Math212a1410
The square well,
The discrete and the essential spectrum,
Weyl’s theorem on the stability of the essential spectrum.

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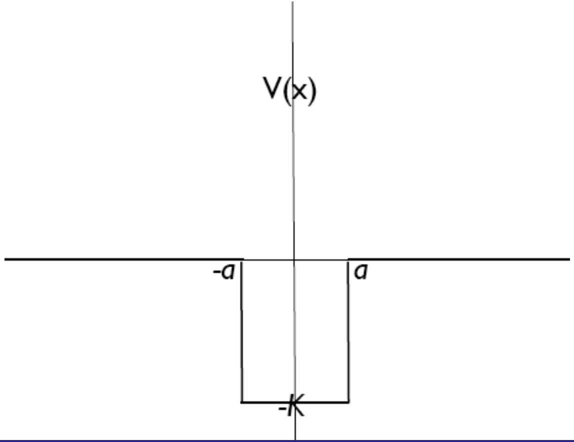
In today's lecture will be devoted to computing the spectrum of the Hamiltonian (= self adjoint operator)

$$H = H_0 + V$$

where $H_0 = -\frac{\hbar}{2m}\frac{d^2}{dx^2}$ is the "free Hamiltonian" in one dimension and the "potential" V is identically zero for $|x| > a$ and equal to $-K$ for $|x| \leq a$. See Figure 1 on the next slide. In writing $H = H_0 + V$ the "V" means multiplication by the function V. The general Schrödinger operator in non-relativistic quantum mechanics has the above form with d^2/dx^2 replaced by the Laplace operator Δ in n-dimensions (usually n = 2 or 3) and V replaced by a more general function.

The square well potential



The result

We will conclude that the spectrum of the square well operator consists of a finite number (at least one) of negative eigenvalues and a "continuous spectrum" consisting of $[0, \infty)$. The eigenvectors for the negative eigenvalues are "bound states" in the sense that they die exponentially for $|x| > a$. This result is taught near the beginning of any elementary quantum mechanics course, usually by "hand waving" definitions and methods that are unconvincing to mathematicians. There are a number of mathematical subtleties involved, and one of the purposes of this lecture is to cross some of the t's and dot some of the i's.

I realize that many of you have not taken a course in quantum mechanics and/or are not interested in physics. So just regard this lecture as an exercise in pure mathematics.

I will be hitting this computation with some sledge hammers.

Contents

The Kato-Rellich theorem, the notion of a core

We know from Lecture 8 that H_0 is a self-adjoint operator. We also know that if V is a real valued function which is bounded on bounded sets, multiplication by V is a self-adjoint operator. But is their sum self adjoint? We will prove that under suitable conditions on V the sum is indeed self-adjoint. This will be a consequence of the Kato-Rellich theorem that we will state and prove below. Before stating the theorem we make some definitions:

Definition

If A is a self-adjoint operator with domain $D(A)$, a subspace $\mathcal{D} \subset D(A)$ is called a **core** for A if the closure of the restriction of A to $\mathcal{D}$ is A.

The Kato-Rellich theorem, A boundedness

Definition

Let A and B be densely defined operators on a Hilbert space $\mathfrak{H}$. We say that B is A-**bounded** if

- $D(B) \supset D(A)$ and
- There exist non-negative real numbers a and b such that

$$\|B\phi\| \leq a\|A\phi\| + b\|\phi\| \quad \forall\ \phi \in D(A). \tag{1}$$

Notice that if

$$\|B\phi\|^2 \leq a^2\|A\phi\|^2 + b^2\|\phi\|^2 \tag{2}$$

then (1) holds.

Conversely, the relative bound

On the other hand, if (1) holds, then

$$\|B\phi\|^2 \leq a^2\|A\phi\|^2 + b^2\|\phi\|^2 + 2ab\|A\phi\|\|\phi\|.$$

Writing $ab = (a\epsilon)(b\epsilon^{-1})$ for any $\epsilon > 0$, we get

$$2ab\|A\phi\|\|\phi\| \leq a^2\epsilon^2\|A\phi\|^2 + b^2\epsilon^{-2}\|\phi\|^2.$$

Thus (1) implies (2) with a replaced by $a + \epsilon$ and b replaced by $b + \epsilon^{-1}$. Thus the infimum of a over all (a, b) such that (1) holds is the same as the infimum of a over all (a, b) such that (2) holds. This common infimum is called the **relative bound** of B with respect to A. If this relative bound is 0 we say that B is **infinitesimally small** with respect to A. In verifying (1) or (2) it is sufficient to do so for all ϕ belonging to a core of A.

The Kato-Rellich theorem, statement

The following theorem was proved by Rellich in 1939 and was extensively used by Kato in the 1960's and is known as the **Kato-Rellich theorem**.

Theorem

Let A be a self-adjoint operator and B a symmetric operator which is relatively A-bounded with relative bound $a < 1$. Then $A + B$ is self-adjoint with domain $D(A)$.

Notice that if B is a bounded operator, then it is A bounded with $a < 1$ for any A. So the Kato-Rellich theorem implies that our square well operator is self-adjoint. So at least we would know that its spectrum is real.

