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Existence and uniqueness of the ground state in Schrödinger equations

Supervisor:
Prof. Monti Roberto

Candidate:
Parmeggiani Andrea

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Introduction

In this thesis we prove that, under suitable assumptions, the time-indipendent Schrödinger equation

$$-\Delta\psi(x) + V(x)\psi(x) = E\psi(x)$$

admits a unique solution.
In particular, we prove that, under suitable assumptions, if the energy E is in its ground state E_0, then there exists a unique solution to the equation.

To begin, we notice that finding a solution to this equation means finding an eigenfunction ψ and an eigenvalue E that satisfy it. To tackle this problem, we consider its variational form: we try to minimize the total energy of the system

$$\mathcal{E}(\psi) = \int_{\mathbb{R}^n} |\nabla\psi(x)|^2 dx + \int_{\mathbb{R}^n} V(x)|\psi(x)|^2 dx$$

subject to the normalization condition

$$\|\psi\|_2 = 1.$$

In the first chapter we prove that there exists a minimum (the ground state energy) and, by using the lower semicontinuity of the potential and Sobolev's inequalities, we prove that any minimizer ψ_0 satisfies the Schrödinger equation with $E = E_0$.

In the second chapter, we prove that this minimizer is unique (up to a constant phase), and that this implies the uniqueness of the solutions of the Schrödinger equation in the ground state energy configuration.

These results have an important physical interpretation, especially in quantum mechanics. During our analysis we observe that the ground state energy is the lowest possible eigenvalue for the Schrödinger equation: this agrees with the physical fact that an observed particle will settle eventually into its ground state. The higher eigenvalues are studied in the second chapter, and they also bring an important physical meaning: their difference determine the possible frequencies of light emitted by a quantum-mechanical system. In the last section there is a direct application on the hydrogen atom of the results discussed previously.

Symbols

A^*	Dual of A
$\Re$	Real part
$\Im$	Imaginary part
$\mathbb{R}$	Set of real numbers
$\mathbb{C}$	Set of complex numbers
$C_c^\infty(\Omega)$	Infinitely differentiable functions of compact support $\Omega \subset \mathbb{R}^n$
$D'(\Omega)$	Distributions
$H^1(\Omega)$	Sobolev's space
$\mathbb{S}^{n-1}$	Unit sphere in $\mathbb{R}^n$
∇	Gradient
Δ	Laplacian
χ_A	Characteristic function of a set A
$\rightharpoonup$	Weak convergence
$L^p(\Omega)$	Set of measurable function with finite p norm
$L^{p+\epsilon}(\Omega)$	Set of measurable function with finite q norm for $q > p$

Chapter 1

Existence of ground state energy in Schrödinger's equation

1.1 Schrödinger's equation

The time indipendent Schrödinger equation for a particle in $\mathbb{R}^n$, interacting with a force field $F(x) = -\nabla V(x)$, is

$$-\Delta\psi(x) + V(x)\psi(x) = E\psi(x), \tag{1.1}$$

$x \in \mathbb{R}^n$, where ψ is a complex-valued function in $L^2(\mathbb{R}^n)$ under the normalization condition

$$\|\psi\|_2 = 1, \tag{1.2}$$

$V : \mathbb{R}^n \to \mathbb{R}$ is the potential's function and $E \in \mathbb{R}$ is the minimum state energy. We will often use the notation $\rho_\psi(x) = |\psi(x)|^2$, which is interpreted as the probability density for finding the particle at x.

Next we define the kinetic T_ψ and the potential energy V_ψ as the following:

$$T_\psi = \int_{\mathbb{R}^n} |\nabla\psi(x)|^2 dx,$$
$$V_\psi = \int_{\mathbb{R}^n} V(x)|\psi(x)|^2 dx.$$

Our job consists in proving that (1.1), under suitable conditions, admits solutions. To achieve this, we try to minimize the total energy $\mathcal{E}(\psi)$ which we define as

$$\mathcal{E}(\psi) = T_\psi + V_\psi, \tag{1.3}$$

under the constrain (1.2).
We first prove that the ground state energy

$$E_0 := \inf\{\mathcal{E}(\psi) : \|\psi\|_2 = 1\}$$

exists, in the sense that it is finite and is a minimum; then that it is an eigenvalue for (1.1) associated with an eigenfunction ψ_0, which is called the ground state. To do this, we use the weak lower semicontinuity of $\mathcal{E}(\psi)$ and a minimizing sequence ψ^j to find the ψ_0 that provides the minimum. Next we prove that the minimizer is unique, and hence the uniqueness of the solution of (1.1) with $E = E_0$.

The natural space to consider will be H^1. We remind that $L^p(\mathbb{R}^n)$ is the set of Borel-measurable functions with finite p-norm,$1 \leq p < \infty$, i.e. $\left(\int_{\mathbb{R}^n} |f|^p\right)^{\frac{1}{p}} < \infty$ and $L^p_{Loc}(\mathbb{R}^n)$ is the set of Borel-measurable functions with finite p-norm on every compact set $K \subseteq \mathbb{R}^n$.

Definition 1 (Sobolev's Spaces $H^1(\mathbb{R}^n)$ and $D^1(\mathbb{R}^n)$)**.** *We define the Sobolev's Spaces $H^1(\mathbb{R}^n)$ and $D^1(\mathbb{R}^n)$ as:*

$$\begin{aligned} H^1(\mathbb{R}^n) =& \{f : \mathbb{R}^n \to \mathbb{C}, f \in L^2(\mathbb{R}^n) \text{ and } \nabla f \in L^2(\mathbb{R}^n)\} \\ D^1(\mathbb{R}^n) =& \{f : \mathbb{R}^n \to \mathbb{C}, f \in L^1_{Loc}(\mathbb{R}^n), \nabla f \in L^2(\mathbb{R}^n), \\ & \text{and } f \text{ vanishes at infinity}\} \end{aligned} \tag{1.4}$$

where ∇ refers to the distributional gradient, and f "vanishes at infinity" means that $\{x \in \mathbb{R}^n : |f(x)| > a\}$ has finite measure for all $a > 0$.

1.2 The ground state energy is finite

As we said earlier, the first step is to make sure that E_0 is bounded under suitable conditions. In this regard, our main tool will be Sobolev's inequalities.

