1. Goal and Motivation

The goal of this lecture is use the Spectral Theorem for compact operators to prove the following

Theorem 1.1. Let $V \in C^{\infty}(\mathbb{R})$ be a nonnegative smooth function and I = (0,1). There exist

- an sequence $\{\varepsilon_k\}_{k\in\mathbb{N}}\subset\mathbb{R}_+$ such that $\varepsilon_k\to+\infty$, a sequence $\psi_k\in C^\infty(I)\cap C(\overline{I})$ such that

(1)
$$-\psi_k''(x) + V(x)\psi_k(x) = \varepsilon_k \psi_k(x) \text{ for all } x \in I, \quad \psi_k(0) = \psi_k(1) = 0,$$
 and $\{\psi_k\}_{k \in \mathbb{N}}$ is an Hilbert basis of $L^2(I)$.

Remark 1.2. In the case $V \equiv 0$ we can solve explicitly (1) and find

$$\varepsilon_k = \pi^2 (k+1)^2$$
 and $\psi_k(x) = \frac{1}{\sqrt{\pi}} \sin(\pi (k+1)x)$.

By Fourier theory, $\{\frac{1}{\sqrt{\pi}}\sin(\pi(k+1)x)\}_{k\in\mathbb{N}}$ is an Hilbert basis of $L^2(I)$.

Theorem 1.1 is a far reaching generalisation of this example as, for a general V, there is no hope to give formulas for the ψ_k 's.

Before starting the proof let us show a typical application of Theorem 1.1.

Example 1.3. Consider the Schrödinger equation

$$i\partial_t w = Hw$$
, $H := -\frac{d^2}{dx^2} + V(x)$, $w(t,0) = w(t,1) = 0$, $w(0,x) = f(x)$,

where $w(t,x): \mathbb{R} \times \overline{I} \to \mathbb{C}$ and $f \in L^2(I)^1$. By Theorem 1.1 there is an orthonormal basis $\{\psi_k\}$ such that $H\psi_k = \varepsilon_k \psi_k$, for some "energies" ε_k . If we express then the initial state $f(x) = \sum_{k} \langle f, \psi_k \rangle \psi_k(x)$ we find that the solution w must be given by

$$w(t,x) = \sum_k \langle f, \psi_k \rangle e^{-i\varepsilon_k t} \psi_k(x),$$

where the series converges at least in the L^2 sense (and much better if f is assumed to be more regular).

Notice that if $f = \psi_N$, then $w(t,x) = e^{-i\varepsilon_N t} \psi_N(x)$, and in particular |w| is constant, this is why the ψ_k 's are called *steady states*.

2. Proof of Theorem 1.1

2.1. The Spectral Theorem. As anticipated, the proof of Theorem 1.1 relies on

Theorem 2.1 (Spectral Theorem). Let \mathcal{H} be an Hilbert space and let $T \in \mathcal{L}(\mathcal{H})$ be compact and symmetric. Then there is a real infinitesimal sequence $\{\lambda_k\}_{k\in\mathbb{N}}$ and an Hilbert basis $\{e_k\}_k \in \mathbb{N}$ of \mathcal{H} such that

$$Tv = \sum_{k} \lambda_k \langle v, e_k \rangle e_k$$
 for all $v \in \mathcal{H}$.

Proof. See the Lecture Notes.

¹In Quantum Mechanics, $|w(t,x)|^2 dx$ represents the probability of finding at time t in the interval [x, x + dx] a quantum particle, prepared at time t = 0 in the state f(x), subject to the Hamiltonian H and confined to live in a box $x \in I$.

2.2. An auxiliary Hilbert space. Define the scalar product

(2)
$$\langle u, v \rangle_V := \int_0^1 u'(x)v'(x) + V(x)u(x)v(x) dx, \quad u, v \in C_c^1(I).$$

Notice that for all $0 \le x < y \le 1$ and $u \in C_c^1$ it holds

$$|u(x) - u(y)| = \left| \int_x^y u'(s) \, ds \right| \le \int_x^y |u'| \le ||u'||_{L^2(I)} |x - y|^{\frac{1}{2}} \le ||u||_V |x - y|^{\frac{1}{2}}.$$

So in particular

(3)
$$||u||_{L^{\infty}(I)} + \sup_{x,y \in I} \frac{|u(x) - u(y)|}{|x - y|^{\frac{1}{2}}} \le 2||u||_{V}.$$

We also define the Hilbert space $(\mathcal{H}, \langle u, v \rangle_V)$ where

$$\mathcal{H} := \overline{C_c^1(I)}^{\|\cdot\|_V}.$$

Thanks to (3), we have $\mathcal{H} \subset C^{\frac{1}{2}}(\overline{I})$ and, concretely, $u \in \mathcal{H}$ if and only if there is a sequence $\{u_j\} \subset C_c^1(I)$ such that

$$\{u_j\}$$
 is Cauchy with respect to $\|\cdot\|_V$ and $u_j \to u$ in $L^2(I)$.

