Interacting waves

In the notes on free waves [FW] we studied the basic equations

$$\partial_t^2 u(x,t) - c^2 \Delta u(x,t) = 0, \qquad i\hbar\partial_t u(x,t) = -\frac{\hbar^2}{2m}\Delta u(x,t),$$

where $x \in \mathbb{R}^d$ is the spatial variable and $t \in \mathbb{R}$ is time. They represent well moderate waves in an unvarying medium not subject to any forces beyond the ones used to derive the equations. As the waves become less moderate (for example strong vibrations in the first case, or rapidly moving electrons in the second case) or as changes in the medium or additional forces come into play, the equations must be modified accordingly. In this part we study some of these modifications.

The simplest kind of modification is adding a potential energy term $V(x)u(x,t)$, which in the case of the wave quation gives

$$\partial_t^2 u(x,t) - c^2 \Delta u(x,t) + V(x)u(x,t) = 0.$$

For a vibrating string or membrane this corresponds to a force which is proportional to displacement, with the constant of proportionality depending on the position. For an elastic restoring force, this comes from Hooke's law and V is positive.

The general Schrödinger equation is given by

$$i\hbar\partial_t u(x,t) = -\frac{\hbar^2}{2m}\Delta u(x,t) + V(x)u(x,t), \tag{1}$$

where V is the potential energy arising from forces on the particles represented by u.

Later we will consider more complicated and more general modifications as well, including connections to other physical problems such as fluids, electromagnetic waves, and acoustic waves.

The Schrödinger equation of the seemingly simple form (1), for suitable choices of V, governs very general physical systems, including many-body problems. To explain this, we recall our derivation of (1) for a single particle moving in Euclidean space.

Let $x \in \mathbb{R}^3$ be the position and $\xi \in \mathbb{R}^3$ the momentum of such a particle, and let $m > 0$ be its mass. Suppose it is subject to a force arising from a potential function $V(x)$. The *classical Hamiltonian function*

$$H(x,\xi) = \frac{1}{2m}|\xi|^2 + V(x), \tag{2}$$

gives the total energy (kinetic plus potential) of the particle at position x and momentum ξ. The corresponding quantum Hamiltonian operator is obtained by multiplying by $e^{ix\cdot\xi/\hbar}$ and using $\xi e^{ix\cdot\xi/\hbar} = -i\hbar\nabla e^{ix\cdot\xi/\hbar}$ to get

$$H(x,\xi)e^{ix\cdot\xi/\hbar} = H(x,-i\hbar\nabla)e^{ix\cdot\xi/\hbar},$$

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where

$$H(x, -i\hbar\nabla) = -\frac{\hbar^2}{2m}\Delta + V(x), \tag{3}$$

and (3), applied to $u(x,t)$, is the right hand side of (1).[1] For a two-body system, the classical Hamiltonian is

$$H(x, \xi) = \frac{1}{2m_1}|\xi_1|^2 + \frac{1}{2m_2}|\xi_2|^2 + V(x),$$

where $x_1,\ x_2 \in \mathbb{R}^3$ are the positions of the two particles, $\xi_1,\ \xi_2 \in \mathbb{R}^3$ are their momenta, $m_1,\ m_2 > 0$ are their masses, and we write $x = (x_1, x_2) \in \mathbb{R}^6$, and $\xi = (\xi_1, \xi_2) \in \mathbb{R}^6$. The corresponding quantum Hamiltonian is

$$H(x, -i\hbar\nabla) = -\frac{\hbar^2}{2m_1}\Delta_1 - \frac{\hbar^2}{2m_2}\Delta_2 + V(x),$$

and if we apply it to $u(x,t)$ and make the simplifying assumption that the masses are equal we get the right hand side of (1) again, but this time with $x \in \mathbb{R}^6$. Similarly, taking $x \in \mathbb{R}^{3N}$ in (1) gives an equation for N particles all having the same mass. In the case that there is no force on the particles (non-interacting particles), we have $V = 0$ and (1) becomes the free Schrödinger equation to which our results from Section 5 of the notes on free waves apply directly.