Theorem 1 (Domination of the potential energy by the kinetic energy)**.** *If $\psi \in H^1(\mathbb{R}^n)$ and*

$$V \in \begin{cases} L^{n/2}(\mathbb{R}^n) + L^\infty(\mathbb{R}^n) & n \geq 3 \\ L^{1+\epsilon}(\mathbb{R}^2) + L^\infty(\mathbb{R}^2) & n = 2 \\ L^1(\mathbb{R}) + L^\infty(\mathbb{R}) & n = 1, \end{cases} \tag{1.5}$$

then E_0 is finite, and there exist some constants C and D such that

$$T_\psi \leq C\mathcal{E}(\psi) + D\|\psi\|_2^2. \tag{1.6}$$

Proof. To start, we need to verify that $\mathcal{E}(\psi)$ is well defined:

$$\mathcal{E}(\psi) = \int_{\mathbb{R}^n} |\nabla\psi(x)|^2 dx + \int_{\mathbb{R}^n} V(x)|\psi(x)|^2 dx.$$

The kinetic energy is defined for every function ψ in $H^1(\mathbb{R}^n)$ and, assuming that $V \in L^1_{loc}(\mathbb{R}^n)$, the second term is defined for every $\psi \in C^\infty_c(\mathbb{R}^n)$. We'll need to divide our inspection into three cases, based on the dimension of the space, for each of them we will utilize a different version of Sobolev's inequalities.

Case $n \geq 3$

Theorem 2 (Sobolev's inequality)**.** *For $n \geq 3$ let $f \in D^1(\mathbb{R}^n)$. Then $f \in L^q(\mathbb{R}^n)$ with $q = 2n/(n-2)$ and the following inequality holds:*

$$\|\nabla f\|_2^2 \geq S_n \|f\|_q^2, \tag{1.7}$$

where

$$S_n = \frac{n(n-2)}{4}|\mathbb{S}^n|^{\frac{2}{n}}.$$

For the proof see [LL].
Since we assume that $\psi \in H^1(\mathbb{R}^n)$, certainly $\psi \in D^1(\mathbb{R}^n)$ so we can use (1.7):

$$\begin{aligned} T_\psi = \|\nabla\psi\|_2^2 &\geq S_n \|\psi\|^2_{2n/(n-2)} \\ &= S_n \left(\int_{\mathbb{R}^n} |\psi(x)|^{2n(n-2)} \right)^{\frac{n-2}{n}} \\ &= S_n \|\rho_\psi\|_{\frac{n}{n-2}}. \end{aligned} \tag{1.8}$$

Using Hölder's inequality:

$$|V_\psi| = |(\psi, V\psi)| \leq \int_{\mathbb{R}^n} |V(x)|\psi(x)|^2| dx \leq \|\rho_\psi\|_{\frac{n}{n-2}} \|V(x)\|_{\frac{n}{2}}$$

and combining this result with (1.8)

$$T_\psi \geq \frac{S_n|(\psi, V\psi)|}{\|V\|_{\frac{n}{2}}} = \frac{S_n|V_\psi|}{\|V\|_{\frac{n}{2}}}. \tag{1.9}$$

If $\|V\|_{\frac{n}{2}} \leq S_n$ then

$$T_\psi \geq |V_\psi|,$$

which implies that

$$T_\psi + V_\psi \geq 0. \tag{1.10}$$

Now we need the following proposition:

Proposition 1. *For every* $v \in L^{\frac{n}{2}}(\mathbb{R}^n)$ *there is some constant* λ *such that* $h(x) := \min(v(x) - \lambda, 0)$ *satisfies:*

$$\|h\|_{\frac{n}{2}} \leq \frac{1}{2} S_n.$$

Proof. Let $v(x) = \sum_{i=1}^{\infty} c_i \chi_{A_i}$, without loss of generality we can assume that c_i are a monotone sequence and $c_i \geq 0$. Then by assumption we have

$$\sum_{i=1}^{\infty} c_i^{\frac{n}{2}} \chi_{A_i} < \infty.$$

Since $\lim_{k\to\infty} \sum_{i=k}^{\infty} c_i^{\frac{n}{2}} \chi_{A_i} = 0$ then for all ϵ exists $K \in \mathbb{N}$ such that $\sum_{i=K}^{\infty} c_i^{\frac{n}{2}} \chi_{A_i} < \epsilon$. Now if $\lambda = c_K$ we have

$$v(x) - \lambda = \sum_{i=1}^{\infty} c_i \chi_{A_i} - c_K$$

and so

$$\min(v(x) - \lambda, 0) = \sum_{i=K}^{\infty} (c_i - c_K) \chi_{A_i}.$$

We conclude that

$$\|h\|_{\frac{n}{2}} = \left(\sum_{i=K}^{\infty} (c_i - c_K)^{\frac{n}{2}} \mu(A_i) \right)^{\frac{2}{n}} \leq \left(\sum_{i=K}^{\infty} c_i^{\frac{n}{2}} \mu(A_i) \right)^{\frac{2}{n}} \leq \epsilon^{\frac{2}{n}}.$$

□

We can finally trace a lower bound on the ground state energy for V if it satisfies

$$V(x) = v(x) + w(x)$$

for some v $\in L^{\frac{n}{2}}(\mathbb{R}^n)$ and $w \in L^{\infty}(\mathbb{R}^n)$.
Recalling (1.10) with $V = h$

$$T_\psi \geq \frac{S_n |(\psi, h\psi)|}{\|h\|_{\frac{n}{2}}} \geq 2|(\psi, h\psi)| = 2|h_\psi|$$

as before we obtain

$$T_\psi + 2h_\psi \geq 0. \tag{1.11}$$

Concluding, an application of (1.3) and (1.11) provides

$$\begin{aligned}\mathcal{E}(\psi) &= T_\psi + V_\psi = T_\psi + (\psi, (v + w + \lambda - \lambda)\psi) \\ &= T_\psi + (\psi, (v-\lambda)\psi) + \lambda\|\psi\|^2 + (\psi, w\psi) \\ &= T_\psi + (v-\lambda)_\psi + \lambda + w_\psi \\ &\geq T_\psi + h_\psi + \lambda + w_\psi \geq \frac{1}{2}T_\psi + \lambda - \|w\|_\infty.\end{aligned}$$

So we see that $\mathcal{E}(\psi)$ is bounded from below by $\lambda - \|w\|_\infty$; we can also draw another conclusion: the total energy bounds the kinetic energy

$$T_\psi \leq 2(\mathcal{E}(\psi) - \lambda + \|w\|_\infty). \tag{1.12}$$

Case $n = 2$

Theorem 3 (Sobolev's inequality)**.** *For $f \in H^1(\mathbb{R}^2)$ the inequality*

$$\|\nabla f\|_2^2 + \|f\|_2^2 \geq S_{2,q}\|f\|_q^2 \tag{1.13}$$

holds for all $2 \leq q < \infty$ with a constant that satisfies

$$S_{2,q} > \left(q^{1-\frac{2}{q}}(q-1)^{-1+\frac{1}{q}}\left(\frac{q-2}{8\pi}\right)^{\frac{1}{2}-\frac{1}{q}}\right)^{-2}.$$