The key observation is the following

Proposition 2.2. The inclusion $\mathcal{H} \subset L^2(I)$ is compact: if $\{w_j\} \subset \mathcal{H}$ is bounded, then a subsequence converges strongly in $C(\overline{I})$ and thus in $L^2(I)$.

Proof. For each $j \in \mathbb{N}$, by definition, we can write $w_j = \tilde{w}_j + \xi_j$ with

$$\tilde{w}_j \in C_c^1(I) \text{ and } \|\xi_j\|_V \le 2^{-j}.$$

If $M := \sup_j \|w_j\|_V$ then $\|\tilde{w}_j\|_V \le M+1$ and so by (3) we have

$$\|\tilde{w}_j\|_{L^{\infty}(I)} + \sup_{x,y \in I} \frac{|\tilde{w}_j(x) - \tilde{w}_j(y)|}{|x - y|^{\frac{1}{2}}} \le 2M + 2.$$

Thus the family of continuous functions $\{\tilde{w}_j\} \subset C(\overline{I})$ is equibounded and equicontinuous, so — by Ascoli-Arzelá — has a subsequence $\tilde{w}_{j'} \to \bar{w}$ uniformly in $C(\overline{I})$. By (3), we also have $\xi_{j'} \to 0$ uniformly, so in conclusion $w_{j'} \to \bar{w}$ in $C(\overline{I})$.

We conclude remarking that every $u \in \mathcal{H}$ must vanish at the endpoints if I.

Exercise 2.3. By approximation, show that $\sin(\pi kx) \in \mathcal{H}$ for all $k \in \mathbb{N}$. More generally, show that if $v \in C^1(I) \cap C(\overline{I})$ with $\int_I \dot{v}^2 < \infty$ and v(0) = v(1) = 0, then $v \in \mathcal{H}$.

2.3. Weak formulation of (1). Given $f \in L^2(I)$, we say that $u \in \mathcal{H}$ solves (1) weakly if

(4)
$$\langle u, w \rangle_V = \langle f, w \rangle_{L^2}$$
 for all $w \in \mathcal{H}$.

Let us motivate this definition, assume for a second that u, f are smooth and

$$-u'' + Vu = f.$$

If we multiply both sides of the equation by $w \in C_c^1(I)$ and integrate over I we find

$$-\int_{I} u''w + Vuw = \int_{I} fw.$$

Now we can integrate by parts the first integral (the boundary term vanish!) and find

$$\langle u, w \rangle_V = \int_I u'w' + Vuw = \int_I fw = \langle f, w \rangle_{L^2}.$$

The following proposition will be crucial to "go back" from the weak formulation (4) to the classical one (1).

Proposition 2.4. Let $f \in L^2(I)$ and $u \in \mathcal{H}$ satisfying (4). Then

$$k^2c_k(u) = c_k(f - Vu) \text{ for all } k \in \mathbb{N}.$$

Proof. Fix $k \in \mathbb{N}$. By the Exercise above $w := \frac{1}{\sqrt{\pi}} \sin(k\pi x) \in \mathcal{H}$. Write $u = \tilde{u}_j + \xi_j$ with $\|\xi_j\|_V \leq 2^{-j}$. Then we have

$$\begin{split} c_k(f) &= \langle f, w \rangle_{L^2(I)} = \langle u, w \rangle_V = \langle \tilde{u}_j, w \rangle_V + \langle \xi_j, w \rangle_V \\ &= \int_I \tilde{u}_j' w' + \int_I V \tilde{u}_j w + \langle \xi_j, w \rangle_V \\ &= k^2 \int_I \tilde{u}_j w + \int_I V \tilde{u}_j w + \langle \xi_j, w \rangle_V. \end{split}$$

Passing to the limit as $j \to \infty$ we find

$$c_k(f) = k^2 c_k(u) + c_k(Vu).$$

2.4. Existence if weak solutions and the operator T. We start solving (4).

Lemma 2.5. Given $f \in L^2(I)$ there exists a unique $u \in \mathcal{H}$ such that (4) holds.

