Uniqueness of the ground state

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Definition 1. Let $f \in L^2(\mathbb{R}^n)$ be a real-valued function. We say that f is

- **positive** if $f \geq 0$ a.e. and $f \neq 0$ (and with a little abuse of notation, we will write $f \geq 0$);
- **strictly positive** if $f > 0$ a. e. .

A bounded operator A is

- **positivity preserving** if for every positive $f \in L^2(\mathbb{R}^n)$, Af is positive;
- **positivity improving** if for every positive $f \in L^2(\mathbb{R}^n)$, Af is strictly positive.

Moreover we say that A is **real** if maps real functions to real functions.

Remark 2 (Characterization of strictly positive functions)**.** Note that there is an easy characterization of the set of strictly positive functions. Namely, a function $f \in L^2(\mathbb{R}^n)$ is strictly positive if and only if

$$\langle g, f \rangle > 0 \qquad \forall g \geq 0.$$

Indeed if $g \geq 0$, then there exists a measurable set Ω with positive measure such that $g > 0$ on Ω. Therefore

$$\langle g, f \rangle \geq \int_\Omega fg > 0.$$

On the other hand, if $\langle g, f \rangle > 0$ for all $g \geq 0$, then f must be strictly positive, otherwise we could find a suitable positive function such that $\langle g, f \rangle = 0$.

Example 3 (Multiplication and convolution operator)**.** Let $g > 0$. Then the multiplication operator $Af \coloneqq gf$ is positivity preserving and the convolution operator $Af \coloneqq g * f$ is positivity improving.

More in general any integral operator with positive (strictly positive) kernel is positivity preserving (positivity improving).

Before stating and proving the main theorem, we need the following preliminary result about positivity.

Theorem 4. *Let $A \in \mathcal{L}(L^2(\mathbb{R}^n))$ be a self-adjoint positivity improving and real operator. If $\|A\|$ is an eigenvalue, then it is simple.*

Proof. Firstly note that if ψ is an eigenfunction for an eigenvalue λ, then both its real and imaginary part are eigenfunction associated to λ. Indeed

$$A \operatorname{Re} \psi + iA \operatorname{Im} \psi = A\psi = \lambda\psi = \lambda \operatorname{Re} \psi + i\lambda \operatorname{Im} \psi$$

and since A is a real operator, $A \operatorname{Re} \psi$ and $A \operatorname{Im} \psi$ are real-valued functions, therefore

$$A \operatorname{Re} \psi = \lambda\psi \qquad \text{and} \qquad A \operatorname{Im} \psi = \lambda \operatorname{Im} \psi.$$

So we can assume w.l.o.g. ψ to be real-valued. If we show that ψ does not change sign, then we are done. Indeed if ψ does not change sign, we can assume w.l.o.g. it is a positive function. Then it is an eigenfunction and since A is positivity improving, ψ is a strictly positive function. Since two strictly positive functions can not be orthogonal to each other, we have that the eigenspace of $\|A\|$ is 1-dimensional.

Let us show ψ does not change sign. Let $\psi_+ \coloneqq \frac{|\psi|+\psi}{2}$ and $\psi_- \coloneqq \frac{|\psi|-\psi}{2}$ be the positive and negative part of ψ respectively. Then we have

$$|A\psi| = |A\psi_+ - A\psi_-| \leq A\psi_+ + A\psi_- = A|\psi|.$$

From this inequality and assuming $\|\psi\| = 1$, it follows that

$$\begin{aligned}
\|A\| &= \|A\|\langle\psi, \psi\rangle = \langle\psi, A\psi\rangle \\
&= \int_{\mathbb{R}^n} \psi A\psi \leq \int_{\mathbb{R}^n} |\psi||A\psi| \leq \int_{\mathbb{R}^n} |\psi|A|\psi| \\
&= \langle|\psi|, A|\psi|\rangle \leq \|A\|.
\end{aligned}$$