As we did in the previous case, $f \in H^1(\mathbb{R}^2)$ and so we can use (1.13)

$$T_\psi + \|\psi\|_2^2 \geq S_{2,p}\|\rho_\psi\|_p$$

and by Hölder's inequality

$$T_\psi + \|\psi\|_2^2 \geq \frac{S_{2,p}(\psi, V\psi)}{\|V\|_{\frac{p}{p-1}}}.$$

Repeating the same process we consider $V = v + w$ with $v \in L^{\frac{p}{p-1}}$ and $w \in L^\infty$. For $\|V\|_{\frac{p}{p-1}} \leq S_{2,p}$ we have

$$T_\psi + \|\psi\|_2^2 \geq V_\psi.$$

As before we define $h = \min(v(x) - \lambda, 0)$ and we choose λ such that $\|h\|_{\frac{p}{p-1}} < S_{2,p}$, which implies:

$$\begin{aligned}h_\psi &\geq -\frac{1}{2}T_\psi - \|\psi\|_2^2 \\ \mathcal{E}(\psi) = T_\psi + V_\lambda &\geq \frac{1}{2}T_\psi + \lambda - \|w\|_\infty - \|\psi\|_2^2.\end{aligned}$$

Since this is true for every $p \geq 2$ we'll say that it's true for every $V \in L^{1+\epsilon}(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$.

Case $n = 1$

Theorem 4 (Sobolev's inequality)**.** *Any $f \in H^1(\mathbb{R})$ is bounded and satisfies the estimate*

$$\left\|\frac{df}{dx}\right\|_2^2 + \|f\|_2^2 \geq 2\|f\|_\infty^2 \tag{1.14}$$

with equality if and only if is a multiple of $e^{-|x-a|}$ for some $a \in \mathbb{R}$. Moreover, f is equivalent to a continous function that satisfies the estimate

$$|f(x) - f(y)| \leq \left\|\frac{df}{dx}\right\|_2 |x-y|^{\frac{1}{2}}.$$

Similarly, $f \in H^1(\mathbb{R})$ so we can use the (1.14)

$$T_\psi + \|\psi\|_2^2 \geq S_1\|\rho_\psi\|_\infty,$$

by using Hölder's inequality and defining h as before with $\|h\|_1 \leq S_1$ we can conclude that

$$\mathcal{E}(\psi) = T_\psi + V_\lambda \geq \frac{1}{2}T_\psi + \lambda - \|w\|_\infty - \|\psi\|_2^2$$

which holds for every $V \in L^1(\mathbb{R}) + L^\infty(\mathbb{R})$. □

1.3 Existence of a minimizer for E_0

In this section, we prove that the minimizer for $\mathcal{E}(\psi)$ exists and satisfies (1.1). To achieve this we first need to prove that V is weakly continous and that $\mathcal{E}$ is weakly lower semicontinous.

Theorem 5. *Let $V(x)$ be a function that satisfies* (1.5) *and assume that it vanishes at infinity. Assume also that*

$$E_0 = \inf\{\mathcal{E}(\psi) : \psi \in H^1(\mathbb{R}^n), \|\psi\|_2 = 1\} < 0. \tag{1.15}$$

Then there is a function $\psi_0 \in H^1(\mathbb{R}^n)$ such that $\|\psi_0\|_2 = 1$,

$$\mathcal{E}(\psi_0) = E_0$$

and it satisfies

$$-\Delta\psi_0 + V\psi_0 = E_0\psi_0. \tag{1.16}$$

Furthermore, every minimizer ψ_0 satisfies (1.16) *in the sense of distribution.*

Remark 1. *The total energy we defined in* (1.3) *can also be obtained from the Schrödinger equation* (1.1) *by testing it with a sequence $\psi^j \in C_0^\infty(\mathbb{R}^n)$ that converges to ψ:*

$$\begin{aligned}\lim_{j\to\infty}(\psi^j, -\Delta\psi + V\psi) &= \lim_{j\to\infty}\left(\int_{\mathbb{R}^n}(-\Delta\psi)\overline{\psi^j} + \int_{\mathbb{R}^n}V\overline{\psi^j}\psi\right)\\ &= \lim_{j\to\infty}\left(\int_{\mathbb{R}^n}\overline{(\nabla\psi^j)}\nabla\psi + \int_{\mathbb{R}^n}V\overline{\psi^j}\psi\right) = T_\psi + V_\psi\\ &= \lim_{j\to\infty}E(\psi,\psi^j) = E\|\psi\|_2^2,\end{aligned}$$

hence

$$\mathcal{E}(\psi) = E\|\psi\|_2^2. \tag{1.17}$$

In general, if f ψ satisfies (1.1) *with E as the eigenvalue associated with the Schrödinger equation, we have that $E \geq E_0$, with equality if and only if ψ is a minimizer, hence, for a generic function $\widetilde{\psi}$:*

$$\mathcal{E}(\widetilde{\psi}) \geq E_0\|\widetilde{\psi}\|_2 \tag{1.18}$$

1.3.1 Weak continuity of the potential

In this section, we prove that the potential is weakly continuous, to do that we need the following theorem; for the proof see [LL].

Theorem 6 (Weak convergence implies strong convergence on small sets)**.** *Let f^j be a sequence in $D^1(\mathbb{R}^n)$ such that ∇f^j converges weakly in $L^2(\mathbb{R}^n)$ to some vector-valued function $v \in L^2(\mathbb{R}^n)$. If n=1,2 we also assume that f^j converges weakly in $L^2(\mathbb{R}^n)$. Then $v = \nabla f$ for some unique function $f \in D^1(\mathbb{R}^n)$.*
Now let $A \subset \mathbb{R}^n$ be any set of finite measure and let χ_A be its characteristic function. Then

$$\chi_A f^j \to \chi_A f \text{ in } L^r(\mathbb{R}^n) \tag{1.19}$$

for every $r < \frac{2n}{n-2}$ when $n \geq 3$, every $p < \infty$ when n=2 and every $p \leq \infty$ when n=1.

