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Osaka J. Math.
30 (1993), 839-853

SPECTRA OF RELATIVISTIC SCHRÖDINGER OPERATORS WITH MAGNETIC VECTOR POTENTIALS

Dedicated to Professor HIROKI TANABE on his sixtieth birthday

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(Recieved June 22, 1992)

1. Introduction

This paper is concerned with the Weyl quantized Hamiltonian of a relativistic spinless particle of mass m interacting with both a magnetic vector potential $a(x)$ and an electric potential $V(x)$:

$$H = h^w(x, D) + V(x)\,, \tag{1.1}$$

where

$$h^w(x, D)u(x) = \iint e^{i(x-y)\cdot\xi}\, h\left(\frac{x+y}{2}, \xi\right) u(y)(2\pi)^{-n} dy d\xi\,,$$
$$h(x, \xi) = \sqrt{|\xi - a(x)|^2 + m^2}\,,$$
$$(x, \xi \in \boldsymbol{R}^n,\ m > 0)\,.$$

When the magnetic potential $a(x)$ is identically zero, the operator (1.1) becomes of the form

$$\sqrt{-\Delta + m^2} + V(x)\,,$$

whose spectral properties have been extensively studied by many authors; see Lieb [10], Carmona, Masters and Simon[1] and the references therein. On the other hand, there have been no results on spectral properties of (1.1) so far as we know.

The aim of this paper is to make an attempt to fill this gap. Our main concern is to locate the essential spectrum of the operator (1.1). Our assumptions on the magnetic vector potential $a(x)$ require the derivatives of $a(x)$ to tend to zero at infinity. Consequently, we are unable to cover the important case where $a(x)$ is linear. Our idea, which will be stated as an abstract lemma in Section 3, is based on a combination of the spectral mapping theorem and Weyl's essential spectrum theorem. To apply the abstract lemma, we calculate the square of $h^w(x, D)$ with the aid of the theory of pseudo-differential operators. The calculation shows in a certain sense that the difference between $h^w(x, D)$ and the operator-square root of the Schrödinger operator T with the same magnetic vector potential $a(x)$ is small. (See Section 2 for the precise definition of T.) However, it is important that the difference is, in general, not equal to zero. If the difference were equal to zero, our main results would be easy consequences of the spectral mapping theorem.

We list here the notations used in this paper. For a self-adjoint operator A in a Hilbert space, $\sigma(A)$, $\sigma_{ess}(A)$ and $\sigma_{disc}(A)$ will denote the spectrum, the essential spectrum and the discrete spectrum of A respectively. For a subset Σ of $[0, \infty)$ we shall write

$$\sqrt{\Sigma} = \{\sqrt{\lambda} \mid \lambda \in \Sigma\} .$$

For a magnetic vector potential $a=(a_1, \cdots, a_n)$ we shall define curl a to be the skewsymmetric matrix valued function with the (j, k)-component $\partial a_k/\partial x_j - \partial a_j/\partial x_k$ $(j, k=1, \cdots, n)$. The space of C^∞-functions having compact supports will be denoted by $C_0^\infty(\boldsymbol{R}^n)$. The Schwartz space of rapidly decreasing functions will be denoted by $\mathcal{S}(\boldsymbol{R}^n)$. By $H^s(\boldsymbol{R}^n)$ we shall mean the Sobolev space of order $s \in \boldsymbol{R}$.

The plan of the paper is as follows. We shall state the main theorems in Section 2. In Section 3 we shall describe our idea in an abstract manner. In Section 4 we shall show that the domain of the self-adjoint realization of $h^w(x, D)$ is $H^1(\boldsymbol{R}^n)$. We shall need this fact to prove our fundamental result (Theorem 1 in Section 2). In Section 5 we shall give proofs of the main theorems with the aid of a key lemma. The proof of the key lemma will be given in Section 6. In Section 7 we shall discuss the the difference between $h^w(x, D)$ and $\sqrt{T}$.

There has recently been a tendancy to call the operator (1.1) a relativistic Schrödinger operator. We follow this tendancy.

2. The Main Results

Let $a(x)=(a_1(x), \cdots, a_n(x))$ be an $\boldsymbol{R}^n$-valued function on $\boldsymbol{R}^n$. We make the following assumptions:

(I) Each $a_j(x)$ is a C^∞-function which is bounded on $\boldsymbol{R}^n$.

(II) For any multi-index $\alpha \neq 0$,

$$\left(\frac{\partial}{\partial x}\right)^\alpha a(x) \to 0 \quad \text{as} \quad |x| \to \infty .$$

Let $V(x)$ be a real-valued measurable function on $\boldsymbol{R}^n$ and let V denote multiplication by $V(x)$. Our assumption on V is

(III) $V(-\Delta+1)^{-1/2}$ is a compact operator on $L^2(\boldsymbol{R}^n)$.

It is a well-known fact that if $|V(x)| \leq c(1+|x|)^{-\varepsilon}$ $(\varepsilon>0)$ then V satisfies

Assumption(III). Furthermore $V(x)$ which obeys Assumption(III) can have singular points. Indeed, one can show, with the aid of Schechter[16, Theorem 9.6, p.144], that $V(x)=|x|^{-\varepsilon}$ with $0<\varepsilon<1$ satisfies Assumption(III).

