H^1 or L^∞ ?

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Summary

- Prof. Martin found that L^2 was not enough and $L^2 \cap L^\infty$ might be too much for the orbitals.
- We are trying to explore what if we use H^1 instead of $L^2 \cap L^\infty$ for the orbitals.

Definition of Sobolev Spaces $W^{k,p}(\Omega)$ and Sobolev Norm

- The Sobolev spaces $W^{k,p}(\Omega)$ are defined over an arbitrary domain $\Omega \subset R^n$ and are vector subspaces of various spaces $L^p(\Omega)$ such that function f and its weak derivatives up to some order k have a finite L^p norm. The Sobolev norm $||\cdot||_{k,p}$, where k is a nonnegative integer and $1 \leq p \leq \infty$, is:

$$||f||_{k,p} = \left(\sum_{0 \leq |a| \leq k}^{k} ||D^a f||_p^p \right)^{1/p}, \quad \text{if } 1 \leq p < \infty$$

$$||f||_{k,\infty} = \max_{0 \leq |a| \leq k} ||D^a f||_\infty, \quad \text{if } p = \infty$$

Definition of Sobolev Spaces $W^{k,p}(\Omega)$ and Sobolev Norm

- Sobolev spaces with $p = 2$ are especially important because they form a Hilbert space. A special notation has arisen to cover this case:
$$H^k = W^{k,2}$$
In addition, the H^k inner product is defined in terms of the L^2 inner product.
$$\langle u, v \rangle_{H^k} = \sum_{i=0}^{k} \langle D^i u, D^i v \rangle_{L^2}$$
Hence, the space H^k becomes a Hilbert space with this inner product.
- In this project, we consider functions in $W^{1,2}$, which is also known as H^1.

Example

Example: Compute $||\varphi(r)||_{H^1}$, where $(x, y, z) \in R^3$,
$r = \sqrt{x^2 + y^2 + z^2}$, and $\varphi(r) = \sqrt{\frac{Z^3}{\pi}} e^{-Zr}$.
By definition, we have:

$$\| \varphi\|_{H^1}^2 = \| \varphi\|_2^2 + \| \nabla\varphi\|_2^2$$

We can compute,

$$\begin{aligned}
\| \varphi\|_2 &= \left(\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \varphi^2 dxdydz \right)^{\frac{1}{2}} \\
&= \left(4\pi \int_0^{+\infty} \varphi^2 (r) r^2 dr \right)^{\frac{1}{2}} \\
&= \left(4Z^3 \int_0^{+\infty} e^{-2Zr} r^2 dr \right)^{\frac{1}{2}} \\
&= 1
\end{aligned}$$

Example

$$\begin{aligned}
\|\nabla\varphi\|_2 &= \left(\int\int\int \nabla\varphi\cdot\nabla\varphi dV\right)^{\frac{1}{2}} \\
&= \left(\int\int\int \left(\frac{\partial\varphi}{\partial x}\right)^2 + \left(\frac{\partial\varphi}{\partial y}\right)^2 + \left(\frac{\partial\varphi}{\partial z}\right)^2 dxdydz\right)^{\frac{1}{2}} \\
&= \left(\int\int\int \frac{Z^5}{\pi} e^{-2Z\sqrt{x^2+y^2+z^2}} dxdydz\right)^{\frac{1}{2}} \\
&= \left(\int_0^{+\infty} 4Z^5 e^{-2Zr} r^2 dr\right)^{\frac{1}{2}} = Z
\end{aligned}$$

Therefore,

$$\|\varphi\|_{H^1} = (1+Z^2)^{1/2}$$

Embedding Theorem

Theorem 1 : $W^{k,p}(R^n) \subseteq W^{l,q}(R^n)$ if $k > l$ and $k - \frac{n}{p} \geq l - \frac{n}{q}$.
Lemma 1: $f,\ g \in\ H^1 \Rightarrow fg \in L^1 \cap L^2$
Proof.

By Theorem 1, let $k = 1$, $p = 2$, $n = 3$, $l = 0$ and $q = 4$, we have $H^1 \subseteq L^4$.

Since $f,\ g \in\ H^1$, $f,\ g \in\ L^4$.

Hence, $||fg||_2^4 \leq ||f^2||_2^2 \cdot ||g^2||_2^2 = ||f||_4^4 \cdot ||g||_4^4 < +\infty$. So, $f,\ g \in\ L^2$.

On the other hand, $||fg||_1 \leq ||f||_2 \cdot ||g||_2 < +\infty$. Hence, $fg \in L^1$.

Therefore, $fg \in L^1 \cap L^2$

Sobolev Inequality

Theorem 2:Assume that $f(x) \in C_0^\infty(R^n)$, a infinitely differentiable function with compact support. Then for $1 \leq p < n$ and $q = \frac{np}{n-p}$, there exists a constant $C(n,p)$ such that

$$||f||_q \leq C(n,p)||\nabla f||_p,$$

where $c(n,p) = \frac{p-1}{n-p}(\frac{n-p}{n(p-1)})^{\frac{1}{q}}(\frac{\Gamma(n+1)}{\Gamma(n/p)\Gamma(n+1-n/p)\omega_{n-1}})^{\frac{1}{n}}$.