Theorem 7 (Weak continuity of the potential)**.** *Let $V(x)$ be a function on $\mathbb{R}^n$ that satisfies* (1.5)*. Assume, in addition, that V(x) vanishes at infinity. Then V_ψ is weakly continuous in $H^1(\mathbb{R}^n)$ i.e if $\psi^j \rightharpoonup \psi$ as $j \to \infty$, weakly in $H^1(\mathbb{R}^n)$, then $V_{\psi^j} \to V_\psi$ as $j \to \infty$.*

Proof. Assuming that $\psi^j \rightharpoonup \psi$ in $H^1(\mathbb{R}^n)$ we have that $L(\psi^j)$ converges for every $L \in H^{1*}(\mathbb{R}^n)$, and hence it is bounded; a direct application of Banach-Steinhaus leads to:

$$\|\psi^j\|_{H^1} \leq C \tag{1.20}$$

for some constant $0 \leq C \geq 0$ that does not depend of j.
Next we define V^δ by:

$$V^\delta = \begin{cases} V(x) & \text{if } |V(x)| \leq \frac{1}{\delta} \\ 0 & \text{if } |V(x)| \geq \frac{1}{\delta}. \end{cases} \tag{1.21}$$

We notice that $V - V^\delta$ tends to zero pointwise as $\delta \to 0$, and, because of (1.5), $V \in L^p(\mathbb{R}^n)$ for a suitable $p \geq 1$. So by dominated convergence $V - V^\delta$ tends to zero in that same $L^p(\mathbb{R}^n)$ norm.
Also, because of (1.20) we have that $\psi^j \in D^1(\mathbb{R}^n)$ and so we can apply the Sobolev's inequality (1.7)(or, if $n = 2, 1$ respectively (1.13) or (1.14)) and find again:

$$C \geq \frac{S_n(\psi^j, (V - V^\delta)\psi^j)}{\|V - V^\delta\|_p},$$

which implies

$$\int_{\mathbb{R}^n} (V - V^\delta)|\psi^j|^2 < \frac{C\|V - V^\delta\|_p}{S_n} \to 0.$$

Thus, to prove that $V_{\psi^j} \to V_\psi$ as $j \to \infty$ we only need to prove that $V^\delta_{\psi^j} \to V^\delta_\psi$ as $j \to \infty$ for each $\delta > 0$.
To achieve this we prove that for every subsequence of $V^\delta_{\psi^j}$ there is a sub-subsequence that converges to V^δ_ψ. We begin by defining

$$A_\epsilon = \{x : |V^\delta(x)| > \epsilon\}$$

for $\epsilon > 0$, and by splitting the integral into two parts:

$$V^\delta_{\psi^j} = \int_{A_\epsilon} V^\delta|\psi^j|^2 + \int_{A^c_\epsilon} V^\delta|\psi^j|^2. \tag{1.22}$$

We notice that

$$\int_{A^c_\epsilon} V^\delta|\psi^j|^2 \leq \int_{\mathbb{R}^n} \epsilon|\psi^j|^2 = \epsilon,$$

and that A_ϵ has finite measure for all ϵ, since V vanishes at infinity by assumption.
To prove that the first term in (1.22) converges to $\int_{A^c_\epsilon} V|\psi^2|$ we can use Theorem 6. In this case we have that $\|\psi^j\|_{H^1(\mathbb{R}^n)}$ is bounded, so every subsequence

ψ^{j^k} is certainly bounded in norm in $H^1(\mathbb{R}^n)$, in particular $\|\nabla\psi^{j^k}\|_{L^2(\mathbb{R}^n)}$ is bounded; since $L^2(\mathbb{R}^n)$ is a reflexive space we know that $\nabla\psi^{j^k}$ admits a weakly convergent subsequence $\nabla\psi^{j^{k^w}} \rightharpoonup v$. By using (1.21) we have that $\psi^{j^{k^w}} \to \psi$ strongly for $w \to \infty$ in $L^r(A_\epsilon)$.

We then notice that $\psi^{j^{k^w}} \to \psi$ strongly for $w \to \infty$ in $L^r(A_\epsilon)$ implies that $|\psi^{j^{k^w}}|^2 \to |\psi|^2$ strongly for $w \to \infty$ in $L^{\frac{r}{2}}(A_\epsilon)$. This can be proven by noticing that $\psi^{j^{k^w}}$ converges to ψ in $L^{\frac{r}{2}}(A_\epsilon)$ and that:

$$\int_{A_\epsilon} ||\psi^{j^{k^w}}|^2 - |\psi|^2|^{\frac{r}{2}} \leq \int_{A_\epsilon} |\psi^{j^{k^w}} - \psi|^{\frac{r}{2}}|\psi^{j^{k^w}} + \psi|^{\frac{r}{2}} \to 0.$$

Since $V^\delta \in L^\infty(\mathbb{R}^n)$ and A_ϵ has finite measure, then $V^\delta \in L^s(A_\epsilon)$ for every $s \geq 1$. So we take s such that $\frac{1}{s} + \frac{2}{r} = 1$ and we can conclude using Hölder's inequality:

$$\int_{A_\epsilon} V^\delta(\left|\psi^{j^{k^w}}\right|^2 - |\psi|^2) \leq \|V^\delta\|_{L^s(A_\epsilon)}\| \left|\psi^{j^{k^w}}\right|^2 - |\psi|^2 \|_{L^{\frac{r}{2}}(A_\epsilon)} \to 0 \qquad (1.23)$$

□

As we stated before, to prove theorem 5 we need to take a minimizing sequence, and, thanks to the weak lower semicontinuity of the energy, prove that its weak limit is a suitable minimizer. We then enounce and prove this last technical result.

Theorem 8 (Weak lower semicontinuity of the energy)**.** *Let V(x) be a function on $\mathbb{R}^n$ satisfying* (1.5)*. Assume, in addition, that V(x) vanishes at infinity, then $\mathcal{E}(\psi)$ is weakly lower semicontinous.*

Proof. We start by observing that T_ψ is weakly lower semicontinous, we can prove it by taking a function $\phi \in H^1(\mathbb{R}^n)$ such that $\|\nabla\phi\|_2 = 1$ and by noticing that:

$$\begin{aligned}(\nabla\psi, \nabla\phi) &= \liminf_{j\to\infty}(\nabla\psi^j, \nabla\phi) = \liminf_{j\to\infty} \int_{\mathbb{R}^n} \overline{\nabla\psi^j}\nabla\phi dx \\ &\leq \liminf_{j\to\infty} \|\nabla\psi^j\|_2\|\nabla\phi\|_2 \leq \liminf_{j\to\infty} \|\nabla\psi^j\|_2.\end{aligned}$$

Since the last term does not depend on ϕ and because $\|\nabla\psi\|_2 = \sup_{\|\nabla\phi\|=1} (\nabla\psi, \nabla\phi)$ we can conclude that

$$\left(\int_{\mathbb{R}^n} |\nabla\psi|^2 dx\right)^{\frac{1}{2}} = \sup_{\|\nabla\phi\|=1} (\nabla\psi, \nabla\phi) \leq \liminf_{j\to\infty} \left(\int_{\mathbb{R}^n} |\nabla\psi^j|^2 dx\right)^{\frac{1}{2}}.$$

We proved in Theorem 7 that V_ψ is weakly continous, so $\mathcal{E}(\psi) = T_\psi + V_\psi$ is weakly lower semicontinous in $H^1(\mathbb{R}^n)$. □

We finally have all the elements to prove Theorem 5.