Before stating our main theorems, we shall show that the operator $h^w(x, D)+V(x)$ admits a self-adjoint realization in $L^2(\boldsymbol{R}^n)$. To this end, we first note that the relativistic Schrödinger operator $h^w(x, D)$ defines a linear operator in $L^2(\boldsymbol{R}^n)$ and is essentially self-adjoint on $C_0^\infty(\boldsymbol{R}^n)$. We shall prove these facts in Section 4. We next define the self-adjoint operator H_1 in $L^2(\boldsymbol{R}^n)$ to be the closure of $h^w(x, D)$ with domain $C_0^\infty(\boldsymbol{R}^n)$. We shall also show in Section 4 that

$$\mathrm{Dom}\,(H_1) = H^1(\boldsymbol{R}^n)\,. \tag{2.1}$$

Assumption(III) together with (2.1) implies that V is H_1-compact, so that V is H_1-bounded with H_1-bound equal to 0 (cf. Reed and Simon[14, Problem 20, p.340]). We finally define the self-adjoint realization H in $L^2(\boldsymbol{R}^n)$ of $h^w(x, D)+V(x)$ by

$$H = H_1+V \quad \text{with} \quad \text{domain} \quad H^1(\boldsymbol{R}^n)\,.$$

Note that $h^w(x, D)+V(x)$ is essentially self-adjoint on $C_0^\infty(\boldsymbol{R}^n)$ (cf. Kato [7, Theorem 4.4, p.288]). Hence H is the unique self-adjoint extension of $h^w(x, D)+V(x)$ with domain $C_0^\infty(\boldsymbol{R}^n)$.

In order to state our basic theorem, we define a self-adjoint operator T to be the clousre of

$$\sum_{j=1}^n \left(\frac{\partial}{i\partial x_j}-a_j(x)\right)^2+m^2 \quad \text{with domain } C_0^\infty(\boldsymbol{R}^n)\,,$$

which is essentially self-adjoint(cf. Ikebe-Kato [5]). The basic theorem is

Theorem 1. *If Assumptions* (I)-(III) *hold, then* $\sigma_{\mathrm{ess}}(H)=\sqrt{\sigma_{\mathrm{ess}}(T)}$.

From Theorem 1 we can deduce several results locating the essential spectra of H and H_1. In general dimension we require, in addition to Assumptions (I) and (II), an assumption on $a(x)$ which is closely related to a gauge transformation:

(IV) There exists a smooth vector potential $b(x)$ such that
- (i) $\mathrm{curl}\, a = \mathrm{curl}\, b$,
- (ii) $b(x)\to 0$ as $|x|\to\infty$.

Theorem 2. *If Assumptions* (I)-(IV) *hold, then* $\sigma_{\mathrm{ess}}(H)=[m, \infty)$.

Theorem 3. *Let* $n=2$ *or* 3. *If Assumptions* (I)-(III) *holds, then the conclusion of Theorem* 2 *holds.*

Theorem 4. *If Assumptions* (I), (II) *and* (IV) *hold, then* $\sigma(H_1)=\sigma_{\mathrm{ess}}(H_1)=[m, \infty)$.

Theorem 5. *Let $n=2$ or 3. If Assumptions* (I) *and* (II) *hold, then the conclusion of Theorem* 4 *holds.*

3. Abstract Lemmas

We prove in this section three lemmas. Even though these lemmas are simple, they are interesting on thier own from the view point of operator theory. We shall use Lemma 3.3 below in proving Theorem 1. We need Lemmas 3.1 and 3.2 only to prove Lemma 3.3.

Let H be a self-adjoint operator in a Hilbert space $\mathcal{H}$ and $\{E(\Lambda)\}$ its spectral measure.

Lemma 3.1. (Spectral mapping theorem) *Suppose $H\geq 0$. Then $\sigma(\sqrt{H})=\sqrt{\sigma(H)}$, $\sigma_{\mathrm{ess}}(\sqrt{H})=\sqrt{\sigma_{\mathrm{ess}}(H)}$, and $\sigma_{\mathrm{disc}}(\sqrt{H})=\sqrt{\sigma_{\mathrm{disc}}(H)}$.*

Proof. Let $\Phi(\lambda)$ be a real-valued continuous function on $\boldsymbol{R}$ such that $\Phi(\lambda)=\sqrt{\lambda}$ for $\lambda\geq 0$. Then $\Phi(H)=\sqrt{H}$. Define a spectral measure $\{E_\Phi(\Lambda)\}$ by

$$E_\Phi(\Lambda)=E(\Phi^{-1}(\Lambda))$$

for any Borel subset Λ of $\boldsymbol{R}$. By elementary calculation in measure theory, we see that

$$\Phi(H)=\int \lambda dE_\Phi(\lambda)\,. \tag{3.1}$$

In other words, $\{E_\Phi(\Lambda)\}$ is the spectral measure of $\sqrt{H}$. Combining this fact and Reed and Simon[13, Proposition and Definition, p.236], we obtain the desired conclusion. Q.E.D.

Lemma 3.2. *Let A be a nonnegative self-adjoint operator in $\mathcal{H}$. Suppose that $H^2=A$ and $H\geq 0$. Then $H=\sqrt{A}$.*

Proof. Let $\Psi(\lambda)=\lambda^2$. Define a spectral measure $\{E_\Psi(\Lambda)\}$ by

$$E_\Psi(\Lambda)=E(\Psi^{-1}(\Lambda)) \tag{3.2}$$

for any Borel subset Λ of $\boldsymbol{R}$. Then, similarly to (3.1), we see that $\{E_\Psi(\Lambda)\}$ is the spectral measure of $\Psi(H)=H^2$. Since $H^2=A$, this is equivalent to the fact that $\{E_\Psi(\Lambda)\}$is the spectral meassure of A. Thus we have

$$\sqrt{A}=\int \sqrt{\lambda}\, dE_\Psi(\lambda)\,. \tag{3.3}$$

By (3.2), the right hand side of (3.3) is equal to H. Q.E.D.

Lemma 3.3. *Let T be a self-adjoint and R a symmetric operators in $\mathcal{H}$.*

Suppose that $R(T+i)^{-1}$ *is compact. If* $H^2=T+R$ *and* $H\geq 0$, *then* $\sigma_{ess}(H)=\sqrt{\sigma_{ess}(T)}$.