The Kato-Rellich theorem, proof, part 1

We know from Lecture 8 that to prove that $A+B$ is self-adjoint, it is enough to show that for some $\mu > 0$ we have that $\mathrm{Ran}(A+B \pm i\mu I) = \mathcal{H}$. We also proved in Lecture 8 the following result for any self-adjoint operator A:

Let $c = \lambda + i\mu$ be any complex number with non-zero imaginary part (i.e. $\mu \neq 0$). Then

$$(cI - A) : D(A) \to \mathfrak{H}$$

is bijective. Furthermore the inverse transformation

$$(cI - A)^{-1} : \mathfrak{H} \to D(A)$$

is bounded with bound

$$\|(cI - A)^{-1}\| \leq \frac{1}{|\mu|}.$$

The Kato-Rellich theorem, proof, part 2

For *any* $\mu > 0$ and any $\phi \in D(A)$ we have

$$\|(A \pm i\mu I)\phi\|^2 = \|A\phi\|^2 + \mu^2\|\phi\|^2.$$

We may write $\phi = (A + i\mu I)^{-1}\psi$ and rewrite the above equality (with $\pm = +$) as

$$\|\psi\|^2 = \|A(A + i\mu I)^{-1}\psi\|^2 + \mu^2\|(A + i\mu)^{-1}\psi\|^2.$$

In particular,

$$\|A(A + i\mu I)^{-1}\psi\| \le \|\psi\| \quad \text{and} \quad \|(A + i\mu I)^{-1}\psi\| \le \frac{1}{\mu}\|\psi\|.$$

The Kato-Rellich theorem, proof, part 3

$$\|A(A+i\mu I)^{-1}\psi\| \leq \|\psi\| \quad \text{and} \quad \|(A+i\mu I)^{-1}\psi\| \leq \frac{1}{\mu}\|\psi\|.$$

Substituting $\phi = (A+i\mu I)^{-1}\psi$ into

$$\|B\phi\| \leq a\|A\phi\| + b\|\phi\| \quad \forall\ \phi \in D(A) \qquad (1)$$

gives

$$\|B(A+i\mu I)^{-1}\psi\| \leq \left(a + \frac{b}{\mu}\right)\|\psi\|.$$

The Kato-Rellich theorem, proof, part 4, conclusion

$$\|B(A+i\mu I)^{-1}\psi\| \le \left(a+\frac{b}{\mu}\right)\|\psi\|.$$

Now $a<1$ by assumption. So for μ sufficiently large the operator $C := B(A+i\mu I)^{-1}$ has norm <1 and hence $I+C$ is invertible. So $\mathrm{Ran}(I+C)=\mathfrak{H}$. Also $\mathrm{Ran}(A+i\mu I)=\mathfrak{H}$ since A is self-adjoint. Hence $\mathrm{Ran}(I+C)(A+i\mu I)=\mathfrak{H}$. But

$$(I+C)(A+i\mu I)\phi=(A+B+i\mu I)\phi.$$

The same argument with $-\mu$ implies that $A+B$ is self-adjoint.

The spectrum of the Laplacian

For a general operator A on a Banach space, we defined its resolvent set to consist of those complex numbers z such that $zI - A$ maps the domain of A onto the entire Banach space, and has a bounded two sided inverse. We defined the spectrum of A as the complement of its resolvent set, and proved in Lecture 8 that the spectrum of a self-adjoint operator is real. Which real numbers belong to the spectrum of Δ? We examine this question at the Fourier transform side where Δ consists of multiplication by $\|k\|^2$. If z is a real number and $z < 0$, then the operator $\hat{f} \mapsto (z - \|k\|^2)^{-1}\hat{f}$ is bounded by $|z|^{-1}$ and maps the entire Hilbert space into the domain of Δ. So no negative real number belongs to the spectrum of Δ. I will now show that all non-negative real numbers **do** belong to the spectrum of Δ so that the spectrum of Δ consists of $[0, \infty)$.

I will use the following useful characterization of the spectrum of a self-adjoint operator as consisting of its "approximate eigenvalues".

A characterization of the spectrum of a self adjoint operator

Theorem

Let A be a self-adjoint operator on a Hilbert space $\mathfrak{H}$. A real number λ belongs to the spectrum of A if and only if there exists a sequence of vectors $u_n \in D(A)$ such that

$$\|u_n\| = 1 \text{ and } \|(\lambda I - A)u_n\| \to 0.$$

We apply this theorem to the spectrum of multiplication by $\|k\|^2$: If $\lambda \geq 0$, we can find, for any $\epsilon > 0$, a bounded function u supported in the region $|\lambda - \|k\|^2| < \epsilon$ with $\|u\| = 1$. Then $\|(\lambda I - \|k\|^2)u\| < \epsilon$. So taking $\epsilon = 1/n$ we get corresponding u_n as in in the theorem. So the theorem implies that $[0, \infty)$ is the spectrum of Δ.

