5.2 Stability of matter

The Hilbert space for the electron is $\mathcal{H} = L^2(\mathbb{R}^d)$ and the Hamiltonian is

$$H = -\frac{\hbar^2}{2m} \Delta - \frac{e^2}{4\pi \varepsilon_0} \kappa.$$ 

That is, the proton is located at the origin and the interaction between proton and electron is Coulomb.

The first question is why $H$ should be bounded below? That is, $(\psi, H\psi)$ cannot be arbitrarily negative. This is the simplest question of the more general problem of stability of matter. There are several ways to prove a lower bound for $H$, and we consider two of them. One is an operator inequality for $-\Delta$, the other is a Sobolev inequality.

**Proposition 5.1** Let $\mathcal{H} = L^2(\mathbb{R}^d)$ with $d \geq 3$. Then

$$-\Delta > \frac{(d-3)^2}{4} \| \psi \|^2.$$

In other words, we have

$$\int_{\mathbb{R}^d} |\nabla \psi|^2 \geq \frac{(d-3)^2}{4} \int_{\mathbb{R}^d} |\psi|^2$$

for all $\psi$ in a dense subspace of $L^2(\mathbb{R}^d)$. Here, the notation $\| \psi \|^2 = \frac{1}{2\pi} \int_{\mathbb{R}^d} |\psi(\omega)|^2$.

**Proof:** Recall that $P^j = -i\frac{\partial}{\partial x^j}$ and that it is self-adjoint.

Using $\frac{\partial}{\partial x^j} \psi = -\frac{\partial}{\partial x^j} \psi$, one can check that

$$\| \psi \|^2 = \int_{\mathbb{R}^d} \psi^* \frac{\partial}{\partial x^j} \psi = \int_{\mathbb{R}^d} \frac{\partial}{\partial x^j} \psi^* \psi = \int_{\mathbb{R}^d} \frac{\partial}{\partial x^j} \psi^* \psi - \int_{\mathbb{R}^d} \psi^* \frac{\partial}{\partial x^j} \psi.$$

It follows that

$$\langle \psi, \frac{\partial}{\partial x^j} \psi \rangle = -\frac{\partial}{\partial x^j} \int_{\mathbb{R}^d} \psi^* \psi = -\frac{\partial}{\partial x^j} \int_{\mathbb{R}^d} \psi^* \psi = -\frac{\partial}{\partial x^j} \int_{\mathbb{R}^d} \psi^* \psi.$$

Next, consider the identity

$$P^j \frac{\partial}{\partial x^j} \psi = \frac{\partial}{\partial x^j} \psi + [P^j, \frac{\partial}{\partial x^j}] = \frac{\partial}{\partial x^j} \psi + i \frac{\partial}{\partial x^j} \psi.$$

An application of the identity then

$$\langle \psi, \frac{\partial}{\partial x^j} \psi \rangle = \langle \psi, \psi \rangle - i \langle \psi, \frac{\partial}{\partial x^j} \psi \rangle.$$

Summing over $j = 1, ..., d$, we get

$$(d-2) \langle \psi, \frac{\partial}{\partial x^j} \psi \rangle = -2 \int_{\mathbb{R}^d} \psi^* \frac{\partial}{\partial x^j} \psi.$$

Then

$$\int_{\mathbb{R}^d} \left( \psi, \frac{\partial}{\partial x^j} \psi \right)^2 = \left| \int_{\mathbb{R}^d} \psi^* \frac{\partial}{\partial x^j} \psi \right|^2 \\
\leq \left| \int_{\mathbb{R}^d} \psi^* \frac{\partial}{\partial x^j} \psi \right|^2 \\
\leq \left( \frac{d}{\int_{\mathbb{R}^d} \psi^* \psi} \right) \left( \frac{d}{\int_{\mathbb{R}^d} \psi^* \psi} \right) \\
= \left( \frac{d}{\int_{\mathbb{R}^d} \psi^* \psi} \right) \left( \frac{d}{\int_{\mathbb{R}^d} \psi^* \psi} \right) \\
= \left( \frac{d}{\int_{\mathbb{R}^d} \psi^* \psi} \right) \left( \frac{d}{\int_{\mathbb{R}^d} \psi^* \psi} \right).$$

\[\square\]
From Proposition 5.1 we immediately obtain a lower bound for $H$:

$$\langle \psi, H \psi \rangle \geq \left( \frac{\hbar^2}{2m} \leq \frac{1}{4} + \frac{\gamma}{8\hbar^2} \right) \langle \psi, \psi \rangle \geq -\frac{2m \epsilon^*}{\hbar^2}.$$ 

This lower bound is four times too negative.

The second method uses a variational principle.

**Exercise 11.** Consider the functional

$$E(\psi) = \int_\mathbb{R} \left( \| \nabla \psi \|^2 + V(\psi)^2 \right) dx$$

Assume that $E(\psi)$ has a unique minimizer in $\{ \psi \in H^1(\mathbb{R}^3) \}$, and that it belongs to $H^2(\mathbb{R}^3)$. Show that it is an eigenvector of the Hamiltonian $H = -\Delta + V$ with the lowest eigenvalue.

**Hint:** $\frac{d}{d\epsilon} E(\psi+\epsilon h)|_{\epsilon=0} = 2 \mathbb{R} \left( \| -\Delta \psi + V \psi \|^2 \right)$, and this is zero if $\psi$ is the minimizer.

It is clear that, if $H = -\Delta + V$, we have $\langle \psi, H \psi \rangle = E(\psi)$. We therefore seek a lower bound for $E(\psi)$. We use a Sobolev inequality.

**Theorem 5.2 (Sobolev inequality for gradients)**

Let $d \geq 3$, and $\mathbb{R}^d \setminus \{ 0 \}$, let $q = \frac{2d}{d-2}$, then any $F \in L^q(\mathbb{R}^d)$ such that $\nabla F$ exists and is in $L^d(\mathbb{R}^d)$ satisfies

$$\| \nabla F \|^q \leq S_d \| F \|^q$$

where $S_d = \frac{d(d-2)}{2} \left( \frac{d}{1+\frac{d}{2}} \right)^{\frac{d}{2}} = \frac{d(d-2)}{2} \frac{2^d}{\pi^{d/2}} \Gamma \left( \frac{d}{2} \right)^{d/2}$.

For the proof, see [Lieb-Loss, Analysis, Theorem 2.5]. Notice that when $d=3$, we have $q = 6$ and $S_3 = 3(\pi)^3$.

For the hydrogen atom, we get from Theorem 5.2 that

$$E(\psi) = \int_\mathbb{R} \left( \| \nabla \psi \|^2 + V(\psi)^2 \right) dx \geq 3(\pi)^3 \| \psi \|^2 - \frac{1}{\hbar^2} \int_\mathbb{R} dx.$$

Let $\rho(\omega) = 14(\omega)^3$. Then

$$E(\psi) \geq \inf_{\rho(\omega) \geq 0, S_3(<1)} \left[ 3(\pi)^3 \| \psi \|^2 - \frac{1}{\hbar^2} \int_\mathbb{R} dx \right].$$

The minimization problem is an easy exercise.” —J. Lieb, “The Skyrme

or Matter: From Atoms to Stars”, 1989 Gibbs Lecture. And one finds $E(\psi) \geq -\frac{1}{3}$. This is even better since the infimum of $C(\psi, H \psi) = E(\psi)$ is $-\frac{1}{3}$. 