Proof of Theorem 5. We begin by taking a minimizing sequence ψ^j such that $\mathcal{E}(\psi^j) \to E_0$ as $j \to \infty$ and $\|\psi^j\|_2 = 1$. Then we note that for (1.6) $\|\nabla\psi^j\|_2$ is bounded by a constant independent of j, and $\|\psi^j\|_2 = 1$, and so $\psi^j \in H^1(\mathbb{R}^n)$.

We also know that $H^1(\mathbb{R}^n)$ is weakly sequentially compact, i.e. every bounded sequence admits a weakly converging subsequence. In our case ψ^j is bounded in $H^1(\mathbb{R}^n)$ so there is a subsequence ψ^{j^k} such that $\psi^{j^k} \rightharpoonup \psi_0$ in $H^1(\mathbb{R}^n)$, this also implies that

$$\|\psi_0\|_2 \leq \|\psi^{j^k}\|_2 = 1.$$

Notice that because of Theorem 8 we have

$$E_0 = \lim_{k\to\infty} \mathcal{E}(\psi^{j^k}) \geq \mathcal{E}(\psi_0).$$

Because of (1.18) we have:

$$0 > E_0 \geq \mathcal{E}(\psi_0) \geq E_0\|\psi_0\|_2^2.$$

By (1.15) it follows that $\|\psi_0\|_2 = 1$ and that $E_0 = \mathcal{E}(\psi_0)$, proving the existence of a minimizer for $\mathcal{E}(\psi)$.

We now have to prove that every minimizer ψ_0 satisfies (1.16) in the sense of distribution. To start we take a function $f \in C_c^\infty(\mathbb{R}^n)$ and we set $\psi^\epsilon := \psi_0 + \epsilon f$ for $\epsilon \in \mathbb{R}$. Then we define $R(\epsilon) = \dfrac{\mathcal{E}(\psi^\epsilon)}{(\psi^\epsilon, \psi^\epsilon)}$ and note that it is the ratio of two polynomials of degree two, and hence differentiable for small ϵ. We also note that, because $\mathcal{E}(\psi)$ contains the restraint $\|\psi\|_2 = 1$, by defining $R(\epsilon)$ in this way we are basically avoiding the restraint on the norm. On the other hand, $R(\epsilon)$ still maintains the fundamental properties of $\mathcal{E}(\psi)$, which are to have E_0 as a minimum, and to reach it in $\epsilon = 0$. This manipulation is well defined because both $\mathcal{E}(\psi)$ and (ψ, ψ) are quadratic forms. This implies that $\left.\dfrac{dR(\epsilon)}{d\epsilon}\right|_{\epsilon=0} = 0$ and so

$$\begin{aligned}\frac{dR(\epsilon)}{d\epsilon} &= \frac{d\mathcal{E}(\psi^\epsilon)}{d\epsilon}\frac{1}{(\psi^\epsilon, \psi^\epsilon)} + \mathcal{E}(\psi^\epsilon)\frac{d}{d\epsilon(\psi^\epsilon, \psi^\epsilon)} \\ &= \frac{d\mathcal{E}(\psi^\epsilon)}{d\epsilon} - \frac{\mathcal{E}(\psi^\epsilon)}{(\psi^\epsilon, \psi^\epsilon)}\frac{d(\psi^\epsilon, \psi^\epsilon)}{d\epsilon},\end{aligned}$$

which leads, when $\epsilon = 0$ to

$$\left.\frac{d\mathcal{E}(\psi^\epsilon)}{d\epsilon}\right|_{\epsilon=0} = E_0 \left.\frac{d(\psi^\epsilon, \psi^\epsilon)}{d\epsilon}\right|_{\epsilon=0}.$$

In conclusion we have that

$$\begin{aligned}\frac{d}{d\epsilon}\left(\psi^\epsilon, (-\Delta + V)\psi^\epsilon\right)|_{\epsilon=0} &= \left(\frac{d\psi^\epsilon}{d\epsilon}, (-\Delta + V)\psi^\epsilon\right)|_{\epsilon=0} = (f, (-\Delta + V)\psi_0) \\ &= E_0 \left.\frac{d(\psi^\epsilon, \psi^\epsilon)}{d\epsilon}\right|_{\epsilon=0} = E_0(f, \psi_0),\end{aligned}$$

for every $f \in C_c^\infty(\mathbb{R}^n)$, proving that ψ_0 satisfies (1.16). □

Chapter 2

Uniqueness of the ground state

In the first section of this chapter, we provide an extension to Theorem 5, proving that there exist many more eigenvalues E_k and corresponding eigenfunctions ψ_k that satisfy the Schrödinger equation. In the second section, we prove that ψ_0 can be chosen to be a strictly positive function, and that is the unique minimizer up to a constant phase. In the third and last section, we apply our previous results on the potential of an hydrogen atom.

2.1 Higher eigenvalues

We now extend Theorem 5 in the following manner. In the last chapter we found that if the ground state energy is negative, then there exists an eigenfunction ψ_0 that provides the minimum and satisfy the Schrödinger equation. We now prove that, if the first excited state E_1, defined as

$$E_1 := \inf\{\mathcal{E}(\psi) : \psi \in H^1(\mathbb{R}^n), \|\psi\|_2 = 1 \text{ and } (\psi, \psi_0) = 0\},$$

is negative, then there exists a second eigenfunction ψ_1 that satisfies (1.1) and provides the minimum. In the same fashion we define by recursion the succession

$$E_k := \inf\{\mathcal{E}(\psi) : \psi \in H^1(\mathbb{R}^n), \|\psi\|_2 = 1 \text{ and } (\psi, \psi_i) = 0, i = 0, ..., k-1\}.$$

and prove that, as long as the first n eigenvalues exist and the $(n+1)^{th}$ is negative, then its corresponding eigenfunction exists and satisfies the Schrödinger equation in the sense of distribution.