$[0,\infty)$ lies in the spectrum of the square well Hamiltonian

Here is the idea: On the interval $[a,\infty)$ the equation $(H-\lambda I)\psi = 0$ becomes becomes

$$\psi'' + \gamma^2\psi = 0, \quad \text{where} \quad \gamma^2 = \frac{2m\lambda}{\hbar}.$$

The solutions to this equation are of the form $ae^{i\gamma x} + be^{-i\gamma x}$. No non-zero function of this form can belong to L_2 for $\lambda > 0$. (And it is easy to see from this that no such λ can be an eigenvalue of H.) But we can construct "approximate eigenvectors" in the sense of (our as yet unproved) Theorem: Let ϕ be a non-zero smooth function of compact support in $[0,\infty)$ with $\|\phi\| = 1$. Set

$$\psi_n(x) := n^{-\frac{1}{2}}\phi\left(\frac{x}{n} + a\right)e^{i\gamma x}.$$

$[0,\infty) \subset$ the spectrum of the square well Hamiltonian, 2

$$\psi_n(x) := n^{-\frac{1}{2}}\phi\left(\frac{x}{n}+a\right)e^{i\gamma x}.$$

Then $\|\psi_n\| = 1$ and

$$(\lambda I - H)\psi_n = \frac{\hbar^2}{2m}(\psi_n'' + \gamma^2\psi_n).$$

But

$$\psi_n'' = 2i\gamma n^{-\frac{3}{2}}\phi'\left(\frac{x}{n}+a\right) + n^{-\frac{5}{2}}\phi''\left(\frac{x}{n}+a\right) - \gamma^2\psi_n$$

So

$$\|\lambda I - H)\psi_n\| \leq \text{const.}\left(\frac{1}{n}\|\phi'\| + \frac{1}{n^2}\|\phi''\|\right) \to 0$$

showing that λ is in the spectrum. $\square$

Proof - the easy part

We now turn the proof of the theorem. First the easy direction:

Proof.

By definition, if λ does not belong to the spectrum of A then the operator $(\lambda I - A)^{-1}$ exists and is bounded, so there is a $\mu > 0$ such that

$$\|(\lambda I - A)u\| \geq \mu\|u\| \quad \forall\ u \in D(A).$$

So if $\|u_n\| = 1$ then $\|(\lambda I - A)u_n\| \geq \mu$ and can not approach 0. So if a sequence as in the theorem exists, then λ belongs to the spectrum of A. This is the easy direction; it is practically the definition of the spectrum. □

A lemma

In the other direction, suppose that no such sequence exists.

Lemma

There exists a constant $c > 0$ such that

$$\|u\| \leq c\|(\lambda I - A)u\| \;\; \forall\, u \in D(A). \quad (3)$$

We prove the lemma:

Proof.

If not, there would exist a sequence v_n of non-zero elements of $D(A)$ with

$$\|(\lambda I - A)v_n\|/\|v_n\| \to 0.$$

Replacing v_n by $u_n := v_n/\|v_n\|$ gives a sequence of unit vector in $D(A)$ with $\|\lambda I - A)u_n\| \to 0$. This establishes (3). □

Using the lemma

From the inequality (3) we conclude that the map $\lambda I - A$ is injective. We can also conclude that its image is closed. For if $w_n = (\lambda I - A)u_n,\ u_n \in D(A)$ with $w_n \to w$, then (3) implies that the sequence u_n is Cauchy and so converges to some $u \in \mathfrak{H}$. We want to show that $u \in D(A)$. For any $v \in D(A)$ we have

$$\begin{aligned}(u, (\lambda I - A)v) = \lim_{n\to\infty}(u_n, (\lambda I - A)v) &= \lim((\lambda I - A)u_n, v) \\ &= \lim_{n\to\infty}(w_n, v) = (w, v).\end{aligned}$$

So $u \in D((\lambda I - A)^*) = D(A^*) = D(A)$ since A is self-adjoint. To show that λ is in the resolvent set of A we must show that the image of $(\lambda I - A)$ is all of $\mathfrak{H}$:

Conclusion of the proof of the theorem characterizing the spectrum

Let $f \in \mathfrak{H}$ and consider the linear function on the image of $\lambda I - A$ given by

$$w \mapsto (v, f) \quad \text{where} \quad w = (\lambda I - A)v.$$

Now $|(v, f)| \le \|f\| \|v\|$ and by (3), this is $\le c\|f\|w\|$. So this linear function is bounded on the image of $\lambda I - A$. But this image, being a closed subspace of $\mathfrak{H}$ as we have just proved, is a Hilbert space in its own right, and so we may apply the Riesz representation theorem to conclude that there is a u in the image of $\lambda I - A$ such that

$$((\lambda I - A)v, u) = (v, f) \ \ \forall \ v \in D(A).$$

Since A, and hence $\lambda I - A$ is self-adjoint, this implies that $u \in D(A)$ and $(\lambda I - A)u = f$.

No spectrum of the square well Hamiltonian below $-K$

We will use the proof we just gave to conclude the above fact. Indeed, let us state the result more generally:

Proposition

Suppose (in any dimension) the potential V has the property that the operator $H = H_0 + V$ is self-adjoint and that there is some constant C such that $V \geq C$. Then any $\lambda < C$ is in the resolvent set of H.

Proof of the proposition

Proof.