Proof. Put $A=T+R$. It is obvious that A is a nonnegative self-adjoint operator and $H^2=A$. It follows from Lemma 3.2 that $H=\sqrt{A}$. Applying Lemma 3.1, we see that $\sigma_{ess}(H)=\sqrt{\sigma_{ess}(A)}$. Since R is relatively compact with respect to T, we find by Reed and Simon[15, Corollary 2, p. 113] that $\sigma_{ess}(A)=\sigma_{ess}(T)$. This implies the desired conclusion. Q.E.D.

4. The Domain of the Operator H_1

In this section we prove (2.1) in Section 2. It is a bonus that $h^w(x, D)$ is essentially self-adjoint on $C_0^\infty(\boldsymbol{R}^n)$. The proof is based on a fundamental result in perturbation theory, namely the Kato-Rellich theorem.

Lemma 4.1. *Suppose that Assumptions* (I) *and* (II) *hold. Then:*
(i) $h^w(x, D)$ *is essentially self-adjoint on* $C_0^\infty(\boldsymbol{R}^n)$.
(ii) $\mathrm{Dom}\,(H_1)=H^1(\boldsymbol{R}^n)$.

Proof. First define a self-adjoint operator H_0 in $L^2(\boldsymbol{R}^n)$ by

$$H_0=\sqrt{-\Delta+m^2} \qquad \text{with domain } H^1(\boldsymbol{R}^n)\,.$$

Next define

$$s(x, \xi)=\frac{|a(x)|^2-2\xi\cdot a(x)}{\sqrt{|\xi-a(x)|^2+m^2}+\sqrt{|\xi|^2+m^2}}\,.$$

It is evident that

$$h(x, \xi)=\sqrt{|\xi|^2+m^2}+s(x, \xi)\,. \tag{4.1}$$

Since $a(x)$ is bounded together with its all derivatives, we see that $s(x, \xi)\in S^0$. (See Kumano-go[8, Definition 1.1, p. 54], for the definition of S^0). In view of [8, Theorem 1.6, p. 224], $s^w(x, D)$ can be extended to a bounded self-adjoint operator on $L^2(\boldsymbol{R}^n)$, which will be denoted by S. By Kato [7, Theorem 4.3, p. 287], we see that H_0+S is a self-ajoint operator in $L^2(\boldsymbol{R}^n)$, of which domain is $H^1(\boldsymbol{R}^n)$. Then it follows from (4.1) that H_0+S is a self-adjoint extension of $h^w(x, D)$ with domain $C_0^\infty(\boldsymbol{R}^n)$. Since H_0 is essentially self-adjoint on $C_0^\infty(\boldsymbol{R}^n)$, we find by Kato[7, Theorem 4.4, p. 288] that $h^w(x, D)$ is essentially self-adjoint on $C_0^\infty(\boldsymbol{R}^n)$. Thus we have proved Conclusion (i), which implies that $h^w(x, D)$ with domain $C_0^\infty(\boldsymbol{R}^n)$ has only one self-adjoint extension. Hence $H_1=H_0+S$. In particular $\mathrm{Dom}\,(H_1)=H^1(\boldsymbol{R}^n)$. Q.E.D.

REMARK. It is known that $h^w(x, D)$ is essentially self-adjoint on $C_0^\infty(\boldsymbol{R}^n)$ undeɪ much weaker assumptions on $a(x)$ than Assumptions (I) and (II) stated in Section 2. See Ichinose[4] and Nagase and Umeda [11,12].

5. Proofs of the Main Theorems

The following lemma is crucial for proving Theorem 1 stated in Section 2.

Lemma 5.1. *Suppose that Assumptions* (I) *and* (II) *hold. Then there exists a Weyl symbol* $r(x, \xi)\in \dot{S}^{-1}$ *such that*

$$[h^w(x, D)]^2u =\left\{\sum_{j=1}^{n} \left(\frac{\partial}{i\partial x_j} - a_j(x)\right)^2 +m^2+r^w(x, D)\right\} u$$

for $u\in \mathcal{S}(\boldsymbol{R}^n)$.

For the definition of $\dot{S}^{-1}$, see [8, Definition 5.11, p. 144]. We postpone the proof of Lemma 5.1 until Section 6. We note here that the estimate of the remainder term $r(x, \xi)$ is extremely sharp (cf. Hörmander [3, Theorem 18.5.4, p. 155] and Iwasaki and Iwasaki[6, Theorem A.2.6, p. 647]). We see two reasons for this sharp remainder estimate. The one is that the Poisson bracket $\{h, h\}=0$. The other is that $h(x,\xi)$ is a composite function of $\sqrt{|\xi|^2+m^2}$ and $\xi-a(x)$. See Lemmas 6.2–6.4 and their proofs.

In the proof of Theorem 1, we shall use the fact that

$$H_1\geq m . \tag{5.1}$$

This was proved by Ichinose[4, Theorem 5.1].

Proof of Theorem 1. Defining a compact self-adjoint operator R by

$$R =r^w(x, D) \quad \text{with domain} \quad L^2(\boldsymbol{R}^n)$$

(cf.[8, Theorem 5.14, p. 147]), we find by Lemma 5.1 that

$$H_1^2u = (T+R)u \tag{5.2}$$

for $u\in C_0^\infty(\boldsymbol{R}^n)$. Since $T+R$ is essentially self-adjoint on $C_0^\infty(\boldsymbol{R}^n)$, (5.2) implies that $H_1^2=T+R$. Hence, noting (5.1) and using Lemma 3.3, we see that

$$\sigma_{ess}(H_1) = \sqrt{\sigma_{ess}(T)} \,. \tag{5.3}$$

Since V is H_1-compact, we deduce from (5.3) and Reed-Simon [15, Corollary 2, p. 113] that $\sigma_{ess}(H)=\sqrt{\sigma_{ess}(T)}$. Q.E.D.

