# Remarks on the Hydrogen Atom Schrödinger Operator 

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## 1. Introduction

The Schrödinger operator associated to the hydrogen atom has the form

$$
\begin{equation*}
H=-\Delta+V, \quad V(x)=-\frac{K}{|x|}, \quad K>0 \tag{1.1}
\end{equation*}
$$

acting on functions on $\mathbb{R}^{3}$. More precisely, $H$ is a self-adjoint operator on $L^{2}\left(\mathbb{R}^{3}\right)$, constructed by the Friedrichs process, with domain

$$
\begin{equation*}
\mathcal{D}(H)=\left\{u \in H^{1}\left(\mathbb{R}^{3}\right):-\Delta u-K|x|^{-1} u \in L^{2}\left(\mathbb{R}^{3}\right)\right\} . \tag{1.2}
\end{equation*}
$$

We recall some well known facts about this operator, details on which can be found in $\S 7$ of $[\mathrm{T}]$, and then produce some additional results.

First (cf. Proposition 7.2 of [T]),

$$
\begin{equation*}
\mathcal{D}(H)=H^{2}\left(\mathbb{R}^{3}\right) \tag{1.3}
\end{equation*}
$$

Here and below, $H^{s}\left(\mathbb{R}^{3}\right)$ will denote $L^{2}$-Sobolev spaces of functions or distributions on $\mathbb{R}^{3}$, and $H^{s, p}\left(\mathbb{R}^{3}\right)$ will denote $L^{p}$-Sobolev spaces. Next, (cf. Proposition 7.3 of $[\mathrm{T}])$, the part of Spec $H$ in $(-\infty, 0)$ is a discrete subset, consisting of eigenvalues of finite multiplicity. In more detail (cf. (7.15)-(7.38) of $[\mathrm{T}]$ ), these eigenvalues are

$$
\begin{equation*}
E_{n}=-\frac{K^{2}}{4 n^{2}}, \quad \text { eigenspaces } \quad V_{n}, \quad \operatorname{dim} V_{n}=n^{2} \tag{1.4}
\end{equation*}
$$

for $n=1,2,3, \cdots$, and $V_{n}$ has a basis consisting of functions of the form

$$
\begin{equation*}
p(x) q(|x|) e^{-2 K|x| / n} \tag{1.5}
\end{equation*}
$$

where $p$ is a harmonic polynomial on $\mathbb{R}^{3}$, homogeneous of degree $k$, and $q$ is a polynomial on $\mathbb{R}$ of degree $j$, with $j+k+1=n$.

As is clear from the formula (1.5), these eigenfunctions are Lipschitz, but, in cases where $p(x)$ is constant, they have no higher regularity. In particular, $\mathcal{D}\left(H^{2}\right)$ is not contained in $H^{4}\left(\mathbb{R}^{3}\right)$. In $[\mathrm{T}]$ it is shown that

$$
\begin{equation*}
\mathcal{D}\left(H^{2}\right) \subset H^{5 / 2-\varepsilon}\left(\mathbb{R}^{3}\right), \quad \forall \varepsilon>0 \tag{1.6}
\end{equation*}
$$

This does not quite imply that

$$
\begin{equation*}
\mathcal{D}\left(H^{2}\right) \subset \operatorname{Lip}\left(\mathbb{R}^{3}\right) \tag{1.7}
\end{equation*}
$$

In $\S 2$ we prove (1.7). Part of our motivation for doing this lies in our investigation of functional calculus for $H$, discussed in [T2]. It is shown that interesting LittlewoodPaley results follow if one has an estimate

$$
\begin{equation*}
\left\|e^{-t H}\right\|_{\mathcal{L}\left(L^{2}, \mathrm{Lip}\right)} \leq C t^{-5 / 4}, \quad \text { for } t \in(0,1] \tag{1.8}
\end{equation*}
$$

We discuss conjectural results related to (1.8) in $\S 3$. Work there naturally motivates us to consider fractional powers $\mathcal{H}^{1+a}$, for $a \in(0,1)$, where

$$
\begin{equation*}
\mathcal{H}=H+K^{2} / 4+1, \tag{1.9}
\end{equation*}
$$

a self-adjoint operator with spectrum in $[1, \infty)$. In $\S 4$ we show that, on the one hand,

$$
\begin{equation*}
\mathcal{D}\left(\mathcal{H}^{1+a}\right) \subset \operatorname{Lip}\left(\mathbb{R}^{3}\right), \quad \text { if } 1+a>\frac{5}{4}, \tag{1.10}
\end{equation*}
$$

and, on the other hand,

$$
\begin{equation*}
\mathcal{D}\left(\mathcal{H}^{1+a}\right)=H^{2(1+a)}\left(\mathbb{R}^{3}\right), \quad \text { if } 1+a<\frac{5}{4} \tag{1.11}
\end{equation*}
$$

Section 5 contains some results and conjectures on the orthogonal projection $P$ of $L^{2}\left(\mathbb{R}^{3}\right)$ onto the direct sum of the eigenspaces associated with the negative spectrum of $H$.