We have $(H\psi,\psi) = \frac{\hbar}{2m}\|k\hat{\psi}(k)\|^2 + (V\psi,\psi)$ so

$$((H-\lambda I)\psi,\psi) \geq (V\psi,\psi) - \lambda(\psi,\psi) \geq (C-\lambda)(\psi,\psi)$$

is non-negative and applying Cauchy-Schwarz we get

$$\|\psi\| \leq c\|(\lambda I - A)\psi\| \quad \forall\ \psi \in D(A) \tag{3}$$

with $c = \frac{1}{C-\lambda}$. □

What we know so far

We now know the following facts about the square well:

- All of $[0, \infty)$ lies in the spectrum, and there are no eigenvalues there.
- There is no spectrum below $-K$.

I will now show that the spectrum lying in $[-K, 0)$ consists of eigenvalues which we will then compute.

The idea goes back to a theorem of Hermann Weyl of 1909(!) which asserts that the essential spectrum of a self adjoint operator (definition in a moment) is unchanged by perturbation by a compact operator.

Isolated points of the spectrum, the discrete spectrum, the essential spectrum

We let $\sigma = \sigma(A)$ denote the spectrum of the self-adjoint operator A. A point $\lambda \in \sigma$ is **isolated** if it is an eigenvalue of finite multiplicity with the property that there is an $\epsilon > 0$ such that the interval $(\lambda - \epsilon, \lambda + \epsilon)$ contains no other points of the spectrum of A.

The **discrete spectrum** of A consists of the set of isolated points of the spectrum and is denoted by $\sigma_d(A)$, or simply by σ_d when A is fixed in the discussion.

The complement of the discrete spectrum in $\sigma(A)$ is called the **essential spectrum** of A and is denoted by $\sigma_{\mathrm{ess}}(A)$ or simply by σ_{ess} when A is fixed in the discussion.

Characterizing the essential spectrum, 1

Suppose that λ is an isolated point of the spectrum. Let $\mathfrak{H}_\lambda$ denote the eigenspace with eigenvalue λ so $\mathfrak{H}_\lambda$ is finite dimensional by assumption. Decompose $\mathfrak{H}$ into the direct sum

$$\mathfrak{H} = \mathfrak{H}_\lambda \oplus \mathfrak{H}_\lambda^\perp.$$

The entire interval $(\lambda - \epsilon, \lambda + \epsilon)$ lies in the resolvent set of the restriction of A to $\mathfrak{H}_\lambda^\perp$. So the restriction of $\lambda I - A$ to $\mathfrak{H}_\lambda^\perp$ has a bounded inverse. So if $\psi_n \in D(A)$ is a sequence of elements of $\mathfrak{H}$ with

- $\|\psi_n\| = 1$ and
- $(\lambda I - A)\psi_n \to 0$

then the $\mathfrak{H}_\lambda^\perp$ components of the ψ_n must tend to 0. The $\mathfrak{H}_\lambda$ components then form a bounded sequence in a finite dimensional space, and hence we can extract a convergent subsequence. So we have proved one half of the following

Characterizing the essential spectrum, 2

Theorem

A point λ belongs to the essential spectrum of a self-adjoint operator A if and only if there exists a sequence $\psi_n \in D(A)$ such that

- $\|\psi_n\| = 1$,
- ψ_n *has no convergent subsequence, and*
- $(\lambda I - A)\psi_n \to 0$.

Characterizing the essential spectrum, 3

We have indeed proved that if λ does not belong to the essential spectrum then there can not exist such a sequence, for if λ lies in the resolvent set then $(\lambda I - A)^{-1}$ is bounded and so no sequence with $\|\psi_n\| = 1$ and $(\lambda I - A)\psi_n \to 0$ can exist, while if λ is an isolated point of the spectrum we have already proved that no sequence satisfying the conditions of the theorem can exist.

Characterizing the essential spectrum, 4

Conversely, suppose that λ lies in the essential spectrum. We want to construct a sequence as in the theorem. If λ is an eigenvalue of infinite multiplicity, we can construct an orthonormal sequence of eigenvectors ψ_n so $(\lambda I - A)\psi_n = 0$ and the ψ_n have no convergent subsequence.

Otherwise we can find a sequence of λ_n lying in the spectrum of A with $\lambda_n \neq \lambda$ and $\lambda_n \to \lambda$. So $\lambda - \lambda_n \neq 0$ and $\lambda - \lambda_n$ lies in the spectrum of $A - \lambda_n I$ and hence by our Theorem characterizing the spectrum, we can find ψ_n with $\|\psi_n\| = 1$ and

$$\|(\lambda_n I - A)\psi_n\| \leq \frac{1}{n}|\lambda_n - \lambda|,$$

so $(\lambda I - A)\psi_n \to 0$.

Characterizing the essential spectrum, 5

We wish to prove that ψ_n has no convergent subsequence. If it did, then passing to the subsequence (and relabeling) we would have $\psi_n \to \psi$ with $\|\psi\| = 1$ and ψ an eigenvector of A with eigenvalue λ.
Then

$$(\lambda - \lambda_n)(\psi_n, \psi) = (\psi_n, A\psi) - \lambda_n(\psi_n, \psi) = ((A - \lambda I)\psi_n, \psi),$$

so

$$|\lambda - \lambda_n||(\psi_n, \psi)| \leq \frac{1}{n}|\lambda_n - \lambda|,$$

which is impossible since $(\psi_n, \psi) \to 1$. □

Characterizing the essential spectrum, 6

It will be convenient to replace the middle condition in the theorem by a slightly different one: A sequence ψ_n is said to converge **weakly** to ψ if for every $v \in \mathfrak{H}$

$$(\psi_n, v) \to (\psi, v).$$

It is easy to see that every bounded sequence in a separable Hilbert space has a weakly convergent subsequence. Indeed, if the ψ_n are bounded, then for each fixed v $\{(\psi_n, v)\}$ is a bounded sequence of complex numbers by Cauchy-Schwarz.