Proof of Theorem 2. It follows from Leinfelder[9, Theorem 2.5] that

$$\sigma_{ess}(T) = [m^2, \infty) . \tag{5.4}$$

Theorem 1 together with (5.4) gives the desired result. Q.E.D

Proof of Theorem 3. It follows from Cycon, Froese, Kirsch, and Simon [2, Theorem 6.1, p.117] that (5.4) holds. Then in the same way as in the proof of Theorem 2, we obtain the desired result. Q.E.D.

Proof of Theorem 4. It follows particularly from Theorem 2 that $\sigma_{\text{ess}}(H_1) = [m, \infty)$. Since $\sigma(H_1) \subset [m, \infty)$ by (5.1), we obtain the desired conclusion. Q.E.D.

Proof of Theorem 5. It follows particularly from Theorem 3 that $\sigma_{\text{ess}}(H_1) = [m, \infty)$. In the same way as in the proof of Theorem 4, we get the desired conclusion. Q.E.D.

6. The Remaining Proof

In this section we shall give the proof of Lemma 5.1 by means of a series of lemmas. Throughout this section, we suppose that Assumptions (I) and (II) hold and we use standard notation(cf. [8]) without saying so every time.

Lemma 6.1. *For every multi-index α there exists a positive constant C_α such that*

$$|h^{(\alpha)}(x, \xi)| \leq C_\alpha \langle \xi \rangle^{1-|\alpha|}.$$

Proof. Define

$$\psi(\xi) = \sqrt{|\xi|^2 + m^2}.$$

Then we have $h(x, \xi) = \psi(\xi - a(x))$. It follows that

$$h^{(\alpha)}(x, \xi) = \psi^{(\alpha)}(\xi - a(x)) \tag{6.1}$$

for every α. It is obvious that for every α there exists a constant K_α such that

$$|\psi^{(\alpha)}(\xi)| \leq K_\alpha \langle \xi \rangle^{1-|\alpha|} \tag{6.2}$$

Since $a(x)$ is bounded on $\boldsymbol{R}^n$, we see that

$$M_1 \langle \xi \rangle \leq \langle \xi - a(x) \rangle \leq M_2 \langle \xi \rangle \tag{6.3}$$

for some constants M_1 and M_2. Combining (6.1)-(6.3) gives the lemma.

Q.E.D.

Lemma 6.2. *For every pair of multi-indices α and β with $\beta \neq 0$, there exists a nonnegative function $C_{\alpha\beta}(x)$ such that*

(i) *$C_{\alpha\beta}(x)$ is bounded and continuous,*
(ii) *$C_{\alpha\beta}(x) \to 0$ as $|x| \to \infty$,*
(iii) *$|h^{(\alpha)}_{(\beta)}(x, \xi)| \leq C_{\alpha\beta}(x) \langle \xi \rangle^{-|\alpha|}$.*

Proof. Let ψ be the same function as in the proof of Lemma 6.1. Repeated application of the chain rule for differentiation to (6.1) shows that

$$h_{(\beta)}^{(\alpha)}(x,\xi)=\sum_{1\leq|\gamma|\leq|\beta|}\psi^{(\alpha+\gamma)}(\xi-a(x))A_{\beta\gamma}(x) \tag{6.4}$$

where $A_{\beta\gamma}(x)$ is a linear combination of functions of the forms $\prod_{l=1}^{|\gamma|}\partial_x^{\nu(l)}a_{j(l)}(x)$ with $\nu(1)+\cdots+\nu(|\gamma|)=\beta$, $\nu(l)\neq 0$ and $j(l)\in\{1,2,\cdots,n\}$. It follows from Assumption (II) that $A_{\beta\gamma}(x)\to 0$ as $|x|\to\infty$. Combining this fact with (6.4), (6.3) and (6.2) gives the lemma. Q.E.D.

In the following lemma $(h\circ h)(x,\xi)$ denotes the Weyl symbol of $[h^w(x,D)]^2$.

Lemma 6.3.

$$(h\circ h)(x,\xi)=|\xi-a(x)|^2+m^2+r(x,\xi)$$

where

$$r(x,\xi)=\int_0^1(1-\theta)q(x,\xi,\theta)d\theta\,,$$

and

$$q(x,\xi,\theta)=-\frac{1}{4}\sum_{|\alpha+\beta|=2}(-1)^{|\beta|}\frac{2!}{\alpha!\beta!}\times$$

$$\text{Os}-\iint e^{-i\tau\cdot w}h_{(\beta)}^{(\alpha)}(x+\frac{z}{2},\xi-\theta\eta)h_{(\alpha)}^{(\beta)}(x-\frac{y}{2},\xi-\theta\zeta)(2\pi)^{-2n}dwd\tau\,,$$

$$w=(y,z)\in\boldsymbol{R}^{2n}\,,\quad \tau=(\eta,\zeta)\in\boldsymbol{R}^{2n}\,.$$

Proof. Appealing to [6, Theorem A.2.3, p. 646] with a change of variables, we have

$$(h\circ h)(x,\xi)=\text{Os}-\iint e^{-i\tau\cdot w}h(x+\frac{z}{2},\xi-\eta)h(x-\frac{y}{2},\xi-\zeta)(2\pi)^{-2n}dwd\tau\,. \tag{6.5}$$

