilon(x)^2 + 2^{-1}I_{\{|y|<1\}}y\partial u_\varepsilon(x)^2]n(dy)$$

$= u_\varepsilon(x)(H_o-m)u_\varepsilon(x)$,

pointwise. Integrating the first and last members of (3.1) yields $\mathrm{Re}((H_A-m)u,u) \geq ((H_o-m)u_\varepsilon,u_\varepsilon) \geq 0$. This proves Theorem 1-(ii), since H_A is symmetric by Lemma 1.

On the other hand, dividing the first and last members of (3.1) by u_ε yields

$$(3.2)\qquad \mathrm{Re}[(\overline{u(x)}/u_\varepsilon(x))(H_A-m)u] \geq (H_o-m)u_\varepsilon,$$

pointwise and so in the distribution sense.

(*Second Step*) For general u, let $u^\delta = \rho_\delta * u$, where $\rho_\delta *$ is Friedrichs' mollifier. We obtain from (3.2)

$$(3.3)\qquad \mathrm{Re}\left[\left(\overline{u^\delta}/(u^\delta)_\varepsilon\right)(H_A-m)u^\delta\right] \geq (H_o-m)(u^\delta)_\varepsilon ,$$

where $(u^\delta)_\varepsilon = (|u^\delta|^2+\varepsilon^2)^{1/2}$, $\varepsilon>0$. We let $\delta\downarrow 0$ first and then $\varepsilon\downarrow 0$. As $\delta\downarrow 0$, we have (by taking a subsequence if necessary) $u^\delta \to u$ in L^2 and a.e. so that $(u^\delta)_\varepsilon \to u_\varepsilon$ in L^2 and a.e. It follows that $\{\overline{u^\delta}/(u^\delta)_\varepsilon\}$ is bounded and converges to $\bar{u}/u_\varepsilon$ a.e. and $H_o(u^\delta)_\varepsilon \to H_o u_\varepsilon$ in $\mathcal{D}'$. For the moment, suppose that

$$(3.4)\qquad H_A u^\delta \to H_A u \quad \text{in } L^1_{loc}, \quad \delta\downarrow 0.$$

Then the left-hand side of (3.3) converges in L^1_{loc}. Thus we get

$$(3.5)\qquad \mathrm{Re}[(\mathrm{sgn}\ u)(H_A-m)u] \geq (H_o-m)|u|,$$

in the distribution sense. Finally let $\varepsilon\downarrow 0$. The left-hand side of (3.5) converges to $\mathrm{Re}[(\mathrm{sgn}\ u)(H_A-m)u]$ a.e., while the right-hand side to $(H_o-m)|u|$ in $\mathcal{D}'$. □

To prove the remaining assertion (3.4), we need regularity of a function $u \in L^2$ with $H_A u \in L^1_{loc}$ as in the following lemma.

Lemma 3. If $u \in L^2$ and $H_A u \in L^1_{loc}$, then u has a decomposition $u = u_1 + u_2$ such that, for every $\psi \in C_0^\infty(R^d)$,

$$\psi u_1,\ H_0\psi u_1 \in L^1, \quad \text{and} \quad \psi u_2,\ H_0\psi u_2 \in L^2.$$

First we prove (3.4). By (2.4), $H_A = m + I_1 + I_2$. Let $u \in L^2$ and $H_A u \in L^1_{loc}$. Since I_1 is a bounded operator on $L^2(R^d)$, we have $I_1 u \in L^2$, and hence $I_2 u \in L^1_{loc}$. Since $I_1 u^\delta \to I_1 u$ in L^2 as $\delta \downarrow 0$, we have only to show $I_2 u^\delta \to I_2 u$ in L^1_{loc}. It is clear that $I_2 u^\delta \to I_2 u$ in $\mathcal{D}'$. Therefore it suffices to show

(3.6) $$I_2 u^\delta - I_2 u^{\delta'} \to 0 \quad \text{in } L^1_{loc}, \qquad \delta, \delta' \downarrow 0.$$

To see (3.6), first note that for every compact $K \subseteq R^d$ there is a constant C_K such that, for $\varphi \in C_0^\infty(R^d)$ with supp $\varphi \subseteq K_4$,