On the other hand, suppose that $\psi_n \in \mathfrak{H}$ satisfies

$$\|\psi_n\| = 1 \text{ and } \psi_n \text{ converges weakly to 0.}$$

Then ψ_n can have no (strongly) convergent subsequence because the strong limit of any subsequence would have to equal the weak limit and hence $= 0$ contradicting the hypothesis $\|\psi_n\| = 1$.

Characterizing the essential spectrum, 7

Proposition

A $\lambda \in \mathbb{R}$ belongs to the essential spectrum of a self adjoint operator A if and only if there exists a sequence $\psi_n \in D(A)$ such that

1. $\|\psi_n\| = 1$,
2. ψ_n *converges weakly to* 0, *and*
3. $(\lambda I - A)\psi_n \to 0$.

If the first two conditions are satisfied then the ψ_n can not have a convergent subsequence, as we have just seen. So the conditions of Theorem 6 are satisfied, and hence λ belongs to the essential spectrum of A.

Characterizing the essential spectrum, 8

Conversely, if λ belongs to the essential spectrum of A then we can find a sequence ψ_n satisfying the three conditions of Theorem 6. The first condition implies that the ψ_n are uniformly bounded so we can choose a subsequence which converges weakly to some $\psi \in \mathfrak{H}$. Let us pass to this subsequence (and relabel). Since our ψ_n has no convergent subsequence, there is an $\epsilon > 0$ such that

$$\|\psi_n - \psi\| \geq \epsilon$$

for all n. By the third condition in the Theorem

$$(\psi_n, (A - \lambda I)\phi) = ((A - \lambda I)\psi_n, \phi) \to 0 \quad \forall\ \phi \in D(A)$$

so

$$(\psi, (A - \lambda I)\phi) = 0 \quad \forall \phi \in D(A).$$

Characterizing the essential spectrum, 9

We have proved that

$$(\psi, (A - \lambda I)\phi) = 0 \quad \forall \phi \in D(A).$$

Since A is self-adjoint, this implies that $\psi \in D(A)$ and $A\psi = \lambda\psi$. Consider the sequence

$$\tilde{\psi}_n := \frac{1}{\|\psi_n - \psi\|}(\psi_n - \psi).$$

We have $\|\tilde{\psi}_n\| = 1$ and $(\tilde{\psi}_n, u) \to 0$ for all $u \in \mathfrak{H}$. So the first two conditions of the Proposition are satisfied. So is the third because

$$(A - \lambda I)\tilde{\psi}_n = \frac{1}{\|\psi_n - \psi\|}(A - \lambda I)\psi_n \to 0$$

since $\|\psi_n - \psi\| \geq \epsilon > 0$. □

Weyl's theorem on the stability of the essential spectrum

We now come to the great theorem of Hermann Weyl. Let A be a self adjoint operator. An operator B is called **compact relative to** A or, more simply A-compact if

1. $D(A) \subset D(B)$ and
2. If $u_n \in D(A)$ is a sequence with
$$\|u_n\| + \|Au_n\| \leq C$$
for some constant C then the sequence Bu_n has a convergent subsequence.

For example, a compact operator is A-compact for any A.

Theorem

[Weyl.] *If A is a self-adjoint and B is a symmetric operator which is A compact then $A + B$ is self-adjoint and has the same essential spectrum as A.*

Preview: How we will use Weyl's theorem

We will show that if V is a bounded potential of compact support then it is H_0 compact and hence $H_0 + V$ has the same essential spectrum as H_0 which is $[0, \infty)$. This allows us to conclude that the negative elements of the spectrum of $H_0 + V$ are eigenvalues with finite multiplicity.
In today's lecture I will prove this fact in one dimension, using special facts about H_0 in one dimension. I will discuss the general situation in a much later lecture (I hope). We will be able to use the one dimensional facts to see how to compute the eigenvalues for the square well.

But first to the proof of Weyl's theorem:

Proof that $A + B$ is self-adjoint

We will prove that B is infinitesimally small with respect to A. Then Kato-Rellich implies that $A + B$ is self-adjoint. For this we begin by proving that B is A-bounded. More precisely, we claim that there are constants k and k' such that

$$\|Bu\| \leq k(\|Au\|+\|u\|) \leq k'(\|Au\|+\|(A+B)u|) \quad \forall \ u \in D(A). \quad (4)$$

Indeed, if the first inequality did not hold we would be able to find a sequence of $u_n \in D(A)$ with $\|Au_n\| + \|u_n\| = 1$ and $\|Bu_n\| \to \infty$, so Bu_n has no convergent subsequence.