To prove that ψ_k satisfies (1.1) we need an additional result about distribution.

Theorem 9 (Linear dependence of distributions)**.** *Let $S_1, ..S_N \in D'(\Omega)$ be distribution. Suppose that $T \in D'(\Omega)$ has the property that $T(\phi) = 0$ for all $\phi \in \bigcap_{i=1}^N N_{S_i}$.*
Then there exist complex numbers $c_1, ..c_N$ such that

$$T = \sum_{i=1}^{N} c_i S_i.$$

For the proof see [LL]. Now we can enounce and prove the last theorem about the existence of solutions for the Schrödinger equation.

Theorem 10 (Higher eigenvalues)**.** *Let V as in Theorem 5, assume the first k eigenvalues defined above exist and that E_k is negative. Then E_k exists in the sense that is a minimum, and also his eigenfunction ψ_k satisfies the Schrödinger equation*

$$(-\Delta + V)\psi_k = E_k \psi_k \tag{2.1}$$

in the sense of distribution. Furthermore, every eigenvalue E_k has finite algebraic multiplicity.

Proof. We first prove that E_k exists, i.e., there exists a minimizer $\psi_k \in H^1(\mathbb{R}^n)$ such that $\|\psi_k\|_2 = 1$ and $\mathcal{E}(\psi_k) = E_k$. To achieve this, we take a minimizing sequence ψ_k^j such that $(\psi_k^j, \psi_i) = 0$ for all $i < k$ and $\mathcal{E}(\psi_k^j) \to E_k$. As we did in the first chapter, we extract a weakly converging subsequence, and we call its weak limit ψ_k; repeating the same argument we prove that $\|\psi_k^j\|_2 = 1$ and $\mathcal{E}(\psi_k) = E_k$. Moreover, we have that

$$0 = \lim_{j\to\infty} (\psi_k^j, \psi_i) = (\psi_k, \psi_i) \text{ for all } i < k,$$

proving the existence of E_k.

To prove that ψ_k satisfies (2.1), we first notice that, as in Theorem 5, for every $f \in C_c^\infty(\mathbb{R}^n)$ with the property that $(f, \psi_i) = 0, i < k$, we have that

$$(f, (-\Delta + V)\psi_k) = E_k(f, \psi_k);$$

hence the distribution $D := (-\Delta + V - E_k)\psi_k$ satisfies D(f)=0 for every $f \in C_c^\infty(\mathbb{R}^n)$. We can now use Theorem 9 to find that

$$D = \sum_{i=0}^{k-1} c_i \psi_i \tag{2.2}$$

for suitable numbers $c_0, ...c_{k-1}$. To prove that ψ_k satisfies (2.1), we need to prove that $D \equiv 0$. To achieve this we test (2.2) with a function $f_n \in C_c^\infty(\mathbb{R}^n)$ that converges weakly to some ψ_j with $j < k$:

$$\begin{aligned}
\lim_{n\to\infty} D(f_n) &= \int_{\mathbb{R}^n} \sum_{i=0}^{k-1} c_i \overline{\psi_j} \psi_i = \sum_{i=0}^{k-1} c_i \delta_i^j = c_j \\
&= (\psi_j, (-\Delta + V - E_k)\psi_k) = \int_{\mathbb{R}^n} (-\Delta\psi_k + V\psi_k - E_k\psi_k)\overline{\psi_j} \\
&= \int_{\mathbb{R}^n} \overline{\nabla\psi_j} \cdot \nabla\psi_k + V\overline{\psi_j}\psi_k - E_k\overline{\psi_j}\psi_k \\
&= \int_{\mathbb{R}^n} \overline{\nabla\psi_j} \cdot \nabla\psi_k + V\overline{\psi_j}\psi_k.
\end{aligned} \tag{2.3}$$

On the other hand, if we take the complex conjugate of (2.1) for ψ_j and again test it with a function $f_n \in C_c^\infty(\mathbb{R}^n)$ that converges weakly to $\overline{\psi_k}$, we obtain:

$$\begin{aligned}
0 &= \lim_{n\to\infty}((-\Delta + V + E_k)\overline{\psi_j})(f_n) = (\overline{\psi_k}, (-\Delta + V - E_k)\overline{\psi_j}) \\
&= \int_{\mathbb{R}^n} (-\overline{\Delta\psi_j} + V\overline{\psi_j} - E_k\overline{\psi_j})\psi_k = \int_{\mathbb{R}^n} \overline{\nabla\psi_j} \cdot \nabla\psi_k + V\overline{\psi_j}\psi_k - E_k\overline{\psi_j}\psi_k \\
&= \int_{\mathbb{R}^n} \overline{\nabla\psi_j} \cdot \nabla\psi_k + V\overline{\psi_j}\psi_k.
\end{aligned} \tag{2.4}$$

In conclusion, we have that $c_j = 0$ for all j, proving the first part of Theorem 10.

We now need to prove that E_k has finite multiplicity. We start by assuming that E_k has infinite multiplicity, this would imply that $E_k = E_{k+1} = E_{k+2} = ... < 0$: we want to prove that $E_k \geq 0$.
By Theorem 10 there is an orthonormal sequence ψ_j satisfying (2.1), and, since the succession is orthogonal, it converges weakly to zero in $L^2(\mathbb{R}^n)$. For (1.12) we have that $\|\nabla\psi_j\|_2$ is bounded, and so by Theorem 6 $\psi_j \rightharpoonup 0$ in $H^1(\mathbb{R}^n)$. In Theorem 7 we proved that the potential is weakly continuous, and so $V_{\psi_j} \to 0$. In conclusion we have that

$$E_k = \lim_{j\to\infty} T_{\psi_j} + V_{\psi_j} \geq 0,$$

which is a contradiction. □

2.2 Uniqueness of minimizers

In this section we prove that ψ_0 can be chosen to be a strictly positive function and that ψ_0 is the unique minimizer up to a constant phase. To achieve this, we first prove, using the convexity inequality for gradients, that the real and the imaginary part of the eigenfunction are proportional. Next, we use the Theorem "Lower bounds on Schrödinger's "wave" functions" to prove that they can be chosen as strictly positive. We then state these two theorems, for the proofs see [LL].

Theorem 11 (Convexity inequality for gradients)**.** *Let f be a complex-valued function in $H^1(\mathbb{R}^n)$. Then*

$$\int_{\mathbb{R}^n} |\nabla |f|(x)|^2 \, dx \leq \int_{\mathbb{R}^n} |\nabla f(x)|^2 \, dx.$$

If, moreover, $\Re(f)(x) > 0$ or $\Im(f)(x) > 0$, then equality holds if and only if there exists a constant c such that $\Re(f) = c\Im(f)$ almost everywhere.