## 2. Domain of $H^{2}$

We next examine the domain of $H^{2}$, for $H$ of the form (1.1). As shown in Proposition 7.7 of [T],

$$
\begin{equation*}
\mathcal{D}\left(H^{2}\right) \subset H^{5 / 2-\varepsilon}\left(\mathbb{R}^{3}\right), \quad \forall \varepsilon>0 \tag{2.1}
\end{equation*}
$$

Here we desire to prove the following, which is not quite implied by (2.1).

## Proposition 2.1. We have

$$
\begin{equation*}
\mathcal{D}\left(H^{2}\right) \subset \operatorname{Lip}\left(\mathbb{R}^{3}\right) . \tag{2.2}
\end{equation*}
$$

Proof. We start by recalling the proof of Proposition 7.7 of [T]. Pick $\lambda \notin \operatorname{Spec} H$. Take $u \in \mathcal{D}\left(H^{2}\right)$, and set $(H-\lambda) u=f \in \mathcal{D}(H)=H^{2}\left(\mathbb{R}^{3}\right)$. Also set $R_{\lambda}=$ $(-\Delta-\lambda)^{-1}$. Then

$$
\begin{equation*}
u=-R_{\lambda} V u+R_{\lambda} f, \quad R_{\lambda} f \in H^{4}\left(\mathbb{R}^{3}\right) . \tag{2.3}
\end{equation*}
$$

The next step taken in $[\mathrm{T}]$ is to use the fact that

$$
\begin{equation*}
M_{V}: H^{2}\left(\mathbb{R}^{3}\right) \longrightarrow H^{1 / 2-\varepsilon}\left(\mathbb{R}^{3}\right), \quad \forall \varepsilon>0 \tag{2.4}
\end{equation*}
$$

to deduce that $R_{\lambda} V u \in H^{5 / 2-\varepsilon}\left(\mathbb{R}^{3}\right)$, yielding (2.1) from (2.3).
We modify the last part of this argument as follows. Pick

$$
\begin{gather*}
\chi \in C_{0}^{\infty}\left(\mathbb{R}^{3}\right), \quad \chi(x)=1 \text { for }|x| \leq 1, \quad \chi(x)=0 \text { for }|x| \geq 2,  \tag{2.5}\\
V=\chi V+(1-\chi) V=V_{0}+V_{1} .
\end{gather*}
$$

Then

$$
\begin{equation*}
u \in \mathcal{D}(H)=H^{2}\left(\mathbb{R}^{3}\right) \Rightarrow V_{1} u \in H^{2}\left(\mathbb{R}^{3}\right) \Rightarrow R_{\lambda} V_{1} u \in H^{4}\left(\mathbb{R}^{3}\right) . \tag{2.6}
\end{equation*}
$$

Meanwhile, since

$$
\begin{equation*}
H^{2}\left(\mathbb{R}^{3}\right) \subset C^{\alpha}\left(\mathbb{R}^{3}\right), \quad \alpha=\frac{1}{2}, \tag{2.7}
\end{equation*}
$$

where, for $0<\alpha<1$,

$$
\begin{equation*}
\|v\|_{C^{\alpha}}=\|v\|_{L^{\infty}}+\sup \left\{\frac{|v(x)-v(y)|}{|x-y|^{\alpha}}: x \neq y \in \mathbb{R}^{3},|x-y| \leq 1\right\}, \tag{2.8}
\end{equation*}
$$

we can write, for $u \in \mathcal{D}(H)$,

$$
\begin{equation*}
u=u(0) \chi+u_{1}, \quad u_{1} \in C^{\alpha}\left(\mathbb{R}^{3}\right), u_{1}(0)=0 \tag{2.9}
\end{equation*}
$$

Hence, given $u \in \mathcal{D}(H)$,

$$
\begin{equation*}
R_{\lambda} V_{0} u=u(0) R_{\lambda} V_{0} \chi+R_{\lambda} V_{0} u_{1} . \tag{2.10}
\end{equation*}
$$