If the second inequality did not hold, we could find a sequence of $u_n \in D(A)$ with $\|Au_n\| + \|u_n\| = 1$ and $\|u_n\| + \|(A + B)u_n\| \to 0$. By passing to a subsequence we may assume that $Bu_n \to u$ in which case we must have $Au_n \to -u$. We also must have $u_n \to 0$, so $u = 0$. But then $Au_n \to 0$ and $u_n \to 0$ contradicts the hypothesis $\|Au_n\| + \|u_n\| = 1$.

Proof that $A + B$ is self-adjoint, 2

We know that there are constants k and k' such that

$$\|Bu\| \leq k(\|Au\|+\|u\|) \leq k'(\|Au\|+\|(A+B)u|) \quad \forall \; u \in D(A). \quad (4)$$

We can now prove that B is infinitesimally small with respect to A, i.e. that for any $\epsilon > 0$ there is a K_ϵ such that

$$\|Bu\| \leq \epsilon\|Au\| + K_\epsilon\|u\| \quad \forall \; u \in D(A).$$

Suppose not. This means that there is some $\epsilon > 0$ such that for any n we can find a $u_n \in D(A)$ with $\|u_n\| + \|Au_n\| = 1$ (so $\|Bu_n\| \leq k$) and

$$\|Bu_n\| > \epsilon\|Au_n\| + n\|u_n\|.$$

Proof that $A + B$ is self-adjoint, 3

So $u_n \to 0$ and hence $\|Au_n\| \to 1$. By passing to a convergent subsequence, we may assume that $Bu_n \to w$, and hence $w = 0$, since $(Bu_n, v) = (u_n, Bv) \to 0$ for any $v \in D(A)$ because B is symmetric. On the other hand,

$$\|w\| = \lim \|Bu_n\| \geq \lim \epsilon \|Au_n\| \to \epsilon > 0.$$

So we now know from Kato-Rellich that $A + B$ is self adjoint with domain $D(A)$.

Proof that the essential spectrum of A is contained in the essential spectrum of $A+B$

Proof.

Suppose that $\lambda \in \sigma_{\mathrm{ess}}(A)$. Choose ψ_n as in the proposition. Condition 1 says that the $\|\psi_n\| = 1$, and condition 3, which says that $(\lambda I - A_n) \to 0$ then implies that $\|A\psi_n\| + \|\psi_n\|$ is bounded. Since B is A compact, we can pass to a subsequence so that now $B\psi_n$ converges, say to u. For any $\phi \in D(A)$ we have

$$(u, \phi) = \lim(B\psi_n, \phi) = \lim(\psi_n, B\phi) = 0$$

by condition 2) which says that ψ_n converges weakly to 0. Since $D(A)$ is dense in $\mathfrak{H}$ this implies that $u = 0$. Thus

$$\lim((A + B - \lambda I)\psi_n = 0$$

which is condition 3 of the Proposition for $A + B$. □

Proof that the essential spectrum of A contains the essential spectrum of $A+B$

To prove this, by the preceding result, it is enough to prove that B (and hence $-B$) is compact relative to $A+B$.

Proof.

So suppose that

$$\|u_n\| \leq C(\|u_n\| + \|(A+B)u_n\|$$

for some constant C. Then it follows from the second inequality in

$$\|Bu\| \leq k(\|Au\| + \|u\|) \leq k'(\|Au\| + \|(A+B)u|) \quad \forall \quad u \in D(A) \quad (4)$$

that

$$\|u_n\| \leq C'(\|u_n\| + \|Au_n\|$$

with $C' = (k'/k)C$, completing the proof of Weyl's theorem. □

The domain of H_0 in one dimension

Recall that (in any dimension) we defined the domain of H_0 as the set of all $u \in L_2(\mathbb{R}^n)$ such that its Fourier transform $\hat{u}$ is such that $k^2 u \in L_2$ in which case $H_0 u$ is the inverse Fourier transform of $k^2 \hat{u}(k)$.

In one dimension we will see that if $u \in D(H_0)$ then u "is" a continuous function with a continuous derivative. Since elements of L_2 are equivalence classes of functions rather than actual functions, I have to be a bit careful about how I say this. I will borrow language from measure theory (which we have not yet studied) and use the phrase "almost everywhere equal to" (which you can safely ignore) so that I don't get fired from my job.

Continuity

Lemma

If $\hat{u}$ and $k\hat{u}(k)$ are both in L_2 then u is (almost everywhere equal to) a continuous function.

By the Fourier inversion formula

$$u(x) - u(y) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} (e^{ikx} - e^{iky})\hat{u}(k)dk.$$

Apply Cauchy-Schwarz to the right hand side written in the form

$$\int_{\mathbb{R}} (e^{ikx} - e^{iky})(1+k^2)^{-1/2} \times (1+k^2)^{1/2}\hat{u}(k)dk.$$

and use the facts that $1/(1+k^2)$ is integrable in one dimension and the function $x \mapsto e^{ikx}$ is continuous.

Differentiablilty

Theorem

The elements of $D(H_0)$ are (almost everywhere equal to) continuously differentiable functions.

If $\hat{u}$ and $k^2\hat{u}(k)$ are in L_2 so is $k\hat{u}(k)$ so we know from the lemma that u is (almost everywhere equal to) a continuous function. Let

$$w(x) := \frac{i}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{ikx} k\hat{u}(k) dk.$$

By the argument we gave for the lemma, this is "continuous".