For a concrete example, take $x \in \mathbb{R}^3$ and $V(x) = -1/|x|$ to study one electron interacting with one proton. Here we are ignoring the movement and size of the proton (this is the *Born–Oppenheimer* approximation) and $V(x)$ is the Coulomb potential arising from the attractive electric force between the electron and the proton. The simplest and most important solution in this case is the one which has the form

$$u(x,t) = e^{-iEt/\hbar}e^{-|x|/R}, \tag{4}$$

for suitable energy $E \in \mathbb{R}$ and length scale $R > 0$. This is called the *ground state* of the electron in the hydrogen atom. It is called a stationary state because the probability density $|u(x,t)|^2$ is independent of t. It is the state occupied by the electron when the atom is at rest.

Exercise 1. Use the fact that the Laplacian in polar coordinates on $\mathbb{R}^d$ is given by $\Delta = \partial_r^2 + \frac{d-1}{r}\partial_r + \frac{1}{r^2}\Delta_{\mathbb{S}^{d-1}}$, where $\Delta_{\mathbb{S}^{d-1}}$ is an appropriate differential operator in the angular variables (the Laplacian on the unit sphere) to find E and R such that (4) solves (1) with $x \in \mathbb{R}^3$ and $V(x) = -1/|x|$.

The hydrogen atom is the simplest and most important atom. If we move on to the next one up, the helium atom, the corresponding form of V is

$$V(x) = \frac{1}{|x_1 - x_2|} - \frac{2}{|x_1|} - \frac{2}{|x_2|},$$

and there is no longer any simple formula for the ground state or for any other state. More generally, we may consider a system of N electrons in a molecule made up of M atoms. Then the corresponding form of V is

$$V(x) = \sum_{1 \le j < k \le N} \frac{1}{|x_j - x_k|} - \sum_{j=1}^{N}\sum_{\ell=1}^{M} \frac{Z_\ell}{|x_j - X_\ell|},$$

[1] See Section 5 of [FW] and the Further Discussion and References there for more on this.

where X_k is the position of the kth nucleus and Z_k is the number of protons it has. The problem of finding good ways to analyze such a system, and particularly to calculate its ground state energy to reasonable accuracy, has been a very important one, going back to the time it was first able to be formulated and right down to the present day.

An operator of the form (3) is called a *Schrödinger operator*. We begin our study of them with the simplest one, the *harmonic oscillator*. It is important both as a concrete example where the results and formulas are fairly explicit and simple, and as a tool in the analysis of the more complicated problems we will consider afterwards.

1. Harmonic Oscillator. The harmonic oscillator potential energy function is $V(x) = \frac{1}{2}k|x|^2$, where $k > 0$. The classical equations of motion are given by Newton's law $m\frac{d^2x}{dt^2} = -\nabla V(x) = -kx$, and they are solved by $x(t) = A\cos(\sqrt{k/mt}) + B\sin(\sqrt{k/mt})$. This is the *classical harmonic oscillator problem*. It describes small oscillations about a nondegenerate stable equilibrium, such as those of a pendulum or spring.

The corresponding quantum problem is

$$i\hbar\partial_t u(x,t) = Hu(x,t) = -\frac{\hbar^2}{2m}\Delta u(x,t) + \frac{1}{2}k|x|^2 u(x,t). \tag{5}$$

We begin by finding the stationary states, and then construct general solutions as superpositions of those. To make the calculations as simple as possible we begin with dimension $d = 1$ and we take $\hbar = 1$, $m = 1/2$, and $k = 2$.

