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THE REGULARITY OF ELECTRONIC WAVE FUNCTIONS IN BARRON SPACES

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Abstract. The electronic Schrödinger equation describes the motion of a finite number of electrons under Coulomb interaction forces in the field of a finite number of clamped nuclei. It is proved that its solutions for negative eigenvalues, below the essential spectrum, lie in the spectral Barron spaces $\mathcal{B}^s$ for $s < 1$. Examples show that this limit generally cannot be reached or surpassed.

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1. Introduction

In these years, the Schrödinger equation celebrates its centenary. It forms the basis of quantum mechanics and is fundamental for the study of atomic and molecular systems. Because the nuclei are much heavier than the electrons, the electrons follow their motion almost instantaneously. Therefore, it is common to separate the motion of the nuclei from that of the electrons and to start from the electronic Schrödinger equation, the equation that describes the motion of a finite number of electrons in the field of a finite number of clamped nuclei, or in other words, to look for the eigenvalues and eigenfunctions of the Hamilton operator

$$H = -\frac{1}{2}\sum_{i=1}^{N}\Delta_i - \sum_{i=1}^{N}\sum_{\nu=1}^{K}\frac{Z_\nu}{\|x_i - a_\nu\|} + \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\frac{1}{\|x_i - x_j\|} \tag{1.1}$$

expressed here in dimensionless form or in atomic units. It acts on functions with arguments $x_1, \ldots, x_N$ in $\mathbb{R}^3$, which are associated with the positions of the considered electrons. The $a_1, \ldots, a_K$ in $\mathbb{R}^3$ are the fixed positions of the nuclei and the values $Z_\nu > 0$ the charges of the nuclei in multiples of the electron charge. The solution space of the equation is the Hilbert space $H^1(\mathbb{R}^{3N})$. The multiplication with the potential

$$V(x) = -\sum_{i=1}^{N}\sum_{\nu=1}^{K}\frac{Z_\nu}{\|x_i - a_\nu\|} + \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\frac{1}{\|x_i - x_j\|} \tag{1.2}$$

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is a bounded mapping from $H^1(\mathbb{R}^{3N})$ to $L_2(\mathbb{R}^{3N})$ as can be shown by means of a Hardy inequality. This will play an important role later on and allows to express the eigenvalue problem in weak form. The weak formulation fixes the solutions at the singular points of the interaction potential (1.2) and at infinity.

The regularity properties of the eigenfunctions have been of interest to mathematicians for a long time, beginning with Kato's seminal work [6] almost seventy years ago. Far-reaching results on the regularity of the eigenfunctions in Hölder spaces can be found in [4, 5]. The study of the regularity in Hilbert spaces of mixed derivatives began with Yserentant [11]. See Kreusler and Yserentant [7], Meng [8] and Yserentant [12, 13], for further developments. The regularity properties of the solutions in Hilbert spaces of mixed derivatives constitute the basis for interesting complexity estimates and attempts to break the curse of dimensionality [12].

Inspired by the extensive recent work on the approximation properties of neural networks, the present paper is dedicated to the regularity of the eigenfunctions in Barron spaces. Let $B_s(\mathbb{R}^n)$, for any real number s, be the Banach space that consists of the measurable functions $u : \mathbb{R}^n \to \mathbb{C}$ with finite norm

$$\|u\|_{1,s} = \int_{\mathbb{R}^n} (1 + \|\omega\|^2)^{s/2} |u(\omega)| \,\mathrm{d}\omega. \tag{1.3}$$

The infinitely differentiable functions with rapidly, superpolynomially decreasing derivatives of all orders, in the following referred to shortly as rapidly decreasing functions, form a dense subset of these spaces. The spectral Barron space $\mathcal{B}^s(\mathbb{R}^n)$, $s \geq 0$, is the space of the functions that possess a then also unique representation

$$u(x) = \left(\frac{1}{\sqrt{2\pi}}\right)^n \int_{\mathbb{R}^n} \widehat{u}(\omega)\, \mathrm{e}^{\,\mathrm{i}\,\omega\cdot x} \,\mathrm{d}\omega \tag{1.4}$$

in terms of a function $\widehat{u} \in B_s(\mathbb{R}^n)$, their Fourier transform. They are Banach spaces under the norm (1.3) of the Fourier transforms. Because every rapidly decreasing function is the Fourier transform of another rapidly decreasing function, the rapidly decreasing functions are dense in $\mathcal{B}^s(\mathbb{R}^n)$. The functions in $\mathcal{B}^s(\mathbb{R}^n)$ are uniformly continuous and vanish at infinity by the Riemann–Lebesgue theorem. If $s \geq m$, m a natural number, they are m-times continuously differentiable and their derivatives up to order m vanish at infinity.