Proof of the theorem

We have

$$\frac{u(x)-u(y)}{x-y} - w(y) = \frac{i}{\sqrt{2\pi}} \int_{\mathbb{R}} \left[\frac{e^{ikx}-e^{iky}}{ik(x-y)} - e^{iky} \right] k\hat{u}(k)dk.$$

Again by Cauchy-Schwarz

$$\left| \frac{u(x)-u(y)}{x-y} - w(y) \right|^2 \leq$$

$$\frac{1}{2\pi} \int_{\mathbb{R}} \left| \frac{e^{ikx}-e^{iky}}{ik(x-y)} - e^{iky} \right|^2 \frac{dk}{k^2+1} \times \int_{\mathbb{R}} (k^2+1)k^2|\hat{u}(k)|^2 dk.$$

The second factor is finite and independent of x and y and the first factor tends to zero. This shows that the derivative of u equals w which is continuous. $\square$

Since $D(H) = D(H_0)$ for the operators of the form $H = H_0 + V$ that we shall consider, we will be able to use the continuity of u and u' to prove that V is H_0 bounded and to determine the eigenfunctions of H. In all the usual physics texts that I have seen, the continuity of u and u' is taken for granted as "physical property" that is need for a state.

In what follows we will use a familiar argument - that since $\left(\frac{1}{\sqrt{2}} - \frac{k^2}{\sqrt{2}}\right)^2 \geq 0$ we have the inequality

$$k^2 \leq \frac{1}{2} + \frac{1}{2}k^4.$$

A Gårding style estimate

Let us go back to the Fourier inversion formula which tells us that

$$u(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{ikx} \hat{u}(k) dk \quad \text{and} \quad u'(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{ikx} k \hat{u}(k) dk$$

from which we deduce that for $u \in D(H_0)$ we have

$$|u(x)|^2 \leq \frac{1}{2\pi} \int_{\mathbb{R}} (1+k^2)|\hat{u}(k)|^2 dk \times \int_{\mathbb{R}} (1+k^2)^{-1} dk$$

and from which we deduce that for $u \in D(H_0)$ we have

$$|u'(x)|^2 \leq \frac{1}{2\pi} \int_{\mathbb{R}} (1+k^2)k^2|\hat{u}(k)|^2 dk \times \int_{\mathbb{R}} (1+k^2)^{-1} dk.$$

Since $k^2 \leq \frac{1}{2} + \frac{1}{2}k^4$ we conclude that there is a constant C such that for any $u \in D(H_0)$ we have

$$|u(x)|^2 + |u'(x)|^2 \leq C(\|u\|^2 + \|H_0 u\|^2) \quad \forall\, x \in \mathbb{R}. \tag{5}$$

Using $|u(x)|^2 + |u'(x)|^2 \leq C(\|u\|^2 + \|H_0 u\|^2) \ \ \forall\, x \in \mathbb{R}$ (5)

Let u_n be a sequence of elements in $D(H_0)$ such that

$$\|H_0 u_n\| + \|u_n\| \leq k$$

for some constant k. Then for any bounded interval I on the real line we can choose a subsequence of the u_n which converge uniformly on I by Arzela-Ascoli.

Let V be a bounded (say piecewise continuous or even Lebesgue measurable) function of compact support (meaning that it vanishes outside some bounded interval) I. Let u_{n_k} be the subsequence as above. Then the uniform convergence of the u_{n_k} implies that the sequence Vu_{n_k} converges in L_2. We have proved that

V is H_0 compact.

Using symmetry

Here is the simplest example of the use of group theory to facilitate the computation of eigenvalues: Let U be a unitary operator on $\mathfrak{H}$ that satisfies $U^2 = I$. So $\mathfrak{H}$ decomposes as a direct sum

$$\mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-$$

where $\mathfrak{H}_+$ consists of those $u \in \mathfrak{H}$ which satisfy $Uu = u$ and $\mathfrak{H}_-$ consists of those $u \in \mathfrak{H}$ which satisfy $Uu = -u$. Indeed, writing

$$u = \frac{1}{2}(u + Uu) + \frac{1}{2}(u - Uu)$$

gives such a decomposition.

Using symmetry, 2

If H is a self-adjoint operator which commutes with U then H leaves each of the subspaces $\mathfrak{H}_\pm$ invariant. Furthermore if $Hu = \lambda u$ and we decompose $u = u_+ + u_-$ according to the above decomposition of $\mathfrak{H}$, then each of the components $u_\pm$ also satisfies $Hu_\pm = \lambda u_\pm$.

A key tool in replacing the two element group $\mathbb{Z}/\mathbb{Z}_2$ by a more general compact group is the Peter-Weyl theorem which you will study in the problem set as a consequence of the theorem about the spectrum of compact self-adjoint operators.

Using symmetry, 3

We apply this to $\mathfrak{H} = L_2(\mathbb{R})$ and U given by

$$(Uf)(x) = f(-x).$$

Clearly H_0 commutes with U. If $V(x) = V(-x)$ then multiplication by V commutes with U. So, for example, every eigenvector of the Schrödinger operator for the square well potential can be decomposed as above, and so we need only study even eigenvectors (those lying in $\mathfrak{H}_+$ or odd eigenvectors, (those lying in $\mathfrak{H}_-$).