By the Taylor expansion formula with respect to the variables $\tau=(\eta,\zeta)$, we get

$$h(x+\frac{z}{2},\xi-\eta)h(x-\frac{y}{2},\xi-\zeta)=h(x+\frac{z}{2},\xi)h(x-\frac{y}{2},\xi)$$

$$-\sum_{|\alpha|=1}\{h^{(\alpha)}(x+\frac{z}{2},\xi)\eta^\alpha h(x-\frac{y}{2},\xi)+\zeta^\alpha h(x+\frac{z}{2},\xi)h^{(\alpha)}(x-\frac{y}{2},\xi)\}$$

$$+\sum_{\substack{|\alpha|=1\\|\beta|=1}}\int_0^1(1-\theta)\{h^{(\alpha+\beta)}(x+\frac{z}{2},\xi-\theta\eta)\eta^{\alpha+\beta}h(x-\frac{y}{2},\xi-\theta\zeta)$$

$$+2\zeta^\beta h^{(\alpha)}(x+\frac{z}{2},\zeta-\theta\eta)\eta^\alpha h^{(\beta)}(x-\frac{\eta}{2},\xi-\theta\zeta)$$

$$+\zeta^{\alpha+\beta}h(x+\frac{z}{2},\xi-\theta\eta)h^{(\alpha+\beta)}(x-\frac{y}{2},\xi-\theta\zeta)\}d\theta\,.$$

Then an oscillatory integral and Kumano-go [8, Theorem 6.7, p. 50] give

$$\text{Os}-\iint e^{-i\tau\cdot w}h(x+\frac{z}{2},\ \xi-\eta)h(x-\frac{y}{2},\ \xi-\zeta)(2\pi)^{-2n}dwd\tau$$

$$(6.6)\quad \begin{aligned}&=[h(x,\ \xi)]^2+\frac{1}{2i}\sum_{|\alpha|=1}\{h^{(\alpha)}(x,\ \xi)h_{(\alpha)}(x,\ \xi)-h_{(\alpha)}(x,\ \xi)h^{(\alpha)}(x,\ \xi)\}\\&+\left(\frac{1}{2i}\right)^2\sum_{|\alpha+\beta|=2}(-1)^{|\beta|}\frac{2!}{\alpha!\beta!}\text{Os}-\iint e^{-i\tau\cdot w}\left[\int_0^1(1-\theta)h^{(\alpha)}_{(\beta)}(x+\frac{z}{2},\ \xi-\theta\eta)\right.\\&\qquad\left.\times h^{(\beta)}_{(\alpha)}(x-\frac{y}{2},\ \xi-\theta\zeta)d\theta\right](2\pi)^{-2n}dwd\tau\,.\end{aligned}$$

Here we have used the fact that

$$\text{Os}-\iint e^{-i\tau\cdot w}f(w)(2\pi)^{-2n}dwd\tau=f(0)$$

for functions $f(w)$ of polynomial growth (cf. Kumano-go [8, Example, p.52]). Since the second term on the right hand side of (6.6) equals zero, (6.5) and (6.6) imply the lemma. Q.E.D.

For multi-indices $\alpha,\ \beta,\ \mu,\ \nu$ we write

$$\begin{aligned}&\varphi(x,\ \xi,\ \theta;\ \alpha,\ \beta,\ \mu,\ \nu)\\&\quad=\text{Os}-\iint e^{-i\tau\cdot w}h^{(\nu)}_{(\beta)}(x+\frac{z}{2},\ \xi-\theta\eta)h^{(\mu)}_{(\alpha)}(x-\frac{y}{2},\ \xi-\theta\zeta)(2\pi)^{-2n}dwd\tau\,.\end{aligned}$$

Lemma 6.4. *Suppose that* $|\alpha+\beta|\geq 1$. *Then for* $\alpha,\ \beta,\ \mu$ *and* ν, *there corresponds a nonnegative measurable function* $C_{\alpha\beta\mu\nu}(x)$ *such that*
(i) $C_{\alpha\beta\mu\nu}(x)$ *is bounded,*
(ii) $C_{\alpha\beta\mu\nu}(x)\to 0$ *as* $|x|\to\infty$,
(iii) $|\varphi(x,\ \xi,\ \theta;\ \alpha,\ \beta,\ \mu,\ \nu)|\leq C_{\alpha\beta\mu\nu}(x)\langle\xi\rangle^{1-|\mu+\nu|}$.

Simple inequalities which will be used in the proof of Lemma 6.4 are as follows:

$$(6.7)\qquad \frac{1}{2}\langle\xi\rangle\leq\langle\xi-\eta\rangle\leq\frac{3}{2}\langle\xi\rangle\quad\text{if}\quad |\eta|\leq\frac{1}{2}|\xi|\,.$$

Proof of Lemma 6.4. We assume without loss of generality that $|\alpha|\geq 1$. Let δ be a constant such that $0<\delta<1$. Choose integers k and l so that

$$(6.8)\qquad 2l>n+|\mu+\nu|,\quad 2k>n+\delta\,.$$

Then, by integration by parts, we have

$$(6.9)\quad \begin{aligned}&\varphi(x,\ \xi,\ \theta;\ \alpha,\ \beta,\ \mu,\ \nu)\\&=\iint e^{-i\tau\cdot w}\langle\eta\rangle^{-2l}\langle\zeta\rangle^{-2l}(1-\Delta_z)^l\{\langle z\rangle^{-2k}(1-\Delta_\eta)^k[h^{(\nu)}_{(\beta)}(x+\frac{z}{2},\ \xi-\theta\eta)]\}\\&\qquad\times(1-\Delta_y)^l\{\langle y\rangle^{-2k}(1-\Delta_\zeta)^k[h^{(\mu)}_{(\alpha)}(x-\frac{y}{2},\ \xi-\theta\zeta)]\}(2\pi)^{-2n}dwd\tau\end{aligned}$$

(cf. Kumano-go[8, Theorem 6.4, p.47]). Choose $\chi\in C_0^\infty(\boldsymbol{R}^n)$ so that

$$\chi(x)=\begin{cases}1 & \text{if } |x|\leq 1\ ;\\ 0 & \text{if } |x|\geq 2\ .\end{cases}$$

Define

$$\chi_j(x)=\chi(x/j) \qquad (j=1,2,\cdots)\ .$$

To decompose the integrand on the right hand side of (6.9), we define

$$E_j=(1-\Delta_y)^l\{\langle y\rangle^{-2k}(1-\Delta_\zeta)^k[(1-\chi_j)(y)h_{(\alpha)}^{(\mu)}(x-\frac{y}{2},\xi-\theta\zeta)]\}\ ,$$

$$F_j=(1-\Delta_y)^l\{\langle y\rangle^{-2k}(1-\Delta_\zeta)^k[\chi_j(y)h_{(\alpha)}^{(\mu)}(x-\frac{y}{2},\xi-\theta\zeta)]\}\ ,$$

$$G=(1-\Delta_z)^l\{\langle z\rangle^{-2k}(1-\Delta_\eta)^k[h_{(\beta)}^{(\nu)}(x+\frac{z}{2},\xi-\theta\eta)]\}\ .$$

Then

$$\text{(6.10)}\quad \varphi(x,\xi,\theta;\alpha,\beta,\mu,\nu)=\iint e^{-i\tau\cdot w}\langle\eta\rangle^{-2l}\langle\zeta\rangle^{-2l}(GE_j+GF_j)(2\pi)^{-2n}dwd\tau\ .$$

To get estimates of E_j and F_j, we set

$$\text{(6.11)}\quad \begin{aligned}\Lambda(r)&:=\{y\in\boldsymbol{R}^n\mid |y|\geq r\}\\ \Omega(r)&:=\{y\in\boldsymbol{R}^n\mid |y|\leq r\}\ .\end{aligned}$$

Since $\alpha\neq 0$, we have by Lemma 6.2

$$\text{(6.11)}\quad \begin{aligned}|E_j|&\leq M_{\alpha\mu}^{(1)}\mathbf{1}_{\Lambda(j)}(y)\langle y\rangle^{-2k}\langle\xi-\theta\zeta\rangle^{-|\mu|}\\ &\leq M_{\alpha\mu}^{(2)}(1+j)^{-\delta}\langle y\rangle^{-2k+\delta}\langle\xi-\theta\zeta\rangle^{-|\mu|}\ .\end{aligned}$$

Here and in the sequel, M with subscripts and a superscript denotes a constant, and for a subset A of $\boldsymbol{R}^n$, $\mathbf{1}_A(y)=1$ if $y\in A$, and $=0$ otherwise. Similarly we have

$$\text{(6.12)}\quad |F_j|\leq M_{\alpha\mu}^{(3)}\mathbf{1}_{\Omega(2j)}(y)C^{\alpha\mu}(x-\frac{y}{2})\langle y\rangle^{-2k}\langle\xi-\theta\zeta\rangle^{-|\mu|}$$

where $C^{\alpha\mu}(x)$ is a linear combination of the functions in Lemma 6.2. Putting

$$\text{(6.13)}\quad C_j^{\alpha\mu}(x):=\sup_{|y|\leq j}C^{\alpha}(x-y)\ ,$$

we see that

$$\text{(6.14)}\quad C_j^{\alpha\mu}(x)\to 0 \quad\text{as}\quad |x|\to\infty$$

and that there exists a nonnegative constant $M_{\alpha\mu}^{(4)}$, independent of j, such that

$$\text{(6.15)}\quad 0\leq C_j^{\alpha\mu}(x)\leq M_{\alpha\mu}^{(4)} \qquad (j=1,2,\cdots)\ .$$

By (6.12) and (6.13), we see that

$$|F_j| \leq M^{(5)}_{\alpha\mu} C^{\alpha\mu}_j(x) \langle y\rangle^{-2k} \langle \xi-\theta\zeta\rangle^{-|\mu|}. \tag{6.16}$$

Lemma 6.1 implies that

$$|G| \leq M^{(6)}_{\alpha\mu} \langle z\rangle^{-2k} \langle \xi-\theta\eta\rangle^{1-|\nu|}. \tag{6.17}$$

In order to estimate the integrand on the right hand side of (6.10), we decompose $\boldsymbol{R}^{2n}_w \times \boldsymbol{R}^{2n}_\tau$ into the following four regions:

$$A(\xi) := \boldsymbol{R}^{2n}_w \times \{\tau \in \boldsymbol{R}^{2n} \mid |\eta| \leq \frac{1}{2}|\xi|,\ |\zeta| \leq \frac{1}{2}|\xi|\},$$

$$B(\xi) := \boldsymbol{R}^{2n}_w \times \{\tau \in \boldsymbol{R}^{2n} \mid |\eta| \leq \frac{1}{2}|\xi|,\ |\zeta| > \frac{1}{2}|\xi|\},$$

$$C(\xi) := \boldsymbol{R}^{2n}_w \times \{\tau \in \boldsymbol{R}^{2n} \mid |\eta| > \frac{1}{2}|\xi|,\ |\zeta| \leq \frac{1}{2}|\xi|\},$$

$$D(\xi) := \boldsymbol{R}^{2n}_w \times \{\tau \in \boldsymbol{R}^{2n} \mid |\eta| > \frac{1}{2}|\xi|,\ |\zeta| > \frac{1}{2}|\xi|\}.$$

If $(w, \tau) \in A(\xi)$ and $0 \leq \theta \leq 1$, then

$$\frac{1}{2}\langle\xi\rangle \leq \langle\xi-\theta\eta\rangle \leq \frac{3}{2}\langle\xi\rangle, \tag{6.18}$$

$$\frac{1}{2}\langle\xi\rangle \leq \langle\xi-\theta\zeta\rangle \leq \frac{3}{2}\langle\xi\rangle, \tag{6.19}$$

so that, by (6.11), (6.16) and (6.17),

$$\begin{aligned} |E_j| &\leq M^{(7)}_{\alpha\mu}(1+j)^{-\delta} \langle y\rangle^{-2k+\delta} \langle\xi\rangle^{-|\mu|}, \\ |F_j| &\leq M^{(8)}_{\alpha\mu} C^{\alpha\mu}_j(x) \langle y\rangle^{-2k} \langle\xi\rangle^{-|\mu|}, \\ |G| &\leq M^{(9)}_{\beta\nu} \langle z\rangle^{-2k} \langle\xi\rangle^{1-|\nu|}. \end{aligned}$$

Thus, noting (6.8), we get

$$\begin{aligned} &\left| \iint_{A(\xi)} e^{-i\tau\cdot w} \langle\eta\rangle^{-2l} \langle\zeta\rangle^{-2l} (GE_j + GF_j)(2\pi)^{-2n} dw d\tau \right| \\ &\qquad \leq M^{(10)}_{\alpha\beta\mu\nu} \{(1+j)^{-\delta} + C^{\alpha\mu}_j(x)\} \langle\xi\rangle^{1-|\mu+\nu|}. \end{aligned} \tag{6.20}$$

If $(w, \tau) \in B(\xi)$ and $0 \leq \theta \leq 1$, then (6.18) holds, so that, by (6.11), (6.16) and (6.17),

$$\begin{aligned} |E_j| &\leq M^{(2)}_{\alpha\mu}(1+j)^{-\delta} \langle y\rangle^{-2k+\delta}, \\ |F_j| &\leq M^{(6)}_{\alpha\mu} C^{\alpha\mu}_j(x) \langle y\rangle^{-2k}, \\ |G| &\leq M^{(11)}_{\beta\nu} \langle z\rangle^{-2k} \langle\xi\rangle^{1-|\nu|}. \end{aligned}$$

In view of (6.8) and the definition of $B(\xi)$, we have

$$\begin{aligned}(6.21)\qquad &\left|\iint_{B(\xi)} e^{-i\tau\cdot w}\langle\eta\rangle^{-2l}\langle\zeta\rangle^{-2l}(GE_j+GF_j)(2\pi)^{-2n}dwd\tau\right| \\ &\leq M^{(12)}_{\alpha\beta\mu\nu}\{(1+j)^{-\delta}+C^{\alpha\mu}_j(x)\}\langle\xi\rangle^{1-|\nu|}\int_{|\zeta|>(1/2)|\xi|}\langle\zeta\rangle^{-2l}d\zeta \\ &\leq M^{(13)}_{\alpha\beta\mu\nu}\{(1+j)^{-\delta}+C^{\alpha\mu}_j(x)\}\langle\xi\rangle^{1-|\mu+\nu|}.\end{aligned}$$

Similarly we have

$$\begin{aligned}(6.22)\qquad &\left|\iint_{C(\xi)} e^{-i\tau\cdot w}\langle\eta\rangle^{-2l}\langle\zeta\rangle^{-2l}(GE_j+GF_j)(2\pi)^{-2n}dwd\tau\right| \\ &\leq M^{(14)}_{\alpha\beta\mu\nu}\{(1+j)^{-\delta}+C^{\alpha\mu}_j(x)\}\langle\xi\rangle^{1-|\mu+\nu|}.\end{aligned}$$

Since, by (6.8),

$$\int_{|\eta|>(1/2)|\xi|}\langle\eta\rangle^{-2l}d\eta\int_{|\zeta|>(1/2)|\xi|}\langle\zeta\rangle^{-2l}d\zeta\leq M^{(15)}_{\mu\nu}\langle\xi\rangle^{1-|\mu+\nu|},$$

we get

$$\begin{aligned}(6.23)\qquad &\left|\iint_{D(\xi)} e^{-i\tau\cdot w}\langle\eta\rangle^{-2l}\langle\zeta\rangle^{-2l}(GE_j+GF_j)(2\pi)^{-2n}dwd\tau\right| \\ &\leq M^{(16)}_{\alpha\beta\mu\nu}\{(1+j)^{-\delta}+C^{\alpha\mu}_j(x)\}\langle\xi\rangle^{1-|\mu+\nu|}.\end{aligned}$$

Put

$$(6.24)\qquad M_{\alpha\beta\mu\nu}=M^{(10)}_{\alpha\beta\mu\nu}+M^{(13)}_{\alpha\beta\mu\nu}+M^{(14)}_{\alpha\beta\mu\nu}+M^{(16)}_{\alpha\beta\mu\nu}$$

$$(6.25)\qquad C_{\alpha\rho\mu\nu}(x)=M_{\alpha\beta\mu\nu}\inf_{1\leq j<\infty}\{(1+j)^{-\delta}+C^{\alpha\mu}_j(x)\}.$$

Then, using (6.14) and (6.15), we see that $C_{\alpha\beta\mu\nu}(x)$ defined in (6.25) satisfies the properties (i), (ii) of the lemma. Finally we conclude from (6.10) and (6.20)–(6.25) that $C_{\alpha\beta\mu\nu}(x)$ satisfies the property (iii) of the lemma. Q.E.D.

Proof of Lemma 5.1. Note that $|\xi-a(x)|^2+m^2$ is the Weyl symbol of $\sum_{j=1}^n(\partial/i\partial x_j-a_j(x))^2+m^2$. In view of Lemma 6.3, it is sufficient to show that for any μ, ν there exists a bounded function $C_{\mu\nu}(x)$, independent of $\theta\in[0, 1]$, such that

$$C_{\mu\nu}(x)\to 0\quad\text{as}\quad |x|\to\infty$$

and

$$(6.26)\qquad |q^{(\nu)}_{(\mu)}(x, \xi, \theta)|\leq C_{\mu\nu}(x)\langle\xi\rangle^{-1-|\nu|}.$$

With the notation introduced right before Lemma 6.4, we see by differentiation under the integral sign that

$$\begin{aligned}(6.27)\qquad q^{(\nu)}_{(\mu)}(x, \xi, \theta)=&-\frac{1}{4}\sum_{|\alpha+\beta|=2}(-1)^{|\beta|}\frac{2!}{\alpha!\beta!} \\ &\times\sum_{\substack{\tilde\mu\leq\mu\\ \tilde\nu\leq\nu}}\binom{\mu}{\tilde\mu}\binom{\nu}{\tilde\nu}\varphi(x, \xi, \theta; \alpha+\mu-\tilde\mu, \beta+\tilde\mu, \beta+\nu-\tilde\nu, \alpha+\tilde\nu)\end{aligned}$$

where

$$\binom{\mu}{\tilde{\mu}} = \mu!/\{\tilde{\mu}!(\mu-\tilde{\mu})!\}\ , \quad \binom{\nu}{\tilde{\nu}} = \nu!/\{\tilde{\nu}!(\nu-\tilde{\nu})!\}\ .$$

Since $|\alpha+\mu-\tilde{\mu}|+|\beta+\tilde{\mu}|>1$, we can apply Lemma 6.4 to each term on the right hand side of (6.27). Thus we get the desired estimate(6.26) Q.E.D.

7. The Difference between $h^w(x, D)$ and $\sqrt{T}$

In this section we shall show that the relativistic Schrödinger operator $h^w(x, D)$, in general, differs from the operator-square root $\sqrt{T}$, where T is the Schrödinger operator defined in Section 2. Throughout this section, we also suppose that Assumptions(I) and (II) hold.

Lemma 7.1. *If* $[h^w(x, D)]^2u \neq Tu$ *for some* $u \in \mathcal{S}(\boldsymbol{R}^n)$, *then* $h^w(x, D)v \neq \sqrt{T}v$ *for some* $v \in \mathcal{S}(\boldsymbol{R}^n)$.

Proof. Suppose, to get a contradiction, that $h^w(x, D)u = \sqrt{T}u$ for all $u \in \mathcal{S}(\boldsymbol{R}^n)$. Then we have

$$[h^w(x, D)]^2u = \sqrt{T}h^w(x, D)u = Tu$$

for all $u \in \mathcal{S}(\boldsymbol{R}^n)$. This contradicts the hypothesis of the lemma. Q.E.D.

As in Section 6, $h\circ h(x, \xi)$ denotes the Weyl symbol of $[h^w(x, D)]^2$. Recall that the Weyl symbol of T is given by $[h(x, \xi)]^2$. Lemma 7.2 below shows that $h\circ h(x, \xi)$ differs from $[h(x, \xi)]^2$ for a large class of vector potentials $a(x)$. Hence we find by Lemma 7.1 and [8, Proposition 1.2, p.56] that $h^w(x, D)$, in general, differs from $\sqrt{T}$.

For each $l \in \{1, \cdots, n\}$ we define a matrix-valued function $A_l(x)$ by

$$A_l(x) = \Big(\sum_{j=1}^{n} \frac{\partial^2 a_l}{\partial x_j^2}(x)\Big)I_n - \Big(\frac{\partial^2 a_l}{\partial x_k \partial x_j}(x)\Big)_{1\le j,k\le n},$$

where I_n is the identity matrix. We write $\hat{\xi} = \xi/|\xi|$.

Lemma 7.2.

$$\lim_{|\xi|\to\infty} |\xi|\,\{h\circ h(x, \xi) - [h(x, \xi)]^2\} = \frac{1}{4}\sum_{l=1}^{n} \hat{\xi}_l(A_l(x)\hat{\xi})\cdot\hat{\xi}\ ,$$

the convergence being uniform in $\boldsymbol{R}^n_x$.

Proof. By [6, Theorem A.2.6, p. 647] we find $q_4(x, \xi) \in S^{-2}$ such that

$$h\circ h = h^2 + (2i)^{-2}(2!)^{-1}\sigma_2(h, h) + (2i)^{-3}(3!)^{-1}\sigma_3(h, h) + q_4\ . \tag{7.1}$$

It follows from Lemmas 6.1 and 6.2 that

$$|\sigma_3(h, h)(x, \xi)| \leq C\langle\xi\rangle^{-2}.$$

Thus we have

$$\sup_x \{|\xi|[|\sigma_3(h, h)(x, \xi)| + |q_4(x, \xi)|]\} \leq C\langle\xi\rangle^{-1}. \tag{7.2}$$

Note that

$$\sigma_2(h, h) = 4\sum_{|\alpha|=2} \frac{1}{\alpha!} h^{(\alpha)} h_{(\alpha)} - 2\sum_{|\alpha|=|\beta|=1} h^{(\alpha)}_{(\beta)} h^{(\beta)}_{(\alpha)}. \tag{7.3}$$

It follows from Lemma 6.2 that

$$\sup_x \{|\xi| |\sum_{|\alpha|=|\beta|=1} h^{(\alpha)}_{(\beta)}(x, \xi) h^{(\beta)}_{(\alpha)}(x, \xi)|\} \leq C\langle\xi\rangle^{-1}. \tag{7.4}$$

By simple calculation, we see that

$$\lim_{|\xi|\to\infty} \frac{\partial^2 h}{\partial x_k \partial x_j}(x, \xi) = -\sum_{l=1}^{n} \hat{\xi}_l \frac{\partial^2 a_l}{\partial x_k \partial x_j}(x), \tag{7.5}$$

$$\lim_{|\xi|\to\infty} |\xi| \frac{\partial^2 h}{\partial \xi_k \partial \xi_j}(x, \xi) = \delta_{jk} - \hat{\xi}_j \hat{\xi}_k, \tag{7.6}$$

where $\delta_{jk}=1$ if $j=k$, and $=0$ otherwise. Since $a(x)$ is bounded on $\boldsymbol{R}^n$ together with its all derivatives, the convergence in (7.5) and (7.6) is uniform in $\boldsymbol{R}^n_x$. Combining (7.1)-(7.6), we get the desired result. Q.E.D.

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