Now $V_{0} u_{1}$ is supported on $\{x:|x| \leq 2\}$, and

$$
\begin{equation*}
\left|V_{0}(x) u_{1}(x)\right| \leq C|x|^{\alpha-1}, \tag{2.11}
\end{equation*}
$$

for $\alpha=1 / 2$.
In fact, given $u \in \mathcal{D}\left(H^{2}\right)$, we can use (2.1) to improve the conclusion of (2.9) to $u_{1} \in C^{\alpha}\left(\mathbb{R}^{3}\right)$ for all $\alpha<1$, and we also have (2.11) for all $\alpha<1$. Consequently,

$$
\begin{equation*}
V_{0} u_{1} \in L^{p}\left(\mathbb{R}^{n}\right), \quad \forall p \in(1, \infty), \tag{2.12}
\end{equation*}
$$

hence

$$
\begin{equation*}
R_{\lambda} V_{0} u_{1} \in H^{2, p}\left(\mathbb{R}^{3}\right), \quad \forall p \in(1, \infty) \tag{2.13}
\end{equation*}
$$

We deduce that, if $u \in \mathcal{D}\left(H^{2}\right)$, with $(H-\lambda) u=f \in \mathcal{D}(H)$, then

$$
\begin{align*}
u & =-R_{\lambda}\left(u(0) V_{0} \chi+V_{0} u_{1}\right) \quad \bmod H^{4}\left(\mathbb{R}^{3}\right) \\
& =-u(0) R_{\lambda}\left(V_{0} \chi\right) \quad \bmod H^{2, p}\left(\mathbb{R}^{3}\right), \tag{2.14}
\end{align*}
$$

for all $p \in[2, \infty)$. Given that

$$
\begin{equation*}
\Delta|x|=2|x|^{-1}, \quad \text { on } \quad \mathbb{R}^{3}, \tag{2.15}
\end{equation*}
$$

we have

$$
\begin{equation*}
R_{\lambda}\left(V_{0} \chi\right)=\frac{K}{2}|x| \chi^{2}+\frac{\lambda K}{2} R_{\lambda}\left(|x| \chi^{2}\right) \bmod \mathcal{S}\left(\mathbb{R}^{3}\right) \tag{2.16}
\end{equation*}
$$

and

$$
\begin{equation*}
R_{\lambda}\left(|x| \chi^{2}\right) \in \bigcap_{1 \leq q<\infty} H^{3, q}\left(\mathbb{R}^{3}\right) \tag{2.16A}
\end{equation*}
$$

We hence have the following result, which is more precise than Proposition 2.1.

Proposition 2.2. We have

$$
\begin{equation*}
\mathcal{D}\left(H^{2}\right) \subset \operatorname{Span}(|x| \chi(x))+\bigcap_{2 \leq p<\infty} H^{2, p}\left(\mathbb{R}^{3}\right) \tag{2.17}
\end{equation*}
$$

In view of the formula (1.5) for elements of $V_{n}$, which of course belong to $\mathcal{D}\left(H^{k}\right)$ for all $k$, this is a pretty good result. However, we take one more pass through the proof of Propositions 2.1 and 2.2, to obtain an improvement of (2.13)-(2.14). To begin, given $u \in \mathcal{D}\left(H^{2}\right)$, we can now say that $u_{1}$ in (2.9) satisfies

$$
\begin{equation*}
u_{1} \in \operatorname{Lip}\left(\mathbb{R}^{3}\right), \quad u_{1}(0)=0 \tag{2.18}
\end{equation*}
$$

It follows that

$$
\begin{equation*}
\left|\nabla\left(V_{0} u_{1}\right)\right| \leq C|x|^{-1}, \tag{2.19}
\end{equation*}
$$

hence

$$
\begin{equation*}
\nabla\left(V_{0} u_{1}\right) \in L^{3-\varepsilon}\left(\mathbb{R}^{3}\right), \quad \forall \varepsilon \in(0,1] \tag{2.20}
\end{equation*}
$$

so

$$
\begin{equation*}
R_{\lambda} V_{0} u_{1} \in H^{3,3-\varepsilon}\left(\mathbb{R}^{3}\right), \quad \forall \varepsilon \in(0,1] . \tag{2.21}
\end{equation*}
$$

Note that this improves (2.13), since

$$
\begin{equation*}
\bigcap_{1<q<3} H^{1, q}\left(\mathbb{R}^{3}\right) \subset \bigcap_{1<p<\infty} L^{p}\left(\mathbb{R}^{3}\right), \tag{2.22}
\end{equation*}
$$

hence

$$
\begin{equation*}
\bigcap_{1<q<3} H^{3, q}\left(\mathbb{R}^{3}\right) \subset \bigcap_{1<p<\infty} H^{2, p}\left(\mathbb{R}^{3}\right) \tag{2.23}
\end{equation*}
$$