Theorem 12 (Lower bounds on Schrödinger's "wave" functions)**.** *Let $W : \mathbb{R}^n \to \mathbb{R}$ be a measurable function, bounded from above. Suppose that $f : \mathbb{R}^n \to [0, \infty[$ is in $L^1_{Loc}(\mathbb{R})$, Wf is in $L^1_{Loc}(\mathbb{R})$ too and that*

$$-\Delta f + Wf \geq 0 \text{ in } D'(\mathbb{R}) \tag{2.5}$$

is satisfied. Then there is a unique lower semicontinous $\widetilde{f}$ that satisfies (2.5) *and agrees with f almost everywhere. $\widetilde{f}$ has the following property: for each compact set $K \subset \Omega$ there is a constant $C = C(K, \Omega, \mu)$ such that*

$$\widetilde{f}(x) \geq C \int_K f(y) dy$$

for each $x \in K$.

We can finally state the main result of this thesis: proving the uniqueness of the minimizer, we will be able to prove the uniqueness of the solution.

Theorem 13 (Uniqueness of minimizers)**.** *Assume that E_0 exists, in the sense that is finite and there exists a function ψ_0 such that $\mathcal{E}(\psi_0) = E_0$ and $\|\psi_0\|_2 = 1$. Assume also that $V \in L^1_{Loc}(\mathbb{R}^n)$, V is locally bounded from above and that $V|\psi_0|^2$ is summable. Then ψ_0 satisfies* (1.1) *with $E = E_0$. Furthermore ψ_0 can be chosen to be a strictly positive function and is the unique minimizer up to a constant phase.*

Proof. By assumption we have that $V|\psi_0|^2$ is summable, i.e,

$$\int_{\mathbb{R}^n} |V(x)||\psi_0(x)|^2 dx$$

is finite. Since $V\psi_0$ is both a function and a distribution, we also have that $(\phi, V\psi_0)$ is finite for all $\phi \in C_c^\infty(\mathbb{R}^n)$. Then, by (1.18), we have that

$$\mathcal{E}(\psi_0 + \epsilon\phi) \geq E_0 \|\psi_0 + \epsilon\phi\|_2^2,$$

hence

$$\begin{aligned}
\mathcal{E}(\psi_0 + \epsilon\phi) &= (\psi_0 + \epsilon\phi, (-\Delta + V)(\psi_0 + \epsilon\phi)) \\
&= \mathcal{E}(\psi_0) + \epsilon \int_{\mathbb{R}^n} [\nabla\psi_0 \overline{\nabla\phi} + V\psi_0\overline{\phi}] \\
&+ \epsilon \int_{\mathbb{R}^n} [\overline{\nabla\psi_0}\nabla\phi + V\overline{\psi_0}\phi] + \epsilon^2 \int_{\mathbb{R}^n} [|\nabla\phi|^2 + V|\phi|^2] \\
&= \mathcal{E}(\psi_0) + 2\epsilon\Re\left\{\int_{\mathbb{R}^n} [\nabla\psi_0\overline{\nabla\phi} + V\psi_0\overline{\phi}]\right\} \\
&+ \epsilon^2 \int_{\mathbb{R}^n} [|\nabla\phi|^2 + V|\phi|^2] \\
&\geq -(E_0 + 2\epsilon\Re\left\{\int_{\mathbb{R}^n} E_0\psi_0\overline{\phi}\right\} + \epsilon^2 \int_{\mathbb{R}^n} E_0|\psi|^2).
\end{aligned}$$

Every term is finite and so, since ψ_0 is a minimizer by assumption, we have that:

$$2\epsilon\Re\left\{\int_{\mathbb{R}^n} [\nabla\psi_0\overline{\nabla\phi} + (V - E_0)\psi_0\overline{\phi}]\right\} + \epsilon^2 \int_{\mathbb{R}^n} [|\nabla\phi|^2 + (V - E_0)|\phi|^2] \geq 0.$$

Since ϵ can be chosen arbitrarily, in particular it can have any sign, we conclude that the first term must be zero; this implies that:

$$((-\Delta + V - E_0)\psi_0)(\phi) = 0 \tag{2.6}$$

for all $\phi \in C_c^\infty(\mathbb{R}^n)$, hence

$$(-\Delta + V - E_0)\psi_0 = 0 \text{ in } D'(\mathbb{R}^n). \tag{2.7}$$

Next, we want to prove that ψ_0 can be chosen to be a strictly positive function. To achieve this we start by noticing that if $\psi_0 = f + ig$, then both f and g are separately minimizers. This can be proven by taking

$$\mathcal{E}(\psi_0) = \int_{\mathbb{R}^n} |\nabla f + i\nabla g|^2 + V(f + ig)^2 = \int_{\mathbb{R}^n} (|\nabla f|^2 + |\nabla g|^2) + V(|f|^2 + |g|^2),$$

which is equal, up to a normalizing constant, to $\mathcal{E}(f) + \mathcal{E}(g)$.

Then we remind that, if $f \in H^1(\mathbb{R}^n)$ then $|f| \in H^1(\mathbb{R}^n)$ and

$$(\nabla|f|) = \begin{cases} \frac{\Re(x)\nabla\Re(x)+\Im(x)\nabla\Im(x)}{|f|(x)} & \text{if } f(x) \neq 0 \\ 0 & \text{if } f(x) = 0; \end{cases} \tag{2.8}$$

furthermore, if f is real-valued, then $|\nabla|f|| = |\nabla f|$. For this reason, since f and g are both real-valued, we obtain $T_f = T_{|f|}$ and $T_g = T_{|g|}$ and consequently $\mathcal{E}(f) = \mathcal{E}(|f|)$ and $\mathcal{E}(g) = \mathcal{E}(|g|)$, hence $\phi_0 := |f|+i|g|$ is a minimizer. Thanks to Theorem 11 we have that

$$E_0 \leq \mathcal{E}(|\phi_0|) \leq \mathcal{E}(\phi_0) = E_0,$$

and so $|\phi_0|$ is a minimizer too.

We proved in Theorem 5 that every minimizer satisfies the distributional Schrödinger equation, so both $|f|$ and $|g|$ satisfies (2.7); moreover we have that V is locally bounded by assumption, and consequently so is $W := V - E_0$. We can then apply Theorem 12 and find two strictly positive semicontinous functions $\widetilde{f}$ and $\widetilde{g}$, which agree almost always respectively with $|f|$ and $|g|$.