Barron spaces play an increasingly important role in the analysis of partial differential equations and their numerical solution, especially in high space dimensions. An instructive example for this kind of research is [10], a work in which a novel approach for the numerical solution of elliptic equations is presented and analyzed. The review article [2] gives an overview of recent developments from a broader perspective. Chen *et al.* [1] study the regularity of the solutions of Schrödinger-type equations in Barron spaces under rather strong conditions on the potential. The work of Dus and Ehrlacher [3] is based on similar assumptions. The Coulomb potential (1.2) does not fall into the category of the potentials considered in these papers. In fact, one cannot expect a high Barron space regularity of the solutions of the electronic Schrödinger equation, since these solutions are in general not differentiable and possess typical cusps at the singular points of the potential. This can already be seen from the example of the (non-normalized) ground state wave function

$$\psi(x) = \exp(-\|x\|) \tag{1.5}$$

of the hydrogen atom. Its Fourier transform is

$$\widehat{\psi}(\omega) = \sqrt{\frac{2}{\pi}}\, \frac{2}{(1 + \|\omega\|^2)^2}. \tag{1.6}$$

The norms (1.3) of $\widehat{\psi}$ are finite for $s < 1$ and tend like $\sim 1/(1-s)$ to infinity as s goes to one. That is, this wave function is contained in the spaces $\mathcal{B}^s(\mathbb{R}^3)$ for $s < 1$, but not in $\mathcal{B}^1(\mathbb{R}^3)$. The message of the present paper is that this behavior is no exception. The solutions of the electronic Schrödinger equation for eigenvalues below the ionization threshold $\Sigma \leq 0$ lie in the Barron spaces $\mathcal{B}^s(\mathbb{R}^{3N})$, $s < 1$. The weighted L_1-norms of their Fourier transforms are finite for $s < 1$ and do not grow faster than $\sim 1/(1-s)$ as s goes to one.

2. Estimates for the Coulomb potential, three space dimensions

The aim of this and of the next section is to provide representations and norm estimates for the Fourier transforms of the products of Coulomb potentials with in the aforementioned sense rapidly decreasing functions. These results are based on an integral representation of the Fourier transform of such products. The situation is complicated by the fact that the potentials are not integrable and have no Fourier transform in the classical sense. The starting point of our considerations are the following two lemmas, which are borrowed from the theory of Riesz potentials and play an important role there; see Section V.1 in [9], for example.

Lemma 2.1. *Let $0 < \alpha < n$ and $\beta = n - \alpha$. For all rapidly decreasing functions $\varphi : \mathbb{R}^n \to \mathbb{C}$ then*

$$\int_{\mathbb{R}^n} \frac{1}{\|x\|^\alpha}\, \varphi(x)\,\mathrm{d}x = \frac{(\sqrt{2\pi})^n}{\gamma(\alpha)} \int_{\mathbb{R}^n} \frac{1}{\|\omega\|^\beta}\, \widehat{\varphi}(\omega)\,\mathrm{d}\omega \tag{2.1}$$

holds, where the constant $\gamma(\alpha)$ depends on the dimension n and is given by

$$\frac{1}{\gamma(\alpha)} = \left(\frac{1}{\sqrt{\pi}}\right)^n \frac{1}{2^\alpha} \frac{\Gamma(\beta/2)}{\Gamma(\alpha/2)}. \tag{2.2}$$

Proof. The proof starts from the identity

$$\int_{\mathbb{R}^n} \frac{1}{\|x\|^\alpha}\, \varphi(x)\,\mathrm{d}x = \frac{1}{\Gamma(\alpha/2)} \int_0^\infty t^{\alpha/2-1} \left(\int_{\mathbb{R}^n} \varphi(x)\, \mathrm{e}^{-t\,\|x\|^2}\,\mathrm{d}x \right) \mathrm{d}t$$

that results from the integral representation

$$\frac{1}{r^\alpha} = \frac{1}{\Gamma(\alpha/2)} \int_0^\infty t^{\alpha/2-1} \mathrm{e}^{-tr^2}\,\mathrm{d}t$$

by means of the Fubini–Tonelli theorem. If one applies the Parseval identity to the inner integral and reverses the order of integration again, one obtains the representation

$$\int_{\mathbb{R}^n} \frac{1}{\|x\|^\alpha}\, \varphi(x)\,\mathrm{d}x = \frac{1}{\Gamma(\alpha/2)} \int_{\mathbb{R}^n} \widehat{\varphi}(\omega) \left(\int_0^\infty t^{\alpha/2-1} \left(\frac{1}{\sqrt{2t}}\right)^n \exp\left(-\frac{\|\omega\|^2}{4t}\right) \mathrm{d}t \right) \mathrm{d}\omega$$

of the integral. With the function $h(t) = \|\omega\|^2/(4t)$, the inner integrand reads

$$-\,\frac{(\sqrt{2})^n}{2^\alpha} \frac{1}{\|\omega\|^\beta}\, h(t)^{\beta/2-1} \mathrm{e}^{-h(t)} h'(t).$$