Also, since $H^{1}\left(\mathbb{R}^{3}\right) \subset L^{6}\left(\mathbb{R}^{3}\right)$, it follows that $H^{4}\left(\mathbb{R}^{3}\right) \subset H^{3,6}\left(\mathbb{R}^{3}\right) \cap H^{3,2}\left(\mathbb{R}^{3}\right) \subset$ $H^{3, q}\left(\mathbb{R}^{3}\right)$, if $2 \leq q \leq 6$, so we improve (2.14) to

$$
\begin{equation*}
u=-u(0) R_{\lambda}\left(V_{0} \chi\right), \quad \bmod H^{3, q}\left(\mathbb{R}^{3}\right) \tag{2.24}
\end{equation*}
$$

for each $q \in[2,3)$. In light of (2.16)-(2.16A), this gives:
Proposition 2.3. Improving Proposition 2.2,

$$
\begin{equation*}
\mathcal{D}\left(H^{2}\right) \subset \operatorname{Span}(|x| \chi)+\bigcap_{2 \leq q<3} H^{3, q}\left(\mathbb{R}^{3}\right) . \tag{2.25}
\end{equation*}
$$

## 3. Conjectural semigroup and resolvent estimates

Estimates on the semigroup $e^{-t H}$ are of great significance. We state a conjecture which, if true, would have nice applications to Littlewood-Paley theory associated to the operator $H$.

Conjecture 3.1. The semigroup $e^{-t H}$ satisfies, for $t \in(0,1]$,

$$
\begin{align*}
&\left\|e^{-t H}\right\|_{\mathcal{L}\left(L^{2}, L^{\infty}\right)} \leq C t^{-3 / 4}, \quad \text { and } \\
&\left\|e^{-t H}\right\|_{\mathcal{L}\left(L^{2}, \mathrm{Lip}\right)} \leq C t^{-3 / 4-1 / 2} \tag{3.1}
\end{align*}
$$

In connection with this, we have the following.
Proposition 3.2. Set

$$
\begin{equation*}
\mathcal{H}=H+\frac{K^{2}}{4}+1, \tag{3.2}
\end{equation*}
$$

which is self-adjoint with spectrum in $[1, \infty)$. Then there exists $C<\infty$ such that

$$
\begin{equation*}
\sup _{t \geq 1}\left\|e^{-t \mathcal{H}}\right\|_{\mathcal{L}\left(L^{2}, \text { Lip }\right)} \leq C \tag{3.3}
\end{equation*}
$$

Proof. Let $t=1+s, s \geq 0$. Since $e^{-t \mathcal{H}}=e^{-\mathcal{H}} e^{-s \mathcal{H}}$ and $e^{-s \mathcal{H}}$ is a contraction on $L^{2}\left(\mathbb{R}^{3}\right)$, we have

$$
\begin{equation*}
\sup _{t \geq 1}\left\|e^{-t \mathcal{H}}\right\|_{\mathcal{L}\left(L^{2}, \text { Lip }\right)} \leq\left\|e^{-\mathcal{H}}\right\|_{\mathcal{L}\left(L^{2}, \text { Lip }\right)} \tag{3.4}
\end{equation*}
$$

Since

$$
\begin{equation*}
e^{-\mathcal{H}}=\mathcal{H}^{-2}\left(\mathcal{H}^{2} e^{-\mathcal{H}}\right), \tag{3.5}
\end{equation*}
$$

and $\mathcal{H}^{2} e^{-\mathcal{H}}$ is bounded on $L^{2}\left(\mathbb{R}^{3}\right)$, we have

$$
\begin{equation*}
\left\|e^{-\mathcal{H}}\right\|_{\mathcal{L}\left(L^{2}, \mathrm{Lip}\right)} \leq C_{1}\left\|\mathcal{H}^{-2}\right\|_{\mathcal{L}\left(L^{2}, \mathrm{Lip}\right)} \leq C \tag{3.6}
\end{equation*}
$$

the last inequality by Proposition 2.1.
Using $\mathcal{H}$, we can rewrite the second conjectural estimate in (3.1) as

$$
\begin{equation*}
\left\|e^{-t \mathcal{H}}\right\|_{\mathcal{L}\left(L^{2}, \mathrm{Lip}\right)} \leq C\left(t^{-3 / 4-1 / 2}+1\right), \quad t>0 . \tag{3.7}
\end{equation*}
$$

It is useful to connect (3.7) to resolvent estimates.