(3.7) $$\|I_2\varphi\|_{1,K} \equiv \int_K |I_2\varphi|dx \le C_K[\|H_0\varphi\|_i + \|\varphi\|_2], \quad i=1,2,$$

where $K_r = \{x;\ \text{dist}(x,K) \le r\}$. Next let $\psi \in C_0^\infty(R^d)$, $0 \le \psi(x) \le 1$, with $\psi(x)=1$ on K_2 and supp $\psi \subseteq K_3$. By Lemma 3, $u = u_1 + u_2$. ψu and ψu_2 are L^2, and so is ψu_1. If $0<\delta<<1$, the $(\psi u_i)^\delta$ satisfy the condition for φ in (3.7). We have, for i=1,2, $H_0(\psi u_i)^\delta = (H_0\psi u_i)^\delta \in L^i$, and $I_2 u_i^\delta = I_2(\psi u_i)^\delta$ on K. Then, by (3.7),

$$\|I_2 u^\delta - I_2 u^{\delta'}\|_{1,K}$$
$$\le C_K \textstyle\sum_{i=1}^2 \left[\|(H_0\psi u_i)^\delta - (H_0\psi u_i)^{\delta'}\|_i + \|(\psi u_i)^\delta - (\psi u_i)^{\delta'}\|_2\right],$$

whence follows (3.6).

The proof of Lemma 3 needs task. We establish a kind of integral representation for $u \in L^2$ with $H_A u \in L^1_{loc}$ (cf. [5, Appendix]). We get from (2.9)

$$((H_A+1)u,\varphi) = (u,(H_A+1)\varphi), \qquad \varphi \in C_0^\infty(R^d).$$

Take $\varphi(y) = G_\varepsilon(x-y)$ with

$$G_\varepsilon(x) = (2\pi)^{d/2}\chi(x/R)\mathcal{F}^{-1}\left(\frac{\exp[-\varepsilon(\sqrt{p^2+m^2}+1)]}{\sqrt{p^2+m^2}+1}\right)(x), \qquad \varepsilon \geq 0,$$

where $\chi \in C_0^\infty(R^d)$ and $R > 0$ ($\mathcal{F}^{-1}$ denotes the inverse Fourier transform). Then

$$(3.8) \qquad ((H_A+1)u,G_\varepsilon(x-\cdot)) = (u,(H_A+1)G_\varepsilon(x-\cdot)).$$

Write

$$((H_A+1)G_\varepsilon(x-\cdot))(y) = ((H_0+1)G_\varepsilon(x-\cdot))(y) - \overline{E_\varepsilon(x,y)} - \overline{F_\varepsilon(x,y)}$$

and let $\varepsilon\downarrow 0$. Then the right-hand side of (3.8) converges to $u-Qu-Eu-Fu$, while the left-hand side of (3.8) converges to $G[H_A+1]u$, both in L^1_{loc}. Thus $u = G[H_A+1]u+Qu+Eu+Fu$. Here Q, E and F are certain integral operators, and G is the one with kernel $G_0(x-y)$. Then Lemma 3 follows by studing the kernels of G, Q, E and F with the aid of the theory of singular integrals. □

4. Concluding Remarks.

1°. Our Weyl quantized relativistic Hamiltonian H_A generally differs from the square root of the nonnegative selfadjoint operator $(-i\partial-A(x))^2 + m^2$:

$$H_A \neq \sqrt{(-i\partial-A(x))^2+m^2}\ .$$

They coincide for $A(x) = A\cdot x$, with A a real symmetric constant matrix. This can be seen with the composition formula for Weyl pseudo- differential operators (e.g. [1, p.151-2]).

However, we shall not discuss which is physically more appropriate as a relativistic quantum Hamiltonian of a spinless particle. H_A suits better from the path integral point of view, because H_A has an exact classical symbol $h_A(p,x)$ as a Weyl pseudo-differential operator (cf. [9]). But H_A is not gauge-invariant, though $\sqrt{(-i\partial-A(x))^2+m^2}$ is.

2^o. When $A(x)\equiv 0$, Theorem 2 turns out: If $u \in L^2$ and $\sqrt{-\Delta+m^2}\, u \in L^1_{loc}$, then

$$\text{(4.1)} \qquad \mathrm{Re}[(\mathrm{sgn}\, u)\sqrt{-\Delta+m^2}\, u] \geq \sqrt{-\Delta+m^2}\, |u|,$$

in the distribution sense. It appears that Theorem 2 should follow immediately from (4.1) and (2.9) by substituting the function $\exp\left[i(x-\cdot)A\left(\frac{x+\cdot}{2}\right)\right]u(\cdot)$ into u in (4.1). However, it is a problem whether (2.9) is true for $A(x)$ not satisfying (2.6) or $u(x)$ not belonging to $\mathcal{S}(\mathbf{R}^d)$.

3^o. An analogue of Kato's inequality will be shown for the operator L corresponding to the Lévy process (e.g. [13]):

$$(Lu)(x) = -\left[\sum_{j,k=1}^d \partial_j a_{jk}(x)\partial_k + \sum_{j=1}^d b_j(x)\partial_j + c(x)\right]u(x) - \int_{|y|>0} [u(x+y)-u(x)-I_{\{|y|<1\}}y\partial u(x)]n(x,dy).$$

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