The inner integral therefore takes the value

$$\frac{(\sqrt{2})^n}{2^\alpha} \frac{1}{\|\omega\|^\beta} \int_0^\infty t^{\beta/2-1} \mathrm{e}^{-t}\,\mathrm{d}t = \frac{(\sqrt{2})^n}{2^\alpha} \frac{1}{\|\omega\|^\beta}\, \Gamma\left(\frac{\beta}{2}\right),$$

which yields (2.1) and proves the lemma. □

In the distributional sense, the function $\widehat{f}(\omega) = c(\alpha)/\|\omega\|^\beta$, $c(\alpha) = (\sqrt{2\pi})^n/\gamma(\alpha)$, is therefore the Fourier transform of the function $f(x) = 1/\|x\|^\alpha$. If $u : \mathbb{R}^n \to \mathbb{C}$ is a rapidly decreasing function, the functions

$$V_\alpha u : x \to \frac{1}{\|x\|^\alpha}\, u(x), \qquad 0 < \alpha < n, \tag{2.3}$$

are integrable. Their Fourier transforms are convolution integrals, Riesz potentials.

Lemma 2.2. *If $u:\mathbb{R}^n\to\mathbb{C}$ is a rapidly decreasing function, the Fourier transform of the function (2.3) is*

$$\widehat{V_\alpha u}(\omega)=\frac{1}{\gamma(\alpha)}\int_{\mathbb{R}^n}\frac{1}{\|\omega-\eta\|^\beta}\,\widehat{u}(\eta)\,\mathrm{d}\eta, \tag{2.4}$$

where $\gamma(\alpha)$ is the dimension-dependent constant (2.2).

Proof. One only needs to insert the function $\varphi(x)=u(x)\,\mathrm{e}^{-\mathrm{i}\,\omega\cdot x}$ into the equation (2.1). □

In the following, we restrict ourselves to three dimensions and study the product of the Coulomb potential

$$V(x)=\frac{1}{\|x\|} \tag{2.5}$$

with rapidly decreasing functions $u:\mathbb{R}^3\to\mathbb{C}$. From Lemma 2.2 we know the Fourier transform

$$\widehat{Vu}(\omega)=\frac{1}{2\pi^2}\int_{\mathbb{R}^3}\frac{1}{\|\omega-\eta\|^2}\,\widehat{u}(\eta)\,\mathrm{d}\eta \tag{2.6}$$

of the then integrable functions Vu. In terms of the integral operator

$$\mathcal{K}f(\omega)=\frac{1}{2\pi^2}\int_{\mathbb{R}^3}\frac{1}{\|\omega-\eta\|^2}\,f(\eta)\,\mathrm{d}\eta \tag{2.7}$$

and the operator $\mathcal{F}$ mapping a function u to its Fourier transform $\mathcal{F}u=\widehat{u}$, (2.6) succinctly reads

$$\mathcal{F}Vu=\mathcal{K}\mathcal{F}u. \tag{2.8}$$

The key to our further reasoning is the following norm estimate for the operator $\mathcal{K}$.

Lemma 2.3. *Let $f:\mathbb{R}^3\to\mathbb{C}$ be a rapidly decreasing function, and let ϑ be greater than one. Then*

$$\int_{\mathbb{R}^3}\frac{1}{(1+\|\omega\|^2)^{\vartheta/2}}\,|\mathcal{K}f(\omega)|\,\mathrm{d}\omega\;\leq\;\kappa(\vartheta)\int_{\mathbb{R}^3}|f(\omega)|\,\mathrm{d}\omega, \tag{2.9}$$

where the constant $\kappa(\vartheta)$ tends to infinity as ϑ goes to one and is given by

$$\kappa(\vartheta)=\frac{2\,\Gamma((\vartheta-1)/2)}{\sqrt{\pi}\,\Gamma(\vartheta/2)}. \tag{2.10}$$

Proof. As a rapidly decreasing function, f is integrable and bounded and $\mathcal{K}f$ therefore bounded. It is

$$\int_{\mathbb{R}^3}\frac{1}{(1+\|\omega\|^2)^{\vartheta/2}}\,|\mathcal{K}f(\omega)|\,\mathrm{d}\omega\;\leq\;\int_{\mathbb{R}^3}\frac{1}{(1+\|\omega\|^2)^{\vartheta/2}}\left(\frac{1}{2\pi^2}\int_{\mathbb{R}^3}\frac{1}{\|\omega-\eta\|^2}\,|f(\eta)|\,\mathrm{d}\eta\right)\mathrm{d}\omega.$$