Therefore

$$\langle\psi, A\psi\rangle = \langle|\psi|, A|\psi|\rangle.$$

If we write out explicitly ψ using the positive and negative part and using the fact that A is self-adjoint, then the previous equality becomes:

$$-2\langle\psi_-, A\psi_+\rangle = 2\langle\psi_-, A\psi_+\rangle.$$

thus

$$\langle \psi_-, A\psi_+ \rangle = 0.$$

This implies that $\psi_- = 0$ or $\psi_+ = 0$. Indeed assume by contradiction $\psi_+ \neq 0$ and $\psi_+ \neq 0$. Then this means ψ_+ and ψ_- are are both positive functions. Since A is positivity improving, we have $A\psi_+$ is strictly positive and from Remark 2 we have $\langle \psi_-, A\psi_+ \rangle > 0$ which is a contradiction.

□

We will use Theorem 4 to show the following result.

Theorem 5 (**Uniqueness of the ground state**)**.** *Let $H = H_0 + V$ be an essentially self-adjoint operator bounded from below with $C_c^\infty(\mathbb{R}^n)$ as a core ($H_0 = -\Delta$).*

If $E_0 = \min \sigma(H)$ is an eigenvalue, it is simple and the corresponding eigenfunction is strictly positive.

The idea of the proof is to apply Theorem 4 to the resolvent $R_H(\lambda)$. The biggest part of the work will be to show that the resolvent is positivity improving.

Before giving the proof of Theorem 5, let us recall some concept and results that we will need.

Definition 6 (Strong resolvent convergence)**.** Let $(A_n)_{n\in\mathbb{N}}$ be a sequence of self-adjoint operators and let A be a self-adjoint operator. We say that $(A_n)_{n\in\mathbb{N}}$ converges to A in the **strong resolvent sense**, and we will write $A_n \xrightarrow{SR} A$, if there exists $z \in \mathbb{C} \setminus \mathbb{R}$ such that

$$\text{s-lim}_{n\to\infty} R_{A_n}(z) = R_A(z),$$

i.e. if the sequence of resolvents of the operators A_n strongly converge to the resolvent of A.

For a strong resolvent convergence sequence, the following property holds.

Theorem 7. *Let $A_n \xrightarrow{SR} A$ and let f a bounded and continuous function defined on $\mathbb{R}$. Then*

$$\text{s-lim}_{n\to\infty} f(A_n) = f(A).$$

Proof. For a proof, see Theorem VIII.20 in [2]. □

Another tool needed for proving Theorem 5 is the Trotter formula.

Theorem 8 (Trotter product formula)**.** *Let A and B be self-adjoint operators bounded from below. Then*

$$e^{-t(A+B)} = \text{s-lim}_{n\to\infty} \left(e^{-\frac{t}{n}A}e^{-\frac{t}{n}B}\right)^n, \qquad t \geq 0. \tag{1}$$

Proof. See Theorem 5.12 in [3] and the previous seminar talk. □

We can finally prove Theorem 5.

Proof of Theorem 5. **Step 1: e^{-tH} is positivity preserving for $t > 0$.**

Let us define new operators H_n as follows

$$H_n \coloneqq H_0 + V_n,$$

where $V_n \coloneqq V\chi_{\{x\in\mathbb{R}^n:|V(x)|\leq n\}}$. Observe that V_n is bounded.

Recall that we have an explicit formula for e^{-tH_0}, i.e.

$$\left(e^{-tH_0}\psi\right)(x) = e^{-\frac{\pi}{4}x}\frac{1}{(2\pi|t|)^{\frac{n}{2}}}\int_{\mathbb{R}^n} e^{\frac{(x-y)^2}{2t}}\psi(y)\,dy.$$

Therefore the operator e^{-tH_0} is the convolution with a strictly positive function, therefore it is positivity improving.

Moreover the multiplication operator

$$\left(e^{-tV_n}\psi\right)(x) = e^{-tV_n}\psi(x)$$

is positivity preserving, because it is the product with a strictly positive function.