Sobolev Inequality

Example: Consider $n = 3$ and $p = 2$, then $q = 6$ and we have:

$$||f||_6 \leq C(3,2)||\nabla f||_2$$

We computed and get: C(3,2)=0.616216.
Suppose $f, g \in H^1$, we can show that:

$$\begin{aligned} ||fg||_2^4 &\leq ||f^2||_2^2 \cdot ||g^2||_2^2 \\ &= ||f||_4^4 \cdot ||g||_4^4 \\ &\leq ||f||_2 \cdot ||f||_6^3 \cdot ||g||_2 \cdot ||g||_6^3 \\ &\leq C(3,2)^6 \cdot ||f||_2 \cdot ||g||_2 \cdot ||\nabla f||_2^3 \cdot ||\nabla g||_2^3 \end{aligned}$$

Theorem 3:

$$\int \frac{|f(x)| \cdot |h(y)|}{|x-y|^\lambda} d^n x d^n y \leq C_{p,r,\lambda,n} \| f \|_p \cdot \| h \|_q,$$

where $f \in L^p(R^n), h \in L^q(R^n)$ and $\frac{1}{p} + \frac{1}{q} + \frac{\lambda}{n} = 2$ with $\lambda < n$.
We concern the case that $\lambda = 1$ and n=3. So, we have:

$$\int \frac{|f(x)| \cdot |h(y)|}{|x-y|} d^3 x d^3 y \leq C_{p,q} \| f \|_p \cdot \| h \|_q,$$

where $f \in L^p(R^3), h \in L^q(R^3)$ and $\frac{1}{p} + \frac{1}{q} = \frac{5}{3}$.
For example, we can have p=1 and $q = \frac{3}{2}$.

Application of L^∞ and H_1 Spaces

Professor Martin did:
Case 1. Define $W_p[f](r) = \int \frac{1}{||r-r'||} f(r')dr'$.
$\int f_1 g_1 W_p[fg]dr$ may be unbounded, when $f, g \in L^2$.
Suppose $f(r) = \sqrt{\frac{Z^3}{\pi}} e^{-Zr}$, we have:

$$\int f^2 W_p[f^2]dr = \int \frac{Z^3}{\pi} e^{-2Zr} (\int \frac{1}{||r - r'||} \cdot \frac{Z^3}{\pi} e^{-2Zr'} dr')dr = \frac{5}{8} Z$$

Professor Martin did:
Case 2. We assume that both f and g are in $L^2 \cap L^\infty$. Using Hölder's inequality with (L^2, L^2) we have

$$||fg||_1 \leq ||f||_2||g||_2$$

and also

$$||fg||_2 \leq ||f||_\infty||g||_2$$

Thus $fg \in L^1 \cap L^2$.

$W_p[\cdot]$ is unbounded $L^1 \cap L^2 \to L^2$, but bounded $L^1 \cap L^2 \to L^\infty$

Application of L^∞ and H_1 Spaces

We did:
Case 3. We assume that both f and g are in H^1. According to Lemma 1, if $f,\ g \in H^1$, then $fg \in L^1 \cap L^2$. Hence, $W_p[fg]$ is bounded in L^∞.
Hence, when $f_1, g_1, f, g \in H^1$, we have:

$$\begin{aligned}\int f_1 g_1 W_p[fg] dr &\leq ||f_1||_2 \cdot ||g_1 \cdot W_p[fg]||_2 \\ &\leq ||f_1||_2 \cdot ||g_1||_2 \cdot ||W_p[fg]||_\infty \\ &< +\infty.\end{aligned}$$

We did:
Case 4. Since $f, g \in H^1 \Rightarrow fg \in L^{3/2}$, we consider if we can use $fg \in L^{3/2}$ instead of $fg \in L^1 \cap L^2$.
Prove: $f, g \in H^1 \Rightarrow fg \in L^{3/2}$
Proof :

$$\begin{aligned} ||fg||_{3/2} &\leq ||\nabla(fg)||_1 \\ &= ||\nabla f \cdot g + \nabla g \cdot f||_1 \\ &\leq ||\nabla f \cdot g||_1 + ||\nabla g \cdot f||_1 \\ &\leq ||\nabla f||_2 \cdot ||g||_2 + ||\nabla g||_2 \cdot ||f||_2 \end{aligned}$$

However, when $fg \in L^{3/2}$, we have:

$$\int f_1 g_1 W_p[fg] dr = +\infty$$

Hence, we give up this attempt.

We derived:

$$\infty > C \geq \sup_{f,g} \frac{\int\int \frac{f(x)g(x)}{||x-y||} dxdy}{||f||_1 ||g||_{3/2}} \qquad (Theorem\ 3)$$

$$= \sup_{f,g} \int \frac{f(x)}{||f||_1} \int \frac{\frac{g(y)}{||x-y||}}{||g||_{3/2}} dydx \qquad (Fubini)$$

$$= \sup_{g} || \frac{\int \frac{g(y)}{||x-y||} dy}{||g||_{3/2}} ||_\infty \qquad (L^1 \ and\ L^\infty \ are\ dual\ spaces)$$

$$= \sup_{g} || \int \frac{g(y)}{||g||_{3/2}} \cdot \frac{1}{||x-y||} dy ||_\infty$$

$$= \sup_g || \int \frac{g(z-x)}{||g||_{3/2}} \cdot \frac{1}{||z||} dz ||_\infty$$

$$= \sup_g \int \frac{g(z)}{||g||_{3/2}} \cdot \frac{1}{||z||} dz$$

$$= || \frac{1}{||z||} ||_3 = \infty \quad (L^{3/2} \textit{ and } L^3 \textit{ are dual spaces})$$

Can you find the mistake?