Tonelli's theorem allows us to reverse the order of integration and leads to

$$\int_{\mathbb{R}^3}\frac{1}{(1+\|\omega\|^2)^{\vartheta/2}}\,|\mathcal{K}f(\omega)|\,\mathrm{d}\omega\;\leq\;\frac{1}{2\pi^2}\int_{\mathbb{R}^3}\left(\int_{\mathbb{R}^3}\frac{1}{\|\omega-\eta\|^2}\,\frac{1}{(1+\|\omega\|^2)^{\vartheta/2}}\,\mathrm{d}\omega\right)|f(\eta)|\,\mathrm{d}\eta,$$

where equality holds for real-valued, nonnegative f. To estimate the inner integral, we subdivide the $\mathbb{R}^3$ into the set Ω_1 that consists of the ω for which $\|\omega\|\leq\|\omega-\eta\|$ holds and the set Ω_2 on which $\|\omega-\eta\|<\|\omega\|$. The integration over each of these two subdomains contributes a value not greater than

$$\int_{\mathbb{R}^3}\frac{1}{\|\omega\|^2}\,\frac{1}{(1+\|\omega\|^2)^{\vartheta/2}}\,\mathrm{d}\omega=4\pi\int_0^\infty\frac{1}{(1+r^2)^{\vartheta/2}}\,\mathrm{d}r$$

to the inner integral. With the function $h(r)=r^2/(1+r^2)$ and the constants $a=1/2$ and $b=(\vartheta-1)/2$,

$$\frac{1}{(1+r^2)^{\vartheta/2}} = \frac{1}{2}\, h(r)^{a-1}(1-h(r))^{b-1}h'(r).$$

The above integral can therefore be reduced to Euler's beta integral

$$\int_0^1 t^{a-1}(1-t)^{b-1}\,\mathrm{d}t = \frac{\Gamma(a)\,\Gamma(b)}{\Gamma(a+b)}\cdot$$

This leads to the constant (2.10) and concludes the proof. □

It is not very difficult to show that $\kappa(\vartheta)$ exceeds the best possible constant by a factor of two at most, considering functions $f\geq 0$ with supports that are concentrated around the origin. In fact, the inner integral takes its maximum value at $\eta=0$. Therefore, the best possible constant is $\kappa(\vartheta)/2$, and $\kappa(-s)/2$ is the norm of $\mathcal{K}$ seen as an operator from the space of the rapidly decreasing functions equipped with the L_1-norm to the space B_s, $s<-1$. The constant $\kappa(\vartheta)$ possesses the representation

$$\kappa(\vartheta) = \frac{2\,q(\vartheta)}{\pi}\,\frac{2}{\vartheta-1}, \quad q(\vartheta) = \frac{\Gamma(1/2)\,\Gamma((\vartheta+1)/2)}{\Gamma(\vartheta/2)}. \tag{2.11}$$

The function q increases strictly, on the interval $1\leq\vartheta\leq 2$ from $q(1)=1$ to $q(2)=\pi/2$.

3. Estimates for the Coulomb potential, the multi-particle case

Now we have the tools to study the Fourier transform of the product of the interaction potential (1.2) with rapidly decreasing functions and to estimate the corresponding norms. Let V_i and $\mathcal{K}_i$, $i=1,\ldots,N$, be operators as in the previous section, but now acting electron-wise and given by

$$V_i u(x) = \frac{1}{\|x_i\|}\,u(x), \quad \mathcal{K}_i f(\omega_i,\omega') = \frac{1}{2\pi^2}\int_{\mathbb{R}^3}\frac{1}{\|\omega_i-\eta_i\|^2}\,f(\eta_i,\omega')\,\mathrm{d}\eta_i, \tag{3.1}$$

where in the definition of the second we have decomposed the vectors $\omega\in(\mathbb{R}^3)^N$ into a part $\omega_i\in\mathbb{R}^3$ and a residual part $\omega'\in(\mathbb{R}^3)^{N-1}$. First, we transfer the results from the previous section to the N-particle case.

Lemma 3.1. *If $f:(\mathbb{R}^3)^N\to\mathbb{C}$ is rapidly decreasing, $\mathcal{K}_i f$ lies in the spaces $B_s(\mathbb{R}^{3N})$, $s<-1$, and*

$$\|\mathcal{K}_i f\|_{1,s} \leq \kappa(-s)\|f\|_{1,0}, \tag{3.2}$$

where the norms are those from (1.3) and the constant is given by (2.10).

Proof. Let $\vartheta=-s$. The functions $\omega_i\to f(\omega_i,\omega')$ are rapidly decreasing and

$$\int_{\mathbb{R}^3}\frac{1}{(1+\|\omega_i\|^2)^{\vartheta/2}}\,|\mathcal{K}_i f(\omega_i,\omega')|\,\mathrm{d}\omega_i \;\leq\; \kappa(\vartheta)\int_{\mathbb{R}^3}|f(\omega_i,\omega')|\,\mathrm{d}\omega_i$$

by Lemma 2.3. Since $\|\omega_i\|\leq\|\omega\|$, this implies the weaker, for our purposes sufficient estimate

$$\int_{\mathbb{R}^3}\frac{1}{(1+\|\omega\|^2)^{\vartheta/2}}\,|\mathcal{K}_i f(\omega_i,\omega')|\,\mathrm{d}\omega_i \;\leq\; \kappa(\vartheta)\int_{\mathbb{R}^3}|f(\omega_i,\omega')|\,\mathrm{d}\omega_i.$$