The eigenvector equation in each region

Let

$$\alpha := \left(\frac{2m(\lambda + K)}{\hbar^2}\right)^{\frac{1}{2}} \quad \text{and} \quad \beta := \left(\frac{-2m\lambda}{\hbar^2}\right)^{\frac{1}{2}}$$

where $-K \leq \lambda < 0$ and we take the positive square roots. For $|x| < a$ the equation $Hu = \lambda u$ is

$$u'' = -\alpha^2 u \tag{6}$$

while for $|x| > a$ the equation $Hu = \lambda u$ is

$$u'' = \beta^2 u. \tag{7}$$

For $x > a$ the only solution of (7) which belongs to L_2 is of the form

$$u(x) = Ce^{-\beta x}.$$

The even eigenvectors

The even solutions of (6) are of the form

$$u(x) = B\cos \alpha x.$$

The logarithmic derivative, u'/u of this function at $x = a$ is $-\alpha \tan \alpha a$. The logarithmic derivative of $Ce^{-\beta x}$ at $x = a$ is $-\beta$. These must be equal by the differentiability properties of elements of the domain of H_0. So we obtain the condition:

The eigenvalues of the even eigenvectors

$$\alpha \tan \alpha a = \beta. \tag{8}$$

To understand the solutions of this equation set

$$\xi := \alpha a \quad \text{and} \quad \eta = \beta a$$

so that

$$\xi^2 + \eta^2 = \frac{2mKa^2}{\hbar^2}, \tag{9}$$

the equation of a circle in the (ξ, η) plane.

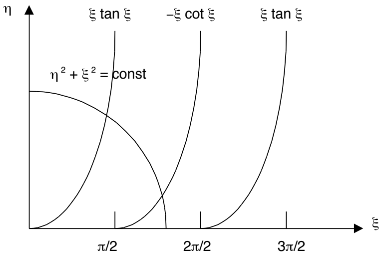
The even eigenvectors, 2

Equation (8) becomes

$$\xi \tan \xi = \eta \qquad (10)$$

and we are interested is solutions with positive values of ξ and η. The solutions of this equation are the intersections of the curves $(\xi, \xi \tan \xi)$ with the circle (9). As ξ varies from 0 to $\pi/2$, $\xi \tan \xi$ increases from 0 to ∞, so the curve $\eta = \xi \tan \xi$ always intersects the circle. This shows that that there always is at least one (even) eigenvector.

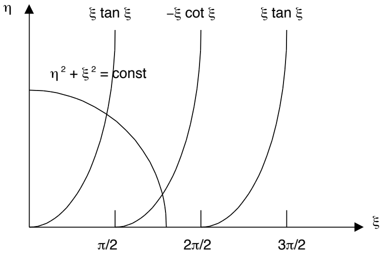
Graphic description of the eigenvalues



The actual values of *E* obtained from the intersections must be determined numerically.

As ξ varies from 0 to $\pi/2$ the value of $\xi \tan \xi$ increases from 0 to ∞ and so $(\xi, \xi \tan \xi)$ intersects the circle. From $\pi/2$ to π, $\xi \tan \xi$ is negative and so makes no appearance in the first quadrant.

Graphic description of the eigenvalues



The actual values of *E* obtained from the intersections must be determined numerically.

From π to $3\pi/2$ the we get a translate of the original curve. So we get the translates of the original curve by multiples of π in the ξ direction. As soon as $n\pi$ exceeds the radius of the circle (9), we no longer can have an intersection. This shows that there are only finitely many eigenvalues corresponding to even eigenvectors.

In fact, the number of "even" eigenvalues is the integer n such that

$$n\pi \leq \frac{2mKa^2}{\hbar^2} < (n+1)\pi.$$

Notice also that the continuity of u at a requires that $Ce^{-\beta a} = B\cos\alpha a$ which shows that each of the eigenvalues has multiplicity one.
I will leave the computation of the odd eigenvalues to you as an exercise, or you can read it in any qm book.

Tunneling

Notice that though the eigenvectors are exponentially decaying, they are not zero outside the well. This is in contrast to a classical particle trapped in a well which can not escape. This phenomenon is known as “tunneling”.

Some comments.

We proved by explicit computation that the eigenvectors of the square well potential die exponentially at infinity. The general theory of such exponential decay can be found the book by my old friend Shmuel Agmon *Lectures on Exponential Decay of Solutions of Second Order Elliptic Equations*, Princeton University Press. (I met Shmuel in 1956 when I was a post doc at NYU.)

A simplified version of the general theory developed by Agmon can be found in Chapter 3 of the excellent book Introduction to Spectral Theory, with application to Schrödinger operators by Hislop and Sigal, Springer (1996).

One can make weaker assumptions on the potential V than those needed to get exponential decay of the eigenvectors but still conclude that they are "bound states" in an appropriate sense. The key result in this direction is due to Ruelle, and an excellent exposition of Ruelle's result, and a nice genealization of it can be found in the paper by W.O. Amrein and V. Georgescu in *Helvetica Physica Acta* **46** (1973) pp. 636 - 658.