Proposition 3.3. If (3.7) holds, then

$$
\begin{equation*}
\left\|\left(1+t^{2} \mathcal{H}^{2}\right)^{-1}\right\|_{\mathcal{L}\left(L^{2}, \mathrm{Lip}\right)} \leq C\left(t^{-3 / 4-1 / 2}+1\right), \quad t>0 . \tag{3.8}
\end{equation*}
$$

Proof. We can use

$$
\begin{equation*}
\left(1+t^{2} \mathcal{H}^{2}\right)^{-1}=(1+t \mathcal{H})^{-2}(1+t \mathcal{H})^{2}\left(1+t^{2} \mathcal{H}^{2}\right)^{-1} \tag{3.9}
\end{equation*}
$$

to reduce our task to showing that (3.7) implies

$$
\begin{equation*}
\left\|(1+t \mathcal{H})^{-2}\right\|_{\mathcal{L}\left(L^{2}, \operatorname{Lip}\right)} \leq C\left(t^{-3 / 4-1 / 2}+1\right) . \tag{3.10}
\end{equation*}
$$

To prove (3.10), we use the identity

$$
\begin{equation*}
(1+t \mathcal{H})^{-\sigma}=\frac{1}{\Gamma(\sigma)} \int_{0}^{\infty} e^{-s} e^{-s t \mathcal{H}} s^{\sigma-1} d s \tag{3.11}
\end{equation*}
$$

Then, given (3.7),

$$
\begin{align*}
\left\|(1+t \mathcal{H})^{-\sigma}\right\|_{\mathcal{L}\left(L^{2}, \mathrm{Lip}\right) \leq} \leq & C \int_{0}^{t^{-2}} e^{-s}(s t)^{-3 / 4-1 / 2} s^{\sigma-1} d s \\
& +C \int_{t^{-2}}^{\infty} e^{-s} s^{\sigma-1} d s  \tag{3.12}\\
\leq & C_{1}\left(t^{-3 / 4-1 / 2}+1\right)
\end{align*}
$$

with $C_{1}<\infty$ if $\sigma>3 / 4+1 / 2$. In particular, this applies for $\sigma=2$.
We also have a converse, derivable via the following useful result.
Proposition 3.4. If (3.8) holds, then

$$
\begin{equation*}
\|\Phi(t \mathcal{H})\|_{\mathcal{L}\left(L^{2}, \mathrm{Lip}\right)} \leq C\left(t^{-3 / 4-1 / 2}+1\right), \quad t>0 \tag{3.13}
\end{equation*}
$$

whenever $\Phi(\lambda)$ satisfies

$$
\begin{equation*}
|\Phi(\lambda)| \leq C(1+|\lambda|)^{-2} . \tag{3.14}
\end{equation*}
$$

Proof. Indeed,

$$
\begin{equation*}
\Phi(t \mathcal{H})=\left(1+t^{2} \mathcal{H}^{2}\right)^{-1}\left(1+t^{2} \mathcal{H}^{2}\right) \Phi(t \mathcal{H}) \tag{3.15}
\end{equation*}
$$

and the product of the last two factors is uniformly bounded on $L^{2}\left(\mathbb{R}^{3}\right)$.
Taking

$$
\begin{equation*}
\Phi(\lambda)=e^{-|\lambda|}, \tag{3.16}
\end{equation*}
$$

we see that

$$
(3.8) \Longrightarrow(3.7)
$$

Remark. Having (3.7), we also see from (3.12) that the estimate (3.13) holds provided

$$
\begin{equation*}
|\Phi(\lambda)| \leq C(1+|\lambda|)^{-\beta}, \quad \beta>\frac{5}{4} . \tag{3.17}
\end{equation*}
$$

## 4. Domain of $\mathcal{H}^{1+a}$

By Proposition 3.4 and the subsequent remark, involving (3.17), we see that if Conjecture 3.1 is true, then the following must hold.

Proposition 4.1. Take $\mathcal{H}$ as in (3.2). Then

$$
\begin{equation*}
\mathcal{D}\left(\mathcal{H}^{1+a}\right) \subset \operatorname{Lip}\left(\mathbb{R}^{3}\right), \quad \text { for } 1+a>\frac{5}{4} \tag{4.1}
\end{equation*}
$$

Our first goal here is to prove (4.1).
To start, take $a \in(0,1)$ and $u \in \mathcal{D}\left(\mathcal{H}^{1+a}\right)$, and write

$$
\begin{equation*}
\mathcal{H} u=f \in \mathcal{D}\left(\mathcal{H}^{a}\right)=H^{2 a}\left(\mathbb{R}^{3}\right), \tag{4.2}
\end{equation*}
$$

the last identification by (1.3) (which implies $\mathcal{D}(\mathcal{H})=H^{2}\left(\mathbb{R}^{3}\right)$ ) and interpolation. Now $\mathcal{H}=H-\lambda$, with $\lambda=-1-K^{2} / 4 \notin \operatorname{Spec} H$, so, parallel to (2.3), we have

$$
\begin{equation*}
u=-R_{\lambda} V u+R_{\lambda} f, \quad R_{\lambda} f \in H^{2(1+a)}\left(\mathbb{R}^{3}\right) \tag{4.3}
\end{equation*}
$$

Note that $H^{2(1+a)}\left(\mathbb{R}^{3}\right) \subset \operatorname{Lip}\left(\mathbb{R}^{3}\right)$ precisely for $1+a>5 / 4$. Taking $V=V_{0}+V_{1}$, as in (2.5), we can rewrite (4.3) as

$$
\begin{align*}
u & =-R_{\lambda} V_{0} u-R_{\lambda} V_{1} u+R_{\lambda} f \\
& =-R_{\lambda} V_{0} u \quad \bmod H^{2(1+a)}\left(\mathbb{R}^{3}\right), \tag{4.4}
\end{align*}
$$

since $u \in \mathcal{D}(\mathcal{H}) \Rightarrow R_{\lambda} V_{1} u \in H^{4}\left(\mathbb{R}^{3}\right)$.
Next, parallel to (2.9),

$$
\begin{equation*}
u=u(0) \chi+u_{1} . \tag{4.5}
\end{equation*}
$$

At this point, we can say the following about $u_{1}$. Since

$$
\begin{equation*}
\mathcal{D}(\mathcal{H})=H^{2}\left(\mathbb{R}^{3}\right) \subset C^{1 / 2}\left(\mathbb{R}^{3}\right), \quad \text { and } \mathcal{D}\left(\mathcal{H}^{2}\right) \subset \operatorname{Lip}\left(\mathbb{R}^{3}\right) \tag{4.6}
\end{equation*}
$$

an interpolation argument gives, for $a \in(0,1)$,

$$
\begin{equation*}
u \in \mathcal{D}\left(\mathcal{H}^{1+a}\right) \Longrightarrow u \in C^{(1+\alpha) / 2}\left(\mathbb{R}^{3}\right), \quad \forall \alpha<a \tag{4.7}
\end{equation*}
$$

so

$$
\begin{equation*}
u_{1} \in C^{(1+\alpha) / 2}\left(\mathbb{R}^{3}\right), \quad \text { and } \quad u_{1}(0)=0 \tag{4.8}
\end{equation*}
$$

Now, by (4.4),

$$
\begin{equation*}
u=-u(0) R_{\lambda}\left(V_{0} \chi\right)-R_{\lambda} V_{0} u_{1}, \quad \bmod H^{2(1+a)}\left(\mathbb{R}^{3}\right) \tag{4.10}
\end{equation*}
$$

and, by (4.8),

$$
\begin{equation*}
\left|V_{0}(x) u_{1}(x)\right| \leq C \chi(x)|x|^{\beta-1}, \quad \forall \beta<\frac{1+a}{2} . \tag{4.11}
\end{equation*}
$$

Next,

$$
\begin{align*}
1+a>\frac{5}{4} & \Rightarrow\left|V_{0}(x) u_{1}(x)\right| \leq C \chi(x)|x|^{-3 / 8+\varepsilon} \quad(\varepsilon>0) \\
& \Rightarrow V_{0} u_{1} \in L^{8}\left(\mathbb{R}^{3}\right) \\
& \Rightarrow R_{\lambda} V_{0} u_{1} \in H^{2,8}\left(\mathbb{R}^{3}\right)  \tag{4.12}\\
& \Rightarrow R_{\lambda} V_{0} u_{1} \in C^{1+r}\left(\mathbb{R}^{3}\right), \quad \forall r<\frac{5}{8}
\end{align*}
$$

Meanwhile, (2.16)-(2.16A) apply to $R_{\lambda}\left(V_{0} \chi\right)$, so we have the desired result (4.1).
Here is an interesting complement to Proposition 4.1.
Proposition 4.2. We have

$$
\begin{equation*}
\mathcal{D}\left(\mathcal{H}^{1+a}\right)=H^{2(1+a)}\left(\mathbb{R}^{3}\right), \quad \text { for } \quad 1 \leq 1+a<\frac{5}{4} . \tag{4.15}
\end{equation*}
$$

Proof. First, take $u \in \mathcal{D}\left(\mathcal{H}^{1+a}\right)$. The first part of the proof of Proposition 4.1 applies in this setting, to yield (4.10), i.e.,

$$
\begin{equation*}
u \in \mathcal{D}\left(\mathcal{H}^{1+a}\right) \Rightarrow u=-u(0) R_{\lambda}\left(V_{0} \chi\right)-R_{\lambda} V_{0} u_{1} \bmod H^{2(1+a)}\left(\mathbb{R}^{3}\right) . \tag{4.16}
\end{equation*}
$$

Also, $1+a \leq 5 / 4 \Rightarrow H^{2(1+a)}\left(\mathbb{R}^{3}\right) \supset H^{5 / 2}\left(\mathbb{R}^{3}\right)$, so $(2.16)-(2.16 \mathrm{~A})$ implies $R_{\lambda}\left(V_{0} \chi\right)=$ $(K / 2)|x| \chi^{2} \bmod H^{2(1+a)}\left(\mathbb{R}^{3}\right)$. Meanwhile, for the Fourier transform of $|x| \chi^{2}$ we have

$$
\begin{align*}
\mathcal{F}\left(|x| \chi^{2}\right)(\xi) & \sim C\langle\xi\rangle^{-2} \mathcal{F}\left(|x|^{-1} \chi^{2}\right)(\xi)  \tag{4.17}\\
& \sim C\langle\xi\rangle^{-4},
\end{align*}
$$

and hence

$$
\begin{equation*}
|x| \chi^{2} \in H^{5 / 2-\varepsilon}\left(\mathbb{R}^{3}\right), \quad \forall \varepsilon>0 \tag{4.18}
\end{equation*}
$$

Hence, as long as $1 \leq 1+a<5 / 4$,

$$
\begin{equation*}
u \in \mathcal{D}\left(\mathcal{H}^{1+a}\right) \Rightarrow u=-R_{\lambda} V_{0} u_{1} \bmod H^{2(1+a)}\left(\mathbb{R}^{3}\right) \tag{4.19}
\end{equation*}
$$

At this point, we have $u_{1} \in \mathcal{D}(\mathcal{H})=H^{2}\left(\mathbb{R}^{3}\right)$ and $V_{0}=|x|^{-1} \chi$. Parallel to (4.17)(4.18), $\widehat{V}_{0}(\xi) \sim C\langle\xi\rangle^{-2}$, so $V_{0} \in H^{1 / 2-\varepsilon}\left(\mathbb{R}^{3}\right), \forall \varepsilon>0$, hence, for all $\varepsilon>0$,

$$
\begin{equation*}
V_{0} \in H^{1 / 2-\varepsilon}\left(\mathbb{R}^{3}\right), \quad \text { hence } \quad V_{0} u_{1} \in H^{1 / 2-\varepsilon}\left(\mathbb{R}^{3}\right), \tag{4.20}
\end{equation*}
$$

so

$$
\begin{equation*}
u \in \mathcal{D}(\mathcal{H}) \Rightarrow R_{\lambda} V_{0} u_{1} \in H^{5 / 2-\varepsilon}\left(\mathbb{R}^{3}\right), \quad \forall \varepsilon>0 \tag{4.21}
\end{equation*}
$$

This proves that $\mathcal{D}\left(\mathcal{H}^{1+a}\right) \subset H^{2(1+a)}\left(\mathbb{R}^{3}\right)$ if $1 \leq 1+a<5 / 4$. Using

$$
\begin{align*}
\mathcal{D}\left(\mathcal{H}^{1+a}\right) & =\left\{u \in \mathcal{D}(\mathcal{H}): \mathcal{H} u \in \mathcal{H}^{a}\right\}  \tag{4.22}\\
& =\left\{u \in H^{2}\left(\mathbb{R}^{3}\right): \mathcal{H} u \in H^{2 a}\left(\mathbb{R}^{3}\right)\right\},
\end{align*}
$$

one can produce a similar argument to establish the converse.

Remark. We have

$$
\begin{equation*}
\left\|e^{-t \mathcal{H}}\right\|_{\mathcal{L}\left(L^{2}, \mathcal{D}\left(\mathcal{H}^{5 / 4}\right)\right)}=\left\|\mathcal{H}^{5 / 4} e^{-t \mathcal{H}}\right\|_{\mathcal{L}\left(L^{2}\right)} \leq C t^{-5 / 4} \tag{4.23}
\end{equation*}
$$

an estimate that, in light of Propositions 4.1-4.2, is tantalizingly close to the conjectured estimate (3.1), but of course not quite on the mark.

## 5. Projection onto the negative spectrum of $H$

Let

$$
\begin{equation*}
P=\text { orthogonal projection of } L^{2}\left(\mathbb{R}^{3}\right) \text { onto } \bigoplus_{n \geq 1} V_{n}, \tag{5.1}
\end{equation*}
$$

where the spaces $V_{n}$ are the eigenspaces of $H$ described in (1.4). Clearly

$$
\begin{equation*}
P: L^{2}\left(\mathbb{R}^{3}\right) \longrightarrow \bigcap_{k \geq 1} \mathcal{D}\left(H^{k}\right) \tag{5.2}
\end{equation*}
$$

In particular,

$$
\begin{equation*}
P: L^{2}\left(\mathbb{R}^{3}\right) \longrightarrow H^{5 / 2-\varepsilon}\left(\mathbb{R}^{3}\right), \quad \forall \varepsilon>0 \tag{5.3}
\end{equation*}
$$

and

$$
\begin{equation*}
P: L^{2}\left(\mathbb{R}^{3}\right) \longrightarrow \operatorname{Lip}\left(\mathbb{R}^{3}\right) \tag{5.4}
\end{equation*}
$$

A special case of (1.5) is

$$
\begin{equation*}
V_{1}=\operatorname{Span} e^{-2 K|x|}, \tag{5.5}
\end{equation*}
$$

so $\operatorname{Lip}\left(\mathbb{R}^{3}\right)$ cannot be replaced by $C^{1}\left(\mathbb{R}^{3}\right)$ in (5.4). Note that (5.3) implies

$$
\begin{equation*}
P: L^{2}\left(\mathbb{R}^{3}\right) \longrightarrow \bigcap_{2 \leq p \leq \infty} L^{p}\left(\mathbb{R}^{3}\right) \tag{5.6}
\end{equation*}
$$

and

$$
\begin{equation*}
P: L^{2}\left(\mathbb{R}^{3}\right) \longrightarrow C_{0}\left(\mathbb{R}^{3}\right) \tag{5.7}
\end{equation*}
$$

By duality, since $P=P^{*}$,

$$
\begin{equation*}
P: L^{q}\left(\mathbb{R}^{3}\right) \longrightarrow L^{2}\left(\mathbb{R}^{3}\right), \quad \forall q \in[1,2] \tag{5.8}
\end{equation*}
$$

and, since also $P^{2}=P$, we then have

$$
\begin{equation*}
P: L^{q}\left(\mathbb{R}^{3}\right) \longrightarrow L^{p}\left(\mathbb{R}^{3}\right), \quad \text { for } \quad 1 \leq q \leq 2 \leq p \leq \infty \tag{5.9}
\end{equation*}
$$

Note that each eigenfunction described in (1.5) belongs to $L^{p}\left(\mathbb{R}^{3}\right)$ for all $p \in$ $[1, \infty]$. Nevertheless, we hazzard the following:

Conjecture 5.1. Given $p \in[1, \infty]$,

$$
\begin{align*}
& P: L^{2}\left(\mathbb{R}^{3}\right) \rightarrow L^{p}\left(\mathbb{R}^{3}\right) \Longrightarrow p \geq 2, \quad \text { and }  \tag{5.10}\\
& P: L^{p}\left(\mathbb{R}^{3}\right) \rightarrow L^{p}\left(\mathbb{R}^{3}\right) \Longrightarrow p=2 . \tag{5.11}
\end{align*}
$$

Note that the operators $H^{k} P$ enjoy the mapping properties (5.2)-(5.4) and (5.6)(5.9). Actually, these operators are milder than $P$. For example, it follows from (1.4) that
$H P$ is Hilbert-Schmidt, and $H^{2} P$ is trace class, on $L^{2}\left(\mathbb{R}^{3}\right)$.
We therefore hazzard the following:
Conjecture 5.2. There exist $p_{0}, p_{1} \in(1,2)$ such that

$$
\begin{align*}
& H P: L^{2}\left(\mathbb{R}^{3}\right) \longrightarrow L^{p}\left(\mathbb{R}^{3}\right), \text { for } p \in\left(p_{0}, 2\right], \text { and }  \tag{5.13}\\
& H P: L^{p}\left(\mathbb{R}^{3}\right) \longrightarrow L^{p}\left(\mathbb{R}^{3}\right), \text { for } p \in\left(p_{1}, p_{1}^{\prime}\right) \tag{5.14}
\end{align*}
$$

[T] M. Taylor, Spectral Theory, Chapter 8 of Partial Differential Equations, Vol. 2, Springer-Verlag, New York, 1996 (2nd ed., 2011).
[T2] M. Taylor, Functional calculus and Littlewood-Paley theory for Schrödinger operators, Preprint, 2017.