Integration over the remaining variables yields the proposition. □

Lemma 3.2. *Let* $u : (\mathbb{R}^3)^N \to \mathbb{C}$ *be rapidly decreasing. The Fourier transform of* $V_i u \in L_1$ *is then*

$$\mathcal{F}V_i u = \mathcal{K}_i \mathcal{F}u. \tag{3.3}$$

Proof. We decompose the full Fourier transform $\mathcal{F}$ into the product $\mathcal{F} = \mathcal{F}^i\mathcal{F}'$ of the partial Fourier transform

$$\mathcal{F}^i u(\omega_i, x') = \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int_{\mathbb{R}^3} u(x_i, x')\, \mathrm{e}^{-\mathrm{i}\omega_i\cdot x_i}\, \mathrm{d}x_i,$$

which acts upon the here relevant part $x_i \in \mathbb{R}^3$, and its correspondingly defined counterpart $\mathcal{F}'$ that acts upon the remaining variables. Both map rapidly decreasing functions to rapidly decreasing functions. The multiplication by V_i and $\mathcal{F}'$ commute, so we have $\mathcal{F}V_i u = \mathcal{F}^i V_i \mathcal{F}' u$ and $\mathcal{F}V_i u = \mathcal{K}_i \mathcal{F}^i \mathcal{F}' u$ by (2.8). □

To calculate the Fourier transform of the product of a rapidly decreasing function u with the potentials

$$V_{i,a}(x) = \frac{1}{\|x_i - a\|}, \qquad a \in \mathbb{R}^3, \tag{3.4}$$

we introduce the operators $\tau_i(a)$ mapping a function f to the function $\tau_i(a)f$ with the values

$$\tau_i(a)f(\omega) = \mathrm{e}^{-\mathrm{i}\,\omega_i\cdot a} f(\omega). \tag{3.5}$$

A short calculation using (3.3) then shows that the Fourier transform of $V_{i,a}u$ is

$$\mathcal{F}V_{i,a}u = \tau_i(a)\mathcal{K}_i\tau_i(-a)\mathcal{F}u. \tag{3.6}$$

Let Q be an orthogonal matrix of corresponding dimension and assign to it the operator Q with the same name mapping an integrable function f to the integrable function Qf with the values

$$Qf(\omega) = f(Q\omega). \tag{3.7}$$

Since the Fourier transform $\mathcal{F}Qf$ of the function Qf is the function $Q\mathcal{F}f$, this operator commutes with the Fourier transform. Let V_{ij} be the potential

$$V_{ij}(x) = \frac{1}{\|x_i - x_j\|} \tag{3.8}$$

and assign to it the orthogonal matrix Q_{ij} that maps the parts in $x_k \in \mathbb{R}^3$ of $x \in (\mathbb{R}^3)^N$ to the vectors

$$x_i \to \frac{x_i - x_j}{\sqrt{2}},\ x_j \to \frac{x_i + x_j}{\sqrt{2}},\ x_k \to x_k \text{ for } k \neq i, j. \tag{3.9}$$

In operator notation, $V_{ij} = Q_{ij}^{-1} V_j Q_{ij}/\sqrt{2}$. With the given commutation relations, the representation

$$\mathcal{F}V_{ij}u = \frac{1}{\sqrt{2}}\, Q_{ij}^{-1}\mathcal{K}_j Q_{ij}\mathcal{F}u \tag{3.10}$$

of the Fourier transform of the product of the potential V_{ij} with a rapidly decreasing function u follows.

Now we are ready, can sum up all the different terms, introduce the operator

$$\mathcal{K} = -\sum_{i=1}^{N}\sum_{\nu=1}^{K} Z_\nu \tau_i(a_\nu)\mathcal{K}_i\tau_i(-a_\nu) + \frac{1}{\sqrt{2}} \sum_{\substack{i,j=1\\ i<j}}^{N} Q_{ij}^{-1}\mathcal{K}_j Q_{ij}, \tag{3.11}$$

and summarize our considerations as follows.

Lemma 3.3. *If $f:\mathbb{R}^{3N}\to\mathbb{C}$ is rapidly decreasing, $\mathcal{K}f$ lies in the spaces $B_s(\mathbb{R}^{3N})$, $s<-1$, and it is*

$$\|\mathcal{K}f\|_{1,s} \leq C\kappa(-s)\|f\|_{1,0}, \tag{3.12}$$

where the constant C depends on the total charge of the nuclei and the number of the electrons, but not on s, and $\kappa(-s)$ is defined as in (2.10). Furthermore,

$$\mathcal{F}Vu = \mathcal{K}\mathcal{F}u \tag{3.13}$$

for all in the given sense rapidly decreasing functions $u:\mathbb{R}^{3N}\to\mathbb{C}$.