We find the stationary states by solving the *eigenvalue equation*

$$Hu_n = -u_n''(x) + x^2 u_n(x) = E_n u_n(x). \tag{6}$$

Then $e^{-itE_n}u_n(x)$ solves (5), and $\cos(t\sqrt{E_n})u_n(x)$ and $\sin(t\sqrt{E_n})u_n(x)$ solve the corresponding wave equation $(\partial_t^2 - \partial_x^2 + x^2)u(x,t) = 0$. The word *stationary* comes from the fact that if $u(x,t) = e^{-itE_n}u_n(x)$, then the probability density $|u(x,t)|^2$ is independent of t, and so in that sense a particle in a stationary state does not move.

To solve (6) we use a variant of the factorization technique we used for the free wave equation $(\partial_t^2 - \partial_x^2)u(x,t) = (\partial_t + \partial_x)(\partial_t - \partial_x)u(x,t)$. We have the almost-factorizations

$$(-\tfrac{d^2}{dx^2} + x^2)u_n = (-\tfrac{d}{dx} + x)(\tfrac{d}{dx} + x)u_n + u_n, \tag{7}$$

and

$$(-\tfrac{d^2}{dx^2} + x^2)u_n = (\tfrac{d}{dx} + x)(-\tfrac{d}{dx} + x)u_n - u_n. \tag{8}$$

These are based on the almost-commutativity property $\frac{d}{dx}xu_n - x\frac{d}{dx}u_n = u_n$; the operator on the left $\frac{d}{dx}x - x\frac{d}{dx}$ is the *commutator* of the operators $\frac{d}{dx}$ and x and it measures how far away the two operators are from commuting with one another.

The simplest solution to (6) is given by using (7) and solving $(\frac{d}{dx} + x)u_0 = 0$. That leads to

$$u_0(x) = e^{-x^2/2}, \qquad E_0 = 1. \tag{9}$$

This is called the *ground state*, because it has the lowest energy of any state: as we shall see momentarily the other eigenfunctions u_n have eigenvalues E_n which are greater than this one.

Applying $(-\frac{d}{dx}+x)$ to (8) and using (7) gives

$$(-\tfrac{d}{dx}+x)Hu_n = (-\tfrac{d}{dx}+x)(\tfrac{d}{dx}+x)(-\tfrac{d}{dx}+x)u_n - (-\tfrac{d}{dx}+x)u_n = H(-\tfrac{d}{dx}+x)u_n - 2(-\tfrac{d}{dx}+x)u_n.$$

If u_n is an eigenfunction with $Hu_n = E_n u_n$, then this becomes

$$E_n(-\tfrac{d}{dx}+x)u_n = H(-\tfrac{d}{dx}+x)u_n - 2(-\tfrac{d}{dx}+x)u_n.$$

We accordingly define recursively

$$u_{n+1} = (-\tfrac{d}{dx}+x)u_n, \qquad E_{n+1} = E_n + 2. \tag{10}$$

The formulas (9) and (10) define the sequence of eigenfunctions of the harmonic oscillator. They, and their corresponding eigenvalues, have the form

$$u_n(x) = H_n(x)e^{-x^2/2}, \qquad E_n = 2n+1,$$

where

$$H_0(x) = 1, \qquad H_1(x) = 2x, \qquad H_2(x) = 4x^2 - 2, \tag{11}$$

and more generally $H_n(x)$ is a polynomial of degree n with leading coefficient 2^n. These polynomials are called the *Hermite polynomials*.

Exercise 2. What do we get if, instead of applying $(-\frac{d}{dx}+x)$ to (8) and using (7), we apply $(\frac{d}{dx}+x)$ to (7) and used (8)? What is the analog of (10) then? How does the resulting sequence of eigenfunctions and eigenvalues simplify?

Exercise 3. Find c (depending on $\hbar$, k, m) such that $v_n(x) = u_n(cx)$ solves $-\frac{\hbar^2}{2m}v_n''(x) + \frac{1}{2}kx^2 v_n(x) = \widetilde{E}_n v_n(x)$ for some $\widetilde{E}_n$, and also find $\widetilde{E}_n$.