Now we define $\widetilde{\phi_0} := \widetilde{f} + i\widetilde{g}$ and apply again Theorem 11 to find

$$E_0 \leq \mathcal{E}(\widetilde{\phi_0}) \leq \mathcal{E}(\phi_0) = E_0.$$

Since there is equality and both $\widetilde{f}$ and $\widetilde{g}$ are strictly positive, Theorem 11 states that there must be some constant $c > 0$ such that $\widetilde{f} = c\widetilde{g}$, and hence there exists a constant $d \in \mathbb{R}$ that satisfies $f = dg$, i.e, $\psi_0 = (1 + id)f$. □

2.3 Uniqueness of positive solutions

In the last section we proved that, under suitable assumptions, the minimizer for $\mathcal{E}(\psi)$ is unique and satisfies the Schrödinger equation with $E = E_0$. Now we prove that the positive solution of the Schrödinger equation satisfies it with $E = E_0$, and that it is the unique minimizer of $\mathcal{E}$. We remind the following result about partial integration of functions in $H^1(\mathbb{R}^n)$, the proof can be found in [LL].

Theorem 14 (Partial integration for functions in $H^1(\mathbb{R}^n)$)**.** *Let u and v be in $H^1(\mathbb{R}^n)$. Then*

$$\int_{\mathbb{R}^n} u\frac{\partial v}{\partial x_i}dx = -\int_{\mathbb{R}^n} \frac{\partial u}{\partial x_i}vdx$$

for $i = 1, ...n$.

Suppose in addition, that Δv can be written as $\Delta v = f + g$ with $f \geq 0$ in

$L^1_{Loc}(\mathbb{R}^n)$ and with g in $L^2(\mathbb{R}^n)$, then $u\Delta v \in L^1(\mathbb{R}^n)$ for all u in $H^1(\mathbb{R}^n)$, furthermore we have that

$$-\int_{\mathbb{R}^n} u\Delta v = \int_{\mathbb{R}^n} \nabla v \cdot \nabla u. \tag{2.9}$$

The fact that the uniqueness of the minimizer imply the uniqueness of the solution is not obvious, and is proved in the following theorem.

Theorem 15 (Uniqueness of positive solutions)**.** *Suppose that V is in $L^1_{Loc}(\mathbb{R}^n)$, V is bounded above (uniformly and not just locally) and that $E_0 > -\infty$. Let $\psi \neq 0$ be any non negative function with $\|\psi\|_2 = 1$ that is in $H^1(\mathbb{R}^n)$ and satisfies the Schrödinger equation* (1.16) *in $D'(\mathbb{R}^n)$. Then $E = E_0$ and ψ is the unique minimizer ψ_0.*

Proof. We first need to prove that $E = E_0$. To achieve this we first prove that, if $E \neq E_0$, then $(\psi, \psi_0) = 0$, which would be impossible since ψ_0 is strictly positive and ψ is nonnegative. Next we note that, since ψ satisfies the Schrödinger equation by assumption, we have that $\Delta\psi$ is a function, and hence in $L^1_{Loc}(\mathbb{R}^n)$. Furthermore, since ψ is nonnegative and V is bounded from above, we can conclude that $\Delta\psi$ is the sum of a nonnegative $L^1_{Loc}(\mathbb{R}^n)$ function with a $L^2(\mathbb{R}^n)$ function.
Now, we take the Schrödinger equation for ψ_0, multiply it by ψ and integrate over $\mathbb{R}^n$ obtaining

$$\int_{\mathbb{R}^n} -\Delta\psi_0\psi + \int_{\mathbb{R}^n} (V - E_0)\psi\psi_0 = 0,$$

hence, thanks to Theorem 14, we can conclude that

$$\int_{\mathbb{R}^n} \nabla\psi_0 \cdot \nabla\psi + \int_{\mathbb{R}^n} (V - E_0)\psi\psi_0 = 0. \tag{2.10}$$

We can repeat the same process interchanging ψ and ψ_0, obtaining (2.10) with E_0 replaced by E. Since $E \neq E_0$ by assumption, we must have that ψ is orthogonal to ψ_0, which is impossible.

□

2.3.1 The hydrogen atom

We can finally exhibit a practical application of these last results. However, to say something about the regularity of the solutions, we need a last result, its proof can be found in [LL].

Theorem 16 (Regularity of Solutions)**.** *Let $\mathcal{B} \subset \mathbb{R}^n$ be an open ball and let u and V be functions in $L^1(\mathcal{B}_1)$ that satisfy*

$$-\Delta u + Vu = 0 \text{ in } D'(\mathcal{B}_1)$$

Then the following hold for any ball $\mathcal{B}$ concentric with $\mathcal{B}_1$ and with strictly small radius:

1. *$n = 1$: Without any further assumption on V, u is continuosly differentiable.*
2. *$n = 2$: Without further assumptions on V, $u \in L^q(\mathcal{B})$ for all $q < \infty$*
3. *$n \geq 3$: Without any further assumptions on V, $u \in L^q(\mathcal{B})$ with $q < \frac{n}{n-2}$*
4. *$n \geq 2$: If $V \in L^p(\mathcal{B})$ for $n \geq p \geq \frac{n}{2}$, then for all $\alpha \neq 2 - \frac{n}{p}$,*

$$|u(x) - u(y)| \leq C|x - y|^\alpha$$

To conclude we consider a real world example. The potential V for the hydrogen atom located at the origin in $\mathbb{R}^3$ is

$$V(x) = -|x|^{-1}.$$

A solution to the Schrödinger equation is found by inspection to be

$$\psi_0(x) = e^{\frac{1}{2}|x|},\ E_0 = -\frac{1}{4}$$

Since is ψ_0 is positive, it is the ground state, i.e., the unique minimizer of

$$\mathcal{E}(\psi) = \int_{\mathbb{R}^3} |\nabla\psi|^2 - \int_{\mathbb{R}^3} \frac{1}{|x|}|\psi(x)|^2 dx.$$

The fact that ψ_0 is unique follows from Theorem 15.

Theorem 16 gives additional insight on ψ_0: since $V \in C^\infty(\mathbb{R}^n \setminus \{0\})$, then $\psi_0 \in C^\infty(\mathbb{R}^n \setminus \{0\})$. We also have that $V \in L^p_{loc}(\mathbb{R}^n)$ for $3 > p > \frac{3}{2}$, and so ψ_0 must also be Holder continuous in the origin.

Bibliography

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