Let ψ be a positive function. Then we have that for every $k \in \mathbb{N}$

$$\left(e^{-\frac{t}{k}H_0}e^{-\frac{t}{k}V_n}\right)^k\psi$$

is a strictly positive function. This implies, using Theorem 8, that

$$e^{-tH_n}\psi = \text{s-lim}_{k\to\infty}\left(e^{-\frac{t}{k}H_0}e^{-\frac{t}{k}V_n}\right)^k\psi$$

is non-negative a.e. . On the other hand, $e^{-tH_n}\psi \neq 0$, because the operator is injective. Therefore $e^{-tH_n}\psi$ is a positive function, and thus e^{-tH_n} a positivity preserving operator.

Now we show that $H_n \xrightarrow{SR} H$.

Firstly observe that for every $\psi \in C_c^\infty(\mathbb{R}^n)$, we have

$$\|\left(H - H_n\right)\psi\|^2 = \int_{\mathbb{R}^n}|V|^2|\psi|^2\left(1 - \chi_{\{|V|\leq n\}}\right)$$

and since $V \in L^2_{loc}(\mathbb{R}^n)$, we can apply the Dominated Convergence Theorem and we get that

$$H_n\psi \longrightarrow H\psi \qquad \forall \psi \in C_c^\infty(\mathbb{R}^n).$$

We need to show that $(H_n - i)^{-1}$ converges strongly to $(H - i)^{-1}$. Let $\psi \in C_c^\infty(\mathbb{R}^n)$ and let $\phi = (H + i)\psi$

$$\begin{aligned}\| \left((H_n - i)^{-1} - (H - i)^{-1}\right) \phi\| &= \| (H_n - i)^{-1} (H - H_n) \psi\| \\ &\leq \| (H_n - i)^{-1} \| \| (H - H_n) \psi\|.\end{aligned}$$

Observe that $\| (H_n - i)^{-1} \| \leq 1$ for every $n \in \mathbb{N}$ (see for example Theorem 2.19 in [3] or Lemma 2.3 in [1]). Therefore we have

$$\| \left((H_n - i)^{-1} - (H - i)^{-1}\right) \phi\| \leq \| (H - H_n) \psi\| \underset{n\to\infty}{\longrightarrow} 0.$$

Thus we proved that $(H_n - i)^{-1}$ converges to $(H - i)^{-1}$ on $\mathrm{Ran}(H + i)$. Since A is essentially self-adjoint, $\mathrm{Ran}(H + i)$ is dense in $L^2(\mathbb{R}^n)$ (see for instance the corollary of Theorem VIII.3 in [2]). This implies that that $(H_n - i)^{-1}$ converges strongly to $(H - i)^{-1}$.

From Theorem 7 we have that e^{-tH_n} is strongly converging to e^{-tH}. Therefore $e^{-tH}\phi$ is a a.e. non-negative function, for every positive ϕ. On the other hand $e^{-tH}\phi \neq 0$. Thus e^{-tH} is positivity preserving.

Step 2: e^{-tH} **is positivity improving for** $t > 0$**.**

Let us fix a positive function ψ and consider the following closed subset of $L^2(\mathbb{R}^n)$:

$$N(\psi) \coloneqq \{\phi \in L^2(\mathbb{R}^n) : \phi \geq 0 \quad \text{and} \quad \langle \phi, e^{-sH}\psi\rangle = 0, \ \forall s > 0\} \cup \{0\}.$$

Observe that $e^{tV_n}(N(\psi)) \subset N(\psi)$, for every $t > 0$. Indeed let $\phi \in N(\psi)$. Then for every $s > 0$ we have, by positivity of the functions,

$$\phi e^{-sH}\psi = 0 \qquad \text{a. e.}$$

and multiplying by e^{tV_n} we trivially have

$$e^{tV_n}\phi e^{-sH}\psi = 0 \qquad \text{a. e.}$$

and thus $e^{tV_n}\phi \in N(\psi)$.

Moreover we have also that $e^{-tH}(N(\psi)) \subset N(\psi)$ for $t > 0$. Indeed if $\phi \in N(\psi)$, then for every $s > 0$:

$$0 = \langle \phi, e^{-(t+s)H}\psi\rangle = \langle e^{-tH}\phi, e^{-sH}\psi\rangle.$$

So we have that the set $N(\psi)$ is invariant set w.r.t. the operators e^{tV_n} and e^{-tH}. We want to show that it is invariant also w.r.t. e^{-tH_0}. Let $\phi \in N(\psi)$ and let $s > 0$. Then using again Theorem 8, we have:

$$0 = \lim_{k\to\infty} \langle \left(e^{-\frac{t}{k}H} e^{\frac{t}{k}V_n} \right)^k \phi, e^{-sH}\psi \rangle = \langle e^{-t(H-V_n)}\phi, e^{-sH}\psi \rangle.$$

Therefore $e^{-t(H-V_n)}\phi \in N(\psi)$. Since $e^{-t(H-V_n)}$ converges strongly to e^{-tH_0} we have that $e^{-tH_0}\phi \in N(\psi)$. Therefore $N(\psi)$ is invariant w.r.t. e^{-tH_0}. This implies that $N(\psi) = \{0\}$. Indeed assume by contradiction that there exists a positive function $\phi \geq 0$ in $N(\psi)$. Since e^{-tH_0} is positivity improving, we have that $e^{-tH_0}\phi > 0$. By Remark 2 we have that for every $s > 0$:

$$\langle e^{-tH_0}\phi, e^{-sH_0}\psi \rangle > 0$$

but this is a contradiction because $\langle e^{-tH_0}\phi, e^{-sH_0}\psi \rangle = 0$, since $e^{-tH_0}\phi \in N(\psi)$.

Therefore e^{-tH} is positivity improving.

Step 3: the resolvent $R_H(\lambda)$ is positivity improving for $\lambda < E_0$.

Observe that from Lemma 4.1 in [3] we can express the resolvent in the following way:

$$\langle \phi, R_H(\lambda)\psi \rangle = \int_0^\infty e^{\lambda t} \langle \phi, e^{-tH}\psi \rangle \, dt$$

where $\lambda < E_0$. This can also be done in a similar way to the proof of Theorem 4.2(Stone's Theorem) in [1] or using the functional calculus. If ϕ and ψ are both positive functions, then the right-hand side is clearly strictly positive. From Remark 2, this implies that $R_H(\lambda)$ is positivity improving.

Step 4: conclusion.

Now let ψ be an eigenfunction of H, i.e.

$$H\psi = E\psi,$$

for an eigenvalue E. Then

$$\begin{aligned} R_H(\lambda)\psi &= (H-\lambda)^{-1}\psi \\ &= (H-\lambda)^{-1}\left(\frac{E\psi}{E}\right) \\ &= (H-\lambda)^{-1}\left(\frac{(H-\lambda)\psi + \lambda\psi}{E}\right) \\ &= \frac{\psi}{E} + \frac{\lambda}{E} R_H(\lambda)\psi \end{aligned}$$

Therefore

$$R_H(\lambda)\psi = \left(\frac{1}{E-\lambda}\right)\psi.$$

Moreover

$$\|R_H(\lambda)\| = \sup_{\|\phi\|=1} |\langle R_H(\lambda)\phi, \phi\rangle| = \sup |\sigma(R_H(\lambda))| = \frac{1}{E_0-\lambda}.$$

From Theorem 4, the (real part and imaginary part of the) eigenfunctions of $R_H(\lambda)$ associated to $\frac{1}{E_0-\lambda}$ do not change sign and those are exactly the eigenfunctions of H associated to E_0. Thus E_0 is simple. □

References

[1] N. Benedikter, *Lecture notes for Advanced Mathematical Physics* 2017

[2] M. Reed and B. Simon, *Methods of Modern Mathematical Physics I: Functional Analysis*

[3] G. Teschl, *Mathematical Methods in Quantum Mechanics*