Proof. The operators $\tau_i(a)$, Q_{ij}, and Q_{ij}^{-1} preserve the norms (1.3). The estimate thus follows from Lemma 3.1 by means of the triangle inequality. The commutation relation results from those for the single parts. □

4. The regularity of the solutions

To prove the Barron space regularity, we switch to the momentum representation of the Schrödinger equation, which is an equation for the Fourier transform of the eigenfunctions. The underlying Hilbert spaces are no longer the Sobolev spaces H^s, but the spaces $\widehat{H}^s$ of the measurable functions u with finite norm given by

$$\|u\|_{2,s}^2 = \int_{\mathbb{R}^{3N}} (1+\|\omega\|^2)^s |u(\omega)|^2 \,\mathrm{d}\omega. \tag{4.1}$$

They consist of the L_2-Fourier transforms $\mathcal{F}_2 u$ of the functions u in the Sobolev spaces H^s as follows from the Parseval identity. A nonzero function $u\in\widehat{H}^1$ is an admissible solution of the electronic Schrödinger equation for the eigenvalue $\lambda<0$ in Fourier or momentum representation if and only if

$$u + G(\lambda)\mathcal{F}_2 V \mathcal{F}_2^{-1} u = 0. \tag{4.2}$$

The operator $G(\lambda)$ denotes the multiplication by the function

$$G(\lambda) = \frac{2}{\|\omega\|^2 - 2\lambda} \tag{4.3}$$

and the bounded linear operator $V: H^1\to L_2$ the multiplication by the potential (1.2). The aim of this section is to show that the solutions of this equation lie in the spaces B_s for $s<1$, that is, are Fourier transforms of functions in the corresponding Barron spaces $\mathcal{B}^s$. Our theory is based on a careful study of the operator

$$T(\lambda) = -\,G(\lambda)\mathcal{F}_2 V \mathcal{F}_2^{-1} \tag{4.4}$$

whose fixed points $u\in\widehat{H}^1$, $u\neq 0$, are the eigenfunctions for the eigenvalue λ.

Lemma 4.1. *The operator $T(\lambda)$ maps the functions $u\in\widehat{H}^1$ to functions in $\widehat{H}^2$ that satisfy the estimate*

$$\|T(\lambda)u\|_{2,2} \leq C\,\|u\|_{2,1}, \tag{4.5}$$

where the constant C depends on the total charge of the nuclei, on the number of electrons, and on λ.

Proof. The estimate is essentially based on the boundedness of the operator $V: u\to Vu$ from the Sobolev space $H^1(\mathbb{R}^{3N})$ to $L_2(\mathbb{R}^{3N})$, which results from the Hardy inequality

$$\int_{\mathbb{R}^3} \frac{1}{\|x\|^2}\,|u(x)|^2\,\mathrm{d}x \leq 4\int_{\mathbb{R}^3} \|\nabla u(x)\|^2\,\mathrm{d}x$$

for functions $u \in H^1(\mathbb{R}^3)$. For $u \in \widehat{H}^1$, the L_2-norm of the function $f = \mathcal{F}_2 V \mathcal{F}_2^{-1} u$ thus satisfies an estimate

$$\|\mathcal{F}_2 V(\mathcal{F}_2^{-1} u)\|_{2,0} \leq c\,\|\mathcal{F}_2(\mathcal{F}_2^{-1} u)\|_{2,1} = c\,\|u\|_{2,1}$$

since the L_2-Fourier transform $\mathcal{F}_2$ preserves the L_2-norm. The rest of the proof is based on the identity

$$\|G(\lambda) f\|_{2,2}^2 = 4 \int_{\mathbb{R}^{3N}} \left(\frac{1 + \|\omega\|^2}{\|\omega\|^2 - 2\lambda} \right)^2 |f(\omega)|^2 \, \mathrm{d}\omega$$

and the in the following repeatedly occurring estimate

$$2\, \frac{1 + \|\omega\|^2}{\|\omega\|^2 - 2\lambda} \leq \max\left(2, -\frac{1}{\lambda}\right).$$

Inserting $f = \mathcal{F}_2 V \mathcal{F}_2^{-1} u$, the proposition follows from the estimate above. □

The most important intermediate step in the proof of the regularity theorem is the following estimate, first only for rapidly decreasing functions, which summarizes our considerations from the last two sections.

Lemma 4.2. *If $u : \mathbb{R}^{3N} \to \mathbb{C}$ is a rapidly decreasing function, $T(\lambda)u$ lies in the L_1-based spaces B_s, $s < 1$, and the norms (1.3) of $T(\lambda)u$ can be estimated as*

$$\|T(\lambda)u\|_{1,s} \leq C_1 \kappa(2 - s) \|u\|_{1,0}, \tag{4.6}$$

where the constant C_1 depends on λ, but is independent of s, and $\kappa(2-s)$ is given by (2.10).