Proof. The linear functional

$$F: \mathcal{H} \to \mathbb{R}, \quad F(w) := \langle f, w \rangle_{L^2(I)},$$

is bounded in \mathcal{H} since for all $w \in \mathcal{H}$ it holds

$$|F(w)| \le ||f||_{L^2(I)} ||w||_{L^2(I)} \le 2||f||_{L^2(I)} ||w||_V.$$

Thus, by Riesz' representation Theorem in \mathcal{H} , there is a unique $u \in \mathcal{H}$ such that

$$\langle u, w \rangle_V = \langle f, w \rangle_{L^2(I)}$$
 for all $w \in \mathcal{H}$.

This means exactly that there is a unique solution u to (4).

This Lemma defines a bounded linear operator $\tilde{T}: L^2(I) \to \mathcal{H}$ as

$$\tilde{T}: L^2(I) \ni f \mapsto u \in \mathcal{H}$$
 which solves (4) for f .

Then we define the compact operator $T: L^2(I) \to L^2(I)$ as the composition

$$T \colon L^2(I) \xrightarrow{\tilde{T}} \mathcal{H} \hookrightarrow L^2(I).$$

This operator is compact because of Proposition 2.2.

Let us check that T is symmetric:

$$\langle f, Tg \rangle_{L^2(I)} = \langle Tf, Tg \rangle_V = \langle Tg, Tf \rangle_V = \langle g, Tf \rangle_{L^2(I)}.$$

2.5. Conclusion of the proof. Since T is compact and symmetric on $L^2(I)$, the Spectral Theorem 2.1 applies: there is a sequence of eigenvalues $\lambda_j \to 0$ and a complete orthonormal system of eigenfunctions $\psi_i \in L^2(I)$ such that

$$\lambda_j \langle \psi_j, w \rangle_V = \langle \psi_j, w \rangle_{L^2(I)}, \text{ for all } w \in \mathcal{H}, j \in \mathbb{N}.$$

Notice that $ran(T) \subset \mathcal{H}$, so we have $\psi_j \in \mathcal{H}$. Taking $w = \psi_j$ we also find that $\lambda_j > 0$ for all $j \in \mathbb{N}$.

In order to conclude the proof of Theorem 1.1 we must prove that each ψ_j is in fact C^{∞} in I. This is done by the so called "bootstrap" procedure, applying repeatedly Proposition 2.4.

First we have $\psi_j - V\psi_j \in L^2(I)$, so

$$\{k^2c_k(\psi_i)\}_k \in \ell^2(\mathbb{N}).$$

This immediately gives $\psi_j \in C^1(I)$ and $\psi_j' \in L^2(I)$, so $\psi_j' - (V\psi_j)' \in L^2(I)$. Then we find

$$\{k^2c_k(\psi_j - V\psi_j)\}_k \in \ell^2(\mathbb{N}).$$

Again Proposition 2.4 gives

$$\{k^4c_k(\psi_j)\}_k \in \ell^2(\mathbb{N}),$$

which in turn implies $\psi_j \in C^2(I)$ and $\psi_j'' \in L^2(I)$. Thus $\psi_j'' - (V\psi_j)'' \in L^2(I)$ and we find

$$\{k^4c_k(\psi_j - V\psi_j)\}_k \in \ell^2(\mathbb{N}).$$

and so

$$\{k^6c_k(\psi_j)\}_k \in \ell^2(\mathbb{N}).$$

It is clear that this procedure never stops and shows

$$k^M c_k(\psi_j) \in \ell^2(\mathbb{N})$$
 for all $M \geq 1$,

so $\psi_i \in C^{\infty}(I)$. Finally, by Proposition 2.4 we find

$$c_k(-\lambda_j\psi_j'' + V\psi_j - \psi_j) = 0 \text{ for all } k \in \mathbb{N},$$

and the only possibility is that each ψ_j solves

$$\lambda_j \psi_j''(x) + V(x)\psi_j(x) = \psi_j(x)$$
 for all $x \in I$.

Theorem 1.1 follows setting $\varepsilon_j := 1/\lambda_j$.

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