The functions u_n are mutually orthogonal because H is symmetric: we have

$$E_n \int u_m u_n = \int u_m H u_n = \int u_n H u_m = E_m \int u_n u_m,$$

and hence

$$n \neq m \qquad \Longrightarrow \qquad E_n \neq E_m \qquad \Longrightarrow \qquad \int u_m u_n = 0.$$

We define a corresponding orthonormal set of eigenfunctions by putting

$$\varphi_n(x) = u_n(x)/\sqrt{\textstyle\int u_n^2}$$

These eigenfunctions form a *complete set* in the sense that nothing is orthogonal to all of them: if v is any function in $L^2(\mathbb{R})$ such that $\int v\varphi_n = 0$ for every n then $v = 0$. To prove this, note that if $\int v\varphi_n = 0$ for every n, then $\int v(x)p(x)e^{-x^2/2}dx = 0$ for any polynomial p because any polynomial p can be written as a linear combination of Hermite polynomials, and so[2]

$$\int v(x)e^{-x^2/2}e^{-ix\xi}dx = \sum_{k=0}^{\infty}\int v(x)e^{-x^2/2}\frac{(-ix\xi)^k}{k!}dx = 0,$$

and hence the Fourier transform of $v(x)e^{-x^2/2}$ is zero, which implies $v = 0$.

[2]To justify switching the order of the integral and sum, use the absolute convergence test, which says that $\sum_{k=0}^{\infty}\int f_k = \int\sum_{k=0}^{\infty} f_k$ provided $\sum_{k=0}^{\infty}\int |f_k|$ converges. See e.g. [Fol, Theorem 2.25].

THEOREM 1. *For any $v \in L^2(\mathbb{R})$, we have*

$$v = \sum_{n=0}^{\infty} c_n \varphi_n, \qquad \text{where } c_n = \langle v, \varphi_n \rangle,$$

in the sense that

$$\lim_{N\to\infty} \Big\| v - \sum_{n=0}^{N} c_n \varphi_n \Big\| = 0. \tag{12}$$

Moreover, we have the following infinite-dimensional version of the Pythagorean theorem:

$$\|v\|^2 = \sum_{n=0}^{\infty} |c_n|^2. \tag{13}$$

Conversely, for any sequence of complex numbers $c_0, c_1, \ldots$ such that $\sum |c_n|^2$ converges, there is a unique $v \in L^2(\mathbb{R})$ with the above properties.

We are using here the L^2 inner product $\langle f, g\rangle = \int f\bar{g}$ and corresponding norm $\|f\| = \sqrt{\langle f, f\rangle}$. The proof only uses the fact that $L^2(\mathbb{R})$ is a Hilbert space with respect to this inner product (i.e. it is complete) and the fact that the φ_n form a complete orthonormal set, and thus works for any complete orthonormal set in any Hilbert space.

In words, (12) says that the partial sums $\sum_{n=0}^{N} c_n\varphi_n$ converge to v *in the L^2 sense*, or *in the Hilbert space*, and (13) says that the length squared of v is equal to the sum of the lengths squared of its components (just like the length squared of the hypotenuse of a right triangle is the sum of the lengths squared of its legs).

Proof. We begin by looking for coefficients c_n which minimize the L^2-distance from v to $\sum c_n\varphi_n$. To do so we write

$$\begin{aligned} \Big\| v - \sum_{n=0}^{N} c_n \varphi_n \Big\|^2 &= \|v\|^2 - \sum_{n=0}^{N} \overline{c_n}\langle v, \varphi_n\rangle - c_n\langle \varphi_n, v\rangle + \sum_{n=0}^{N} |c_n|^2 \\ &= \|v\|^2 - \sum_{n=0}^{N} |\langle v, \varphi_n\rangle|^2 + \sum_{n=0}^{N} \big|c_n - \langle v, \varphi_n\rangle\big|^2, \end{aligned} \tag{14}$$

where for the first equality we expanded $\|v - w\| = \|v\|^2 - