Functional Calculus and Littlewood-Paley Theory For Schrödinger Operators

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Contents

1. Introduction

We aim to study an operator calculus for a class of Schrödinger operators of the form

$$H = -\Delta + V, \tag{1.1}$$

acting on functions on $\mathbb{R}^3$, where V is a real-valued function, subject to certain hypotheses, which will be made below. We particularly want to include the case

$$V(x) = -\frac{K}{|x|}, \quad K > 0, \tag{1.2}$$

arising when H is the Schrödinger operator associated to a hydrogen atom. For such a V, the Friedrichs method yields a self-adjoint operator on $L^2(\mathbb{R}^3)$, with domain given by

$$\mathcal{D}(H) = \{u \in H^1(\mathbb{R}^3) : -\Delta u + Vu \in L^2(\mathbb{R}^3)\}. \tag{1.3}$$

One ingredient of use to show that the Friedrichs method works includes the following estimate: for each $\varepsilon > 0$, there exists $C(\varepsilon) < \infty$ such that

$$\int_{\mathbb{R}^3} |V(x)|\, |u(x)|^2\, dx \le \varepsilon \|\nabla u\|^2_{L^2} + C(\varepsilon)\|u\|^2_{L^2}, \quad \forall\, u \in H^1(\mathbb{R}^3). \tag{1.4}$$

This holds for V of the form (1.2). When (1.4) holds, we have a self-adjoint operator H with domain satisfying (1.3), and H is semi-bounded, i.e., there exists $b \in \mathbb{R}$ such that $H + bI$ is positive definite. It is further the case that, when V has the form (1.2), then

$$\mathcal{D}(H) = H^2(\mathbb{R}^3). \tag{1.5}$$

Here and below, $H^s(\mathbb{R}^3)$ denotes L^2-Sobolev spaces of functions or distributions on $\mathbb{R}^3$. We also use $H^{s,p}(\mathbb{R}^3)$ to denote L^p-Sobolev spaces, for $p \in (1,\infty)$. We formalize the following hypothesis that we place on V.

Hypothesis 1.1. V is a real-valued, measurable function on $\mathbb{R}^3$ satisfying (1.4), and $H = -\Delta + V$ is self-adjoint on $L^2(\mathbb{R}^3)$, with domain $\mathcal{D}(H)$ satisfying (1.3) and (1.5).

For a demonstration that functions V of the form (1.2) satisfy Hypothesis 1.1, one can consult Chapter 8, §7, of [T4].

Given a bounded, continuous function $\Phi : \mathbb{R} \to \mathbb{R}$, $\Phi(H)$ is defined via the spectral theorem as a bounded operator on $L^2(\mathbb{R}^3)$. We want to examine conditions, analogous to those that arise in the Marcinkiewicz theorem, that guarantee that $\Phi(H)$ is bounded on $L^p(\mathbb{R}^3)$ for $1 < p < \infty$. Actually, it is convenient to take

$$\mathcal{H} = H + aI, \tag{1.6}$$

where $a > 0$ is picked so that

$$\operatorname{Spec} \mathcal{H} \subset [1,\infty), \tag{1.7}$$

and examine $\Phi(\sqrt{\mathcal{H}})$. We will also assume that $\Phi(\lambda)$ is an even function of $\lambda \in \mathbb{R}$, which, in view of (1.7), is not a severe restriction.

We say Φ belongs to $S^0_1(\mathbb{R})$ provided that, for each $k \in \mathbb{Z}^+$,

$$|\Phi^{(k)}(\lambda)| \le C_k(1+|\lambda|)^{-k}. \tag{1.8}$$

We aim to prove the following.

Theorem 1.1. *Take $\mathcal{H}$ as in (1.6)–(1.7), and assume that Hypotheses 1.1, 2.1, and 3.1 hold. Given a smooth, even function $\Phi : \mathbb{R} \to \mathbb{C}$,*

$$\begin{aligned} \Phi \in S^0_1(\mathbb{R}) \Rightarrow \Phi(\sqrt{\mathcal{H}}) : L^p(\mathbb{R}^3) \to L^p(\mathbb{R}^3), \quad \forall\, p \in (1,\infty) \\ \textit{and } \Phi(\sqrt{\mathcal{H}}) \textit{ is of weak type (1,1).} \end{aligned} \tag{1.9}$$

Hypothesis 1.1 has been stated above. Hypotheses 2.1 and 3.1 are stated in §§2 and 3, respectively.

Techniques we will use to prove Theorem 1.1 include some that arose in the works [T1], [T2], [CGT], [DST], [T3], [MMV], and [T5], among others. A first step is to bring in the identity

$$\Phi(\sqrt{\mathcal{H}})f = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widehat{\Phi}(t) \cos t\sqrt{\mathcal{H}}\, f\, dt, \tag{1.10}$$

where $\widehat{\Phi}$ is the Fourier transform of Φ, so (1.10) is a consequence of the Fourier inversion formula. We then split $\Phi(\sqrt{\mathcal{H}})$ into two pieces,

$$\Phi(\sqrt{\mathcal{H}}) = \Phi^{\#}(\sqrt{\mathcal{H}}) + \Phi^{b}(\sqrt{\mathcal{H}}), \tag{1.11}$$

obtained by taking

$$\Phi(\lambda) = \Phi^{\#}(\lambda) + \Phi^{b}(\lambda), \tag{1.12}$$

where

$$\widehat{\Phi}^{\#}(t) = \beta(t)\widehat{\Phi}(t), \quad \widehat{\Phi}^{b}(t) = (1-\beta(t))\widehat{\Phi}(t), \tag{1.13}$$

and where we take

$$\beta \in C_0^{\infty}((-1,1)), \quad \beta(t) = \beta(-t), \quad \beta(t) = 1 \text{ for } |t| \le \frac{1}{2}. \tag{1.14}$$

The hypothesis $\Phi \in S^0_1(\mathbb{R})$ implies $\Phi^b(\lambda)$ is rapidly decreasing, while $\Phi^{\#}$ also belongs to $S^0_1(\mathbb{R})$. In §2, we analyze $\Phi^b(\sqrt{\mathcal{H}})$ and show that, under Hypotheses 1.1 and 2.1,

$$\Phi^b(\sqrt{\mathcal{H}}) : L^p(\mathbb{R}^3) \longrightarrow L^p(\mathbb{R}^3), \quad \forall\, p \in [1,\infty]. \tag{1.15}$$

In §3 we analyze $\Phi^{\#}(\sqrt{\mathcal{H}})$ and show that, if in addition Hypothesis 3.1 holds, then $\Phi^{\#}(\sqrt{\mathcal{H}})$ has the properties ascribed to $\Phi(\sqrt{\mathcal{H}})$ in (1.9). As in the references cited above, a major role in estimating these operators is played by finite propagation speed, in the form

$$\operatorname{supp} f \subset K \Longrightarrow \operatorname{supp} \cos t\sqrt{\mathcal{H}}\, f \subset K_{|t|}, \tag{1.16}$$

where, given $K \subset \mathbb{R}^3$,

$$K_{|t|} = \{x \in \mathbb{R}^3 : \operatorname{dist}(x,K) \le |t|\}. \tag{1.17}$$

In §4 we put together the results of §§2–3 to complete the proof of Theorem 1.1.

Given that we do have Hypotheses 1.1, 2.1, and 3.1, there is the matter of verifying them, in cases of interest. As stated above, Hypothesis 1.1 holds for the hydrogen atom operator (1.1)–(1.2). In Appendix A, we show that actually Hypothesis 1.1 implies Hypothesis 2.1. This leaves Hypothesis 3.1. We do not have a proof of Hypothesis 3.1 for the hydrogen atom operator. In §5 we discuss efforts in this direction, referring to [T7] for more on this. In Appendix B we give conditions on V that do imply Hypothesis 3.1, though these conditions do not hold for the hydrogen atom.

2. Estimates on $\Phi^b(\sqrt{\mathcal{H}})$

Throughout this section, Hypothesis 1.1 will be in effect. We start out with a simple but useful observation.

Proposition 2.1. *Assume*

$$|\Phi^b(\lambda)| \le C\langle\lambda\rangle^{-2\sigma}, \quad \sigma > \frac{3}{2}. \tag{2.1}$$

Then $\Phi^b(\sqrt{\mathcal{H}})$ has an integral kernel $K^b(x,y)$,

$$\Phi^b(\sqrt{\mathcal{H}})u(x) = \int\limits_{\mathbb{R}^3} K^b(x,y)u(y)\,dy, \tag{2.2}$$

satisfying

$$|K^b(x,y)| \le C < \infty, \quad \forall\, x,y \in \mathbb{R}^3. \tag{2.3}$$

Proof. We can wrie

$$\Phi^b(\sqrt{\mathcal{H}}) = \mathcal{H}^{-\sigma/2}\Psi(\sqrt{\mathcal{H}})\mathcal{H}^{-\sigma/2}, \tag{2.4}$$

with $\Psi(\sqrt{\mathcal{H}})$ bounded on $L^2(\mathbb{R}^3)$. By (1.5),

$$\mathcal{H}^{-1} : L^2(\mathbb{R}^3) \longrightarrow H^2(\mathbb{R}^3), \tag{2.5}$$

and interpolation and duality yield

$$\mathcal{H}^{-\sigma/2} : L^2(\mathbb{R}^3) \longrightarrow H^\sigma(\mathbb{R}^3), \quad \mathcal{H}^{-\sigma/2} : H^{-\sigma}(\mathbb{R}^3) \longrightarrow L^2(\mathbb{R}^3), \tag{2.6}$$

for $0 \le \sigma \le 2$. It follows that, if $\sigma \le 2$,

$$\begin{aligned} \sigma > \frac{3}{2} &\Longrightarrow \{\delta_y : y \in \mathbb{R}^3\} \text{ bounded in } H^{-\sigma}(\mathbb{R}^3) \\ &\Longrightarrow \{\mathcal{H}^{-\sigma/2}\delta_y : y \in \mathbb{R}^3\} \text{ bounded in } L^2(\mathbb{R}^3) \\ &\Longrightarrow \{\Psi(\sqrt{\mathcal{H}})\mathcal{H}^{-\sigma/2}\delta_y : y \in \mathbb{R}^3\} \text{ bounded in } L^2(\mathbb{R}^3) \\ &\Longrightarrow \{\Phi^b(\sqrt{\mathcal{H}})\delta_y : y \in \mathbb{R}^3\} \text{ bounded in } H^\sigma(\mathbb{R}^3) \\ &\Longrightarrow \{\Phi^b(\sqrt{\mathcal{H}})\delta_y : y \in \mathbb{R}^3\} \text{ bounded in } C_0(\mathbb{R}^3). \end{aligned} \tag{2.7}$$

Thus we have (2.2), with

$$K^b(x,y) = \Phi^b(\sqrt{\mathcal{H}})\delta_y(x), \tag{2.8}$$

which gives (2.3).

Our next task is to obtain finer estimates on $K^b(x,y)$, in terms of $|x-y|$, exhibiting sufficient decay as $|x-y| \to \infty$. For this, we bring in the formula

$$\Phi^b(\sqrt{\mathcal{H}}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{\varphi}(t) \cos t\sqrt{\mathcal{H}}\, dt, \tag{2.9}$$

with

$$\hat{\varphi}(t) = \hat{\Phi}^b(t) = \hat{\Phi}(t)(1-\beta(t)), \tag{2.9A}$$

as in (1.13)–(1.14). To start, let us assume

$$u \in L^2(B_1(x)),\ v \in L^2(B_1(y)), \quad |x-y| = R+2. \tag{2.10}$$

Then, thanks to finite propagation speed for $\cos t\sqrt{\mathcal{H}}$,

$$\begin{aligned} (\varphi(\sqrt{\mathcal{H}})u, v) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{\varphi}(t)\, (\cos t\sqrt{\mathcal{H}}u, v)\, dt \\ &= \frac{1}{\sqrt{2\pi}} \int\limits_{|t|\ge R} \hat{\varphi}(t)\, (\cos t\sqrt{\mathcal{H}}u, v)\, dt. \end{aligned} \tag{2.11}$$

Consequently, since $\cos t\sqrt{\mathcal{H}}$ has operator norm ≤ 1 on $L^2(\mathbb{R}^3)$,

$$|(\varphi(\sqrt{\mathcal{H}})u, v)| \le \frac{1}{\sqrt{2\pi}} \Bigl(\int\limits_{|t|\ge R} |\hat{\varphi}(t)|\, dt \Bigr) \|u\|_{L^2} \|v\|_{L^2}. \tag{2.12}$$

We now bring in the following hypothesis:

Hypothesis 2.1. There exists $C < \infty$ such that, for each $y \in \mathbb{R}^3$, we have $u_y, v_y \in L^2(\mathbb{R}^3)$ such that

$$\begin{aligned} &\operatorname{supp} u_y,\ v_y \subset B_1(y), \quad \|u_y\|_{L^2},\ \|v_y\|_{L^2} \le C, \quad \text{and} \\ &\delta_y = \mathcal{H}u_y + v_y. \end{aligned} \tag{2.13}$$

If this hypothesis holds, then $K^b(x,y)$ in (2.2), (2.8) satisfies

$$\begin{aligned} K^b(x,y) &= (\varphi(\sqrt{\mathcal{H}})\delta_y, \delta_x) \\ &= (\varphi_4(\sqrt{\mathcal{H}})u_y, u_x) + (\varphi_2(\sqrt{\mathcal{H}})u_y, v_x) \\ &\quad + (\varphi_2(\sqrt{\mathcal{H}})v_y, u_x) + (\varphi(\sqrt{\mathcal{H}})v_y, v_x), \end{aligned} \tag{2.14}$$

where $\varphi_4(\sqrt{\mathcal{H}}) = \mathcal{H}^2\varphi(\sqrt{\mathcal{H}})$ and $\varphi_2(\sqrt{\mathcal{H}}) = \mathcal{H}\varphi(\sqrt{\mathcal{H}})$, i.e.,

$$\varphi_4(\lambda) = \lambda^4\varphi(\lambda), \quad \varphi_2(\lambda) = \lambda^2\varphi(\lambda). \tag{2.15}$$

Hence, by (2.12), if $|x-y| = R+2$,

$$|K^b(x,y)| \le C \int\limits_{|t|\ge R} \Bigl\{ |\hat{\varphi}(t)| + |\hat{\varphi}_2(t)| + |\hat{\varphi}_4(t)| \Bigr\}\, dt. \tag{2.16}$$

3. Estimates on $\Phi^{\#}(\sqrt{\mathcal{H}})$

We now analyze

$$\Phi^{\#}(\sqrt{\mathcal{H}}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(t)\, \cos t\sqrt{\mathcal{H}}\, dt, \tag{3.1}$$

with

$$\psi(t) = \widehat{\Phi}^{\#}(t) = \widehat{\Phi}(t)\beta(t), \tag{3.2}$$

as in (1.13)–(1.14). Following a technique used in [MMV], and also in [T5], we replace (2.1) by

$$\Phi^{\#}(\sqrt{\mathcal{H}}) = \frac{1}{2} \int_{-\infty}^{\infty} \psi_k(t) \mathcal{J}_{k-1/2}(t\sqrt{\mathcal{H}})\, dt, \tag{3.3}$$

where

$$\mathcal{J}_\nu(\lambda) = \lambda^{-\nu} J_\nu(\lambda), \tag{3.4}$$

$J_\nu(\lambda)$ denoting the standard Bessel function, and

$$\psi_k(t) = \prod_{j=1}^{k} \Bigl(-t\frac{d}{dt} + 2j - 2\Bigr)\psi(t). \tag{3.5}$$

As is classical,

$$\mathcal{J}_{-1/2}(\lambda) = \sqrt{\frac{2}{\pi}} \cos\lambda, \tag{3.6}$$

and then (3.3) follows from (3.1) by an integration by parts argument, using the inductive formula

$$\Bigl(t\frac{d}{dt} + 2\nu\Bigr)\mathcal{J}_\nu(t\sqrt{\mathcal{H}}) = \mathcal{J}_{\nu-1}(t\sqrt{\mathcal{H}}). \tag{3.7}$$

Compare (3.7)–(3.9) of [T5].

Given (3.2), we have

$$\operatorname{supp} \psi_k \subset [-1, 1]. \tag{3.8}$$

Furthermore, the hypothesis (1.8) implies

$$|(t\partial_t)^j \psi(t)| \le C_j |t|^{-1}, \quad 0 \le j \le 4. \tag{3.9}$$

This in turn implies

$$|\psi_k(t)| \le C_k |t|^{-1}, \quad 0 \le k \le 4. \tag{3.10}$$

Other important ingredients for the analysis of $\Phi^{\#}(\sqrt{\mathcal{H}})$ arise from the classical integral representation

$$\mathcal{J}_\nu(\lambda) = c_\nu \int_{-1}^{1} (1-s^2)^{\nu-1/2} \cos s\lambda \, ds, \quad \nu > -\frac{1}{2}. \tag{3.11}$$

One consequence is the estimate

$$|\mathcal{J}_{k-1/2}(\lambda)| \le C_k (1+|\lambda|)^{-k}, \quad k > 0. \tag{3.12}$$

Another follows from

$$\mathcal{J}_{k-1/2}(t\sqrt{\mathcal{H}}) = c_{k-1/2} \int_{-1}^{1} (1-s^2)^{k-1} \cos st\sqrt{\mathcal{H}} \, ds. \tag{3.13}$$

Finite propagation speed gives

$$\operatorname{supp} f \subset K \Longrightarrow \operatorname{supp} \cos t\sqrt{\mathcal{H}}\, f \subset K_{|t|}, \tag{3.14}$$

where, if $K \subset \mathbb{R}^3$,

$$K_{|t|} = \{x \in \mathbb{R}^3 : \operatorname{dist}(x, K) \le |t|\}. \tag{3.15}$$

Then (3.13) gives

$$\operatorname{supp} f \subset K \Longrightarrow \operatorname{supp} \mathcal{J}_{k-1/2}(t\sqrt{\mathcal{H}}) f \subset K_{|t|}. \tag{3.16}$$

We apply these results to analyze the integral kernel $K^{\#}(x,y)$ for $\Phi^{\#}(\sqrt{\mathcal{H}})$, given by

$$\Phi^{\#}(\sqrt{\mathcal{H}}) f(x) = \int_{\mathbb{R}^3} K^{\#}(x,y) f(y) \, dy. \tag{3.17}$$

By (3.3),

$$K^{\#}(x,y) = \int_0^1 \psi_k(t) B_k(t,x,y) \, dt, \tag{3.18}$$

where $B_k(t,x,y)$ is the integral kernel of $\mathcal{J}_{k-1/2}(t\sqrt{\mathcal{H}})$:

$$\mathcal{J}_{k-1/2}(t\sqrt{\mathcal{H}})f(x) = \int_{\mathbb{R}^3} B_k(t,x,y)f(y)\,dy. \tag{3.19}$$

To proceed, we bring in the following hypothesis on the "heat semigroup" $e^{-t\mathcal{H}}$.

Hypothesis 3.1. For $t > 0$, the semigroup $e^{-t\mathcal{H}}$ satisfies the estimates

$$\begin{aligned} \|e^{-t\mathcal{H}}f\|_{L^\infty} &\le C(t^{-3/4}+1)\|f\|_{L^2}, \quad \text{and} \\ \|\nabla e^{-t\mathcal{H}}f\|_{L^\infty} &\le C(t^{-3/4-1/2}+1)\|f\|_{L^2}. \end{aligned} \tag{3.20}$$

This hypothesis will be in effect for the rest of this section. As a consequence, we have the following related estimates.

Lemma 3.1. *If $G:\mathbb{R}\to\mathbb{R}$ satisfies*

$$|G(\lambda)| \le C(1+|\lambda|)^{-\gamma-1}, \quad \gamma > \frac{3}{2}, \tag{3.21}$$

then

$$\|G(t\sqrt{\mathcal{H}})\|_{\mathcal{L}(L^2,\mathrm{Lip})} \le Ct^{-3/2-1}, \quad t\in(0,1]. \tag{3.22}$$

Proof. We can use

$$G(t\sqrt{\mathcal{H}}) = (1+t^2\mathcal{H})^{-\sigma}(1+t^2\mathcal{H})^{\sigma}G(t\sqrt{\mathcal{H}}), \quad 2\sigma = \gamma+1, \tag{3.23}$$

to reduce our task to showing that

$$\|(1+t^2\mathcal{H})^{-\sigma}\|_{\mathcal{L}(L^2,\mathrm{Lip})} \le C(t^{-3/2-1}+1), \quad \text{if } \ \sigma > \frac{3}{4}+\frac{1}{2}. \tag{3.24}$$

To prove (3.24), we use the identity

$$(1+t^2\mathcal{H})^{-\sigma} = \frac{1}{\Gamma(\sigma)}\int_0^\infty e^{-s}e^{-st^2\mathcal{H}}s^{\sigma-1}\,ds. \tag{3.25}$$

Then, by (3.20),

$$\begin{aligned} \|(1+t^2\mathcal{H})^{-\sigma}\|_{\mathcal{L}(L^2,\mathrm{Lip})} &\le C\int_0^{t^{-2}} e^{-s}(st^2)^{-3/4-1/2}s^{\sigma-1}\,ds \\ &\quad + C\int_{t^{-2}}^\infty e^{-s}s^{\sigma-1}\,ds \\ &\le C_1(t^{-3/2-1}+1), \end{aligned} \tag{3.26}$$

with $C_1 < \infty$ if $\sigma > 3/4 + 1/2$.

Now, by (3.12), Lemma 3.1 applies to $G(\lambda) = \mathcal{J}_{k-1/2}(\lambda)$, provided $k > 3/2 + 1$, i/e., $k \geq 4$, so

$$\|\mathcal{J}_{k+1/2}(t\sqrt{\mathcal{H}})\|_{\mathcal{L}(L^2,\mathrm{Lip})} \leq Ct^{-3/2-1}, \quad \text{for } t \in (0,1], \tag{3.27}$$

and hence, for $k \geq 4$,

$$\|\nabla_x B_k(t,x,\cdot)\|_{L^2} \leq Ct^{-3/2-1}, \quad t \in (0,1]. \tag{3.28}$$

Since $B_k(t,x,y) = B_k(t,y,x)$, we also have the following, analogous to Proposition 2.2 of [MMV]:

Corollary 3.2. *If $k \geq 4$,*

$$\|\nabla_y B_k(t,\cdot,y)\|_{L^2} \leq Ct^{-3/2-1}, \quad \textit{for } t \in (0,1],\ y \in \mathbb{R}^3. \tag{3.29}$$

Using this, we estimate $K^\#(x,y)$, arising in (3.17)–(3.18). In fact, using (3.29) plus the fact that $B_k(t,\cdot,y)$ is supported on the ball $B_{|t|}(y)$ in $\mathbb{R}^3$ (by (3.16)), we have

$$\|\nabla_y B_k(t,\cdot,y)\|_{L^2} \leq C\Big(\mathrm{Vol}(B_{|t|}(y))\Big)^{1/2} t^{-3/2-1} \leq Ct^{-1}. \tag{3.30}$$

Hence, from (3.18) and (3.10), we have, for $k = 4$,

$$\begin{aligned} \|\nabla_y K^\#(\cdot,y)\|_{L^1(B_1(y)\setminus B_s(y))} &\leq \int_s^1 \frac{C}{t}\|\nabla_y B_k(t,\cdot,y)\|_{L^1}\,dt \\ &\leq C\int_s^1 \frac{dt}{t^2} \\ &\leq \frac{C}{s}. \end{aligned} \tag{3.31}$$

This yields the following.

Lemma 3.3. *There exists $C < \infty$, independent of $s \in (0,1]$ and of $y, y' \in \mathbb{R}^3$, such that*

$$|y - y'| \leq \frac{s}{2} \Longrightarrow \|K^\#(\cdot,y) - K^\#(\cdot,y')\|_{L^1(B_1(y)\setminus B_s(y))} \leq C. \tag{3.32}$$

This leads to the following important conclusion.

Proposition 3.4. *Let $\Phi^\#$ satisfy (1.13)–(1.14) and (1.8). Granted Hypothesis 3.1, $\Phi^\#(\sqrt{\mathcal{H}})$ is of weak type $(1,1)$.*

Proof. Given that $\Phi^\#(\sqrt{\mathcal{H}})$ is bounded on $L^2(\mathbb{R}^3)$, and its integral kernel satisfies (3.32), the weak type (1,1) property is a consequence of Proposition 3.1 of [MMV], which in turn is a natural variant of Theorem 2.4 in Chapter III of [CW].

4. Proof of the main theorem

Recall from §2 that $\Phi^b(\sqrt{\mathcal{H}})$ has integral kernel $K^b(x,y)$, satisfying (2.3) and (2.16), hence $|K^b(x,y)| \le C$ for all $x,y \in \mathbb{R}^3$, and

$$|K^b(x,y)| \le C \int\limits_{t\ge|x-y|-2} \Bigl\{|\hat{\varphi}(t)| + |\hat{\varphi}_2(t)| + |\hat{\varphi}_4(t)|\Bigr\}\, dt, \quad |x-y| \ge 2, \tag{4.1}$$

where

$$\hat{\varphi}(t) = (1-\beta(t))\widehat{\Phi}(t), \quad \hat{\varphi}_j(t) = \partial_t^j \hat{\varphi}(t). \tag{4.2}$$

Now

$$\Phi \in S^0_1(\mathbb{R}) \Longrightarrow \hat{\varphi} \in \mathcal{S}(\mathbb{R}), \tag{4.3}$$

so we get

$$|K^b(x,y)| \le C_N(1+|x-y|)^{-N}, \quad \forall\, N \in \mathbb{Z}^+. \tag{4.4}$$

This clearly implies

$$\Phi^b(\sqrt{\mathcal{H}}) : L^p(\mathbb{R}^3) \longrightarrow L^p(\mathbb{R}^3), \quad \forall\, p \in [1,\infty]. \tag{4.5}$$

This result for $p = 1$ is stronger than having type (1,1).

As for $\Phi^{\#}(\sqrt{\mathcal{H}})$, Proposition 3.4 says it is of type (1,1). Since it is clearly bounded on $L^2(\mathbb{R}^3)$, the Marcinkiewicz interpolation theorem yields

$$\Phi^{\#}(\sqrt{\mathcal{H}}) : L^p(\mathbb{R}^3) \longrightarrow L^p(\mathbb{R}^3), \tag{4.6}$$

for $p \in (1,2]$, and then duality gives boundedness for $p \in [2,\infty)$. Together, (4.5) and (4.6) yield the L^p-bounds for $\Phi(\sqrt{\mathcal{H}})$ in (1.9).

5. The hydrogen atom Schrödinger operator

We briefly discuss how the material of §§1–4 applies to the hydrogen atom Schrödinger operator, given by (1.1)–(1.2). As stated in §1, Hypothesis 1.1 applies to this case; a proof can be found in Chapter 8, §7, of [T4]. As we show in Appendix A, Hypothesis 1.1 implies Hypothesis 2.1, so it also applies. This brings us to Hypothesis 3.1.

We have not shown that Hypothesis 3.1 applies to the hydrogen atom. Material bearing on this issue is discussed in [T7]. There is is shown that, for $\mathcal{H}$ as in (1.6), with $a = K^2/4 + 1$,

$$\begin{aligned} 0 < b < \frac{5}{4} &\Longrightarrow \mathcal{D}(\mathcal{H}^b) = H^{2b}(\mathbb{R}^3), \quad \text{and} \\ b > \frac{5}{4} &\Longrightarrow \mathcal{D}(\mathcal{H}^b) \subset \mathrm{Lip}(\mathbb{R}^3). \end{aligned} \tag{5.1}$$

Note that

$$H^s(\mathbb{R}^3) \subset \mathrm{Lip}(\mathbb{R}^3) \Longleftrightarrow s > \frac{5}{2}. \tag{5.2}$$

Formulas for the eigenfunctions of H show that, if $b > 5/4$, then $\mathcal{D}(\mathcal{H}^b)$ is not contained in $H^{2b}(\mathbb{R}^3)$. We also note that

$$\|e^{-t\mathcal{H}}\|_{\mathcal{L}(L^2,\mathcal{D}(\mathcal{H}^{5/4}))} = \|\mathcal{H}^{5/4}e^{-t\mathcal{H}}\|_{\mathcal{L}(L^2)} \le Ct^{-5/4}, \tag{5.3}$$

which is similar to the conjectural estimate (3.20), but does not prove it.

Whether Hypothesis 3.1 holds for the hydrogen atom remains an open problem.

A. Hypothesis 1.1 ⇒ Hypothesis 2.1

We assume Hypothesis 1.1, so

$$\mathcal{H}^{-1} : L^2(\mathbb{R}^3) \longrightarrow H^2(\mathbb{R}^3). \tag{A.1}$$

By duality,

$$\mathcal{H}^{-1} : H^{-2}(\mathbb{R}^3) \longrightarrow L^2(\mathbb{R}^3), \tag{A.2}$$

snd then, by interpolation,

$$\mathcal{H}^{-1} : H^{-2+s}(\mathbb{R}^3) \longrightarrow H^s(\mathbb{R}^3), \quad 0 \le s \le 2. \tag{A.3}$$

Now $\{\delta_y : y \in \mathbb{R}^3\}$ is a bounded subset of $H^{-3/2-\varepsilon}(\mathbb{R}^3)$, for each $\varepsilon > 0$, so

$$w_y = \mathcal{H}^{-1}\delta_y \ \text{ is bounded in } \ H^{1/2-\varepsilon}(\mathbb{R}^3), \quad \forall\, \varepsilon > 0. \tag{A.4}$$

as y runs over $\mathbb{R}^3$. To get u_y in (2.13), we want to set $u_y = \varphi_y w_y$, where φ_y is a cut-off. To show that this works, we need to establish further regularlty of w_y, away from y.

To this end, let ψ be smooth of class C^2, and assume all its derivatives of order ≤ 2 are bounded. If $w \in H^s(\mathbb{R}^3)$, $0 \le s \le 2$, then $\psi w \in H^s(\mathbb{R}^3)$, and $\Delta(\psi w) = \psi\Delta w + (\Delta\psi)w + 2\nabla\psi \cdot \nabla w$, hence

$$\mathcal{H}(\psi w) = \psi\mathcal{H}w + (\Delta\psi)w + 2\nabla\psi \cdot \nabla w. \tag{A.5}$$

Let us take such ψ, equal to 0 for $|x| \le a$, equal to 1 for $|x| \ge 2a$, where $a > 0$ is small, set $\psi_y(x) = \psi(x-y)$, and apply (A.5) with ψ replaced by ψ_y and w replaced by w_y, as in (A.4). Since $\psi_y\delta_y = 0$, we have

$$\mathcal{H}(\psi_y w_y) = (\Delta\psi_y)w_y + 2\nabla\psi_y \cdot \nabla w_y \in H^{-1/2-\varepsilon}(\mathbb{R}^3), \tag{A.6}$$

for all $\varepsilon > 0$, bounded in y. Hence, by (A.3),

$$\psi_y w_y \in H^{3/2-\varepsilon}(\mathbb{R}^3), \quad \forall\, \varepsilon > 0, \tag{A.7}$$

bounded in y. (Though it is not necessary,) we can iterate this argument. Take a similar $\tilde{\psi}$, equal to 0 for $|x| \le 2a$ and 1 for $|x| \ge 4a$, and set $\tilde{\psi}_y(x) = \tilde{\psi}(x-y)$. Then

$$\mathcal{H}(\tilde{\psi}_y w_y) = (\Delta\tilde{\psi})w_y + 2\nabla\tilde{\psi}_y \cdot \nabla w_y \in H^{1/2-\varepsilon}(\mathbb{R}^3), \tag{A.8}$$

so, by (A.3),

$$\tilde{\psi}_y w_y \in H^2(\mathbb{R}^3), \quad \text{bounded in } y. \tag{A.9}$$

We are now ready for the main result of this appendix.

Proposition A.1. *Hypothesis 1.1 implies Hypothesis 2.1.*

Proof. Take $\varphi \in C_0^\infty(B_1(0))$ such that $\varphi(x) = 1$ for $|x| \le 1/2$. Set $\varphi_y(x) = \varphi(x-y)$, and, with w_y as in (A.4), set

$$u_y = \varphi_y w_y, \quad \text{bounded in } \ H^{1/2-\varepsilon}(\mathbb{R}^3). \tag{A.10}$$

Since $\varphi_y \delta_y = \delta_y$, we get from (A.5) that

$$\mathcal{H} u_y = \delta_y + v_y, \tag{A.11}$$

with

$$v_y = (\Delta\varphi_y) w_y + 2\nabla\varphi_y \cdot \nabla w_y. \tag{A.12}$$

Since $\Delta\varphi_y = 0$ and $\nabla\varphi_y = 0$ on $B_{1/2}(y)$, we have from (A.9) that

$$\{v_y : y \in \mathbb{R}^3\} \ \text{ is bounded in } \ H^1(\mathbb{R}^3). \tag{A.13}$$

Remark. As we have stated, Hypothesis 1.1 holds for H as in (1.1), with V given by (1.2). More generally, as shown in Theorem X.15 of [RS], one has H self adjoint, with domain $\mathcal{D}(H) = H^2(\mathbb{R}^3)$, when H is as in (1.1) and $V : \mathbb{R}^3 \to \mathbb{R}$ satisfies

$$V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3). \tag{A.14}$$

B. Sufficient conditions for Hypothesis 3.1

Here we derive a condition on $\mathcal{H}$ that is sufficient for Hypothesis 3.1 to hold, i.e., for $t > 0,\ f \in L^2(\mathbb{R}^3)$,

$$\begin{aligned} \|e^{-t\mathcal{H}} f\|_{L^\infty} &\le C(t^{-3/4}+1)\|f\|_{L^2}, \\ \|\nabla e^{-t\mathcal{H}} f\|_{L^\infty} &\le C(t^{-5/4}+1)\|f\|_{L^2}. \end{aligned} \tag{B.1}$$

In fact, since $e^{-t\mathcal{H}}$ is a contraction semigroup on $L^2(\mathbb{R}^3)$, it suffices to treat $t \in (0,1]$. Recall that

$$\mathcal{H} = -\Delta + W, \quad W = V + a, \tag{B.2}$$

where a is a positive constant, chosen so that $\operatorname{Spec}\mathcal{H} \subset [1,\infty)$.

For our analysis, we write

$$u(t) = e^{-t\mathcal{H}} f \Longrightarrow \partial_t u = \Delta u - Wu, \tag{B.3}$$

so DuHamel's formula gives

$$u(t) = e^{t\Delta} f - \int_0^t e^{(t-s)\Delta} W u(s)\, ds. \tag{B.4}$$

An examination of the integral kernel $(4\pi t)^{-3/2} e^{-|x-y|^2/4t}$ of $e^{t\Delta}$ gives

$$\begin{aligned} \|e^{t\Delta} f\|_{L^\infty} &\le C t^{-3/4}\|f\|_{L^2}, \\ \|\nabla e^{t\Delta} f\|_{L^\infty} &\le C t^{-5/4}\|f\|_{L^2}, \end{aligned} \tag{B.5}$$

for $f \in L^2(\mathbb{R}^3)$. Hence our remaining task is to estimate the second term on the right side of (B.4).

To start, since $\|u(s)\|_{L^2} \le \|f\|_{L^2}$, we have

$$\|e^{(t-s)\Delta} W u(s)\|_{L^\infty} \le C(t-s)^{-3/4}\|W\|_{L^\infty}\|f\|_{L^2}, \tag{B.6}$$

and integrating over $s \in (0,t)$ readily gives the first estimate in (B.1), provided

$$W \in L^\infty(\mathbb{R}^3). \tag{B.7}$$

To proceed, we have

$$\|u(s)\|_{H^1} \le C\|\mathcal{H}^{1/2} e^{-s\mathcal{H}} f\|_{L^2} \le C s^{-1/2}\|f\|_{L^2}. \tag{B.8}$$

Hence, if we assume

$$\|Wg\|_{H^1} \le \mathcal{M}(W)\|g\|_{H^1}, \quad \mathcal{M}(W) < \infty, \tag{B.9}$$

we have

$$\|Wu(s)\|_{H^1} \le Cs^{-1/2}\mathcal{M}(W)\|f\|_{L^2}. \tag{B.10}$$

Now

$$\begin{aligned} \|\nabla e^{(t-s)\Delta}g\|_{L^\infty} &= \|e^{(t-s)\Delta}\nabla g\|_{L^\infty} \\ &\le C(t-s)^{-3/4}\|\nabla g\|_{L^2}, \end{aligned} \tag{B.11}$$

so

$$\|\nabla e^{(t-s)\Delta}Wu(s)\|_{L^\infty} \le C(t-s)^{-3/4}s^{-1/2}\mathcal{M}(W)\|f\|_{L^2}, \tag{B.12}$$

and integrating over $s \in (0,t)$ gives

$$\Big\|\nabla \int_0^t e^{(t-s)\Delta}Wu(s)\,ds\Big\|_{L^\infty} \le Ct^{-5/4}\mathcal{M}(W)\|f\|_{L^2}. \tag{B.13}$$

We have established the following.

Proposition B.1. *Assume $W = V + a$ satisfies (B.7) and (B.9). Then (B.1) holds, i.e., Hypothesis 3.1 holds.*

Remark. For (B.9) to hold, it is necessary that W satisfy (B.7), and it is sufficient that W satisfy both (B.7) and the following:

$$\nabla W \in L^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3). \tag{B.14}$$

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