Proof. For the functions $f \in B_{s-2}$ one has

$$\|G(\lambda) f\|_{1,s} = 2 \int_{\mathbb{R}^{3N}} \frac{1 + \|\omega\|^2}{\|\omega\|^2 - 2\lambda} \, (1 + \|\omega\|^2)^{(s-2)/2} \, |f(\omega)| \, \mathrm{d}\omega,$$

from which as in the proof of Lemma 4.1

$$\|G(\lambda) f\|_{1,s} \leq \max\left(2, -\frac{1}{\lambda}\right) \|f\|_{1,s-2}$$

follows. The inverse Fourier transform $\mathcal{F}_2^{-1} u$ of a rapidly decreasing function u is a rapidly decreasing function. Since the L_1-Fourier transform $\mathcal{F} v$ and the L_2-Fourier transform $\mathcal{F}_2 v$ of functions v in the intersection of both spaces coincide, for rapidly decreasing functions u we have

$$\mathcal{F}_2 V \mathcal{F}_2^{-1} u = \mathcal{F} V \mathcal{F}_2^{-1} u = \mathcal{K} \mathcal{F} \mathcal{F}_2^{-1} u = \mathcal{K} u$$

by Lemma 3.3. Inserting $f = \mathcal{F}_2 V \mathcal{F}_2^{-1} u$ into the above estimate, (4.6) follows from (3.12). □

To proceed, we need to introduce a new scale of functions spaces X_s, the intersections of the space $\widehat{H}^1$ and the spaces B_s from the introduction. We equip them with the norms

$$|\!|\!| u |\!|\!|_s = \|u\|_{2,1} + \|u\|_{1,s} \tag{4.7}$$

that are composed of the norm on the solution space $\widehat{H}^1$ of the equation and the weighted L_1-norms (1.3).

Lemma 4.3. *The spaces X_s are complete and the rapidly decreasing functions lie dense in them.*

Proof. The proof of the completeness of the spaces is almost identical to the proof of the completeness of L_1 itself. Let $u_1, u_2, \dots$ be a Cauchy sequence of functions in X_s and let $v_1, v_2, \dots$ be a subsequence for which

$$|||v_{k+1} - v_k|||_s \leq 2^{-k}$$

holds. The monotonously increasing sequence of the nonnegative measurable functions $f_1, f_2, \dots$ given by

$$f_n(x) = \sum_{k=1}^{n} |v_{k+1}(x) - v_k(x)|$$

then tends pointwise to a measurable limit function f. In the next step the structure of the norms enters. Because the norm of a function in X_s coincides with the norm of its absolute value, the norms

$$|||f_n|||_s \leq \sum_{k=1}^{n} |||v_{k+1} - v_k|||_s \leq \sum_{k=1}^{n} 2^{-k}$$

remain uniformly bounded and by the monotone convergence theorem the norm

$$|||f|||_s = \lim_{n\to\infty} |||f_n|||_s$$

of the limit function f is finite. This means that f is almost everywhere finite, that the v_k converge almost everywhere pointwise to a measurable function v, and that the absolute values of the v_k and of v are almost everywhere bounded by the function $|v_1| + f$ of finite norm. So the dominated convergence theorem leads to

$$\lim_{k\to\infty} |||v - v_k|||_s = 0.$$

That is, v is an accumulation point of the Cauchy sequence of the u_k. The u_k thus converge to v.

The functions in X_s can be approximated by functions with bounded support, as again follows from the dominated convergence theorem, and these by infinitely differentiable functions with bounded support via the convolution with appropriate mollifiers. This shows that the rapidly decreasing functions are dense in X_s. □

The estimate from Lemma 4.2 can be transferred to the functions in $X_0 = \widehat{H}^1 \cap L_1$.

Lemma 4.4. *If $u \in X_0$, the function $T(\lambda)u$ lies in X_s for $s < 1$ and its norms (1.3) can be estimated as*

$$\|T(\lambda)u\|_{1,s} \leq C_1 \kappa(2-s) \|u\|_{1,0}, \tag{4.8}$$

with the same constant C_1 as in (4.6) that is independent of s and $\kappa(2-s)$ as in (2.10).

Proof. Let $u_1, u_2, \dots$ be a sequence of rapidly decreasing functions that converges in X_0 to u. By Lemmas 4.1 and 4.2, the functions $T(\lambda)u_k$ form Cauchy sequences in the given spaces X_s. Since the spaces X_s are complete, the $T(\lambda)u_k$ converge in X_s to a function f_s. Since convergence in X_s implies convergence in B_s,

$$\|f_s\|_{1,s} \leq C_1 \kappa(2-s) \|u\|_{1,0}$$

follows from (4.6). But convergence in X_s also implies convergence in $\widehat{H}^1$. By Lemma 4.1, the $T(\lambda)u_k$ converge in $\widehat{H}^1$ and even in $\widehat{H}^2$ to $T(\lambda)u$. This means $\|f_s - T(\lambda)u\|_{2,1} = 0$ and proves the proposition. □

In the following we split the considered functions into a low-frequency and a high-frequency part. Let $\Omega > 0$ be a given bound that separates the low from the high frequencies and let $\chi(\omega) = 0$ for $\|\omega\| < \Omega$ and $\chi(\omega) = 1$ for $\|\omega\| \geq \Omega$. Let the operator P denote the multiplication with the cut-off function χ. The high-frequency part $v = Pu$ of the solution $u \in \widehat{H}^1$ of the equation (4.2) satisfies the equation

$$v - PT(\lambda)v = PT(\lambda)(u - Pu). \tag{4.9}$$

This equation is the key to our regularity result, which will follow from the contractivity of $PT(\lambda)$ seen as an operator from $\widehat{H}^1$ to $\widehat{H}^1$ as well as from X_0 to X_0 for sufficiently large chosen frequency bounds Ω.

Lemma 4.5. *For $u \in \widehat{H}^1$, the function $PT(\lambda)u \in \widehat{H}^2$ can be estimated as*

$$\|PT(\lambda)u\|_{2,1} \leq C\left(\frac{1}{1+\Omega^2}\right)^{1/2}\|u\|_{2,1}, \tag{4.10}$$

where the constant C is the same as in (4.5).

Proof. This follows from the almost trivial estimate

$$\|Pf\|_{2,1}^2 \leq \frac{1}{1+\Omega^2}\,\|f\|_{2,2}^2$$

for functions $f \in \widehat{H}^2$ and Lemma 4.1 applied to $f = T(\lambda)u$. □

Lemma 4.6. *If $u \in X_0$, the function $PT(\lambda)u$ lies in X_s for $s < 1$ and its norms (1.3) can be estimated as*

$$\|PT(\lambda)u\|_{1,s} \leq C_1\left(\frac{1}{1+\Omega^2}\right)^{\vartheta/2}\kappa(2-(s+\vartheta))\,\|u\|_{1,0}, \tag{4.11}$$

where $\vartheta < 1 - s$ can be chosen arbitrarily and C_1 is the same constant as in (4.6) and (4.8).

Proof. The proposition follows from the estimate

$$\|Pf\|_{1,s} \leq \left(\frac{1}{1+\Omega^2}\right)^{\vartheta/2}\|f\|_{1,s+\vartheta}$$

for functions $f \in B_{s+\vartheta}$ and from Lemma 4.4 applied to $f = T(\lambda)u$. □

Theorem 4.7. *The solutions $u \in \widehat{H}^1$ of the electronic Schrödinger equation (4.2) in momentum representation for eigenvalues $\lambda < 0$ lie in the spaces X_s for $0 \leq s < 1$. For these s, their norms (1.3) satisfy the estimate*

$$\|u\|_{1,s} \leq C_1\kappa(2-s)\|u\|_{1,0}, \tag{4.12}$$

with the same constant C_1 as in (4.6) and (4.8) that depends on the total charge of the nuclei, on the number of electrons, and on the eigenvalue λ, but is independent of s, and with

$$\kappa(2-s) = \frac{2}{\sqrt{\pi}}\frac{\Gamma((1-s)/2)}{\Gamma((2-s)/2)} \leq \frac{2}{1-s}\cdot \tag{4.13}$$

Proof. By Lemmas 4.5 and 4.6, we can choose Ω so large that the assigned operator $PT(\lambda)$ is contractive as an operator from $\widehat{H}^1$ to $\widehat{H}^1$ and from X_0 to X_0. As an eigenfunction $u \in \widehat{H}^1$ for the eigenvalue $\lambda < 0$ is a solution of the equation (4.2), its high-frequency part $v = Pu$ in $\widehat{H}^1$ solves the equation (4.9). Since $PT(\lambda)$ is contractive as an operator from $\widehat{H}^1$ to $\widehat{H}^1$, $v = Pu$ is the only solution of this equation in $\widehat{H}^1$ with $u - Pu$ given. This means that the high-frequency part Pu of the eigenfunction possesses the representation

$$Pu = \sum_{k=1}^{\infty}(PT(\lambda))^k(u - Pu)$$

in form of a Neumann series. The function $u - Pu$ is square integrable and has a bounded support, the ball of radius Ω around the origin. Therefore, it lies in X_0. Thus, the Neumann series converges to an element in X_0. That is, its high frequency part Pu and the eigenfunction $u = Pu + (u - Pu)$ itself lie in X_0. Since $u = T(\lambda)u$ by (4.2) and (4.4), u lies in X_s for $s < 1$ by Lemma 4.4 and its norms (1.3) satisfy the estimate (4.12). The inequality (4.13) follows from (2.11) and the subsequent remark. □

Now we have come to the end and reached the goal of our efforts. Translated back to the representation in position space, the theorem states that the solutions of the electronic Schrödinger equation for eigenvalues below the ionization threshold $\Sigma \leq 0$ lie in the Barron spaces $\mathcal{B}^s$, $s < 1$. The weighted L_1-norm

$$\|u\|_{1,s} = \int_{\mathbb{R}^{3N}} (1 + \|\omega\|^2)^{s/2} |u(\omega)| \, \mathrm{d}\omega \tag{4.14}$$

of their Fourier transforms does not grow faster than $\sim 1/(1-s)$ as s goes to one, as with the hydrogen ground state. The example of the hydrogen ground state shows that the limit $s = 1$ cannot be reached in general. The norms are likely to degenerate if the associated eigenvalue approaches the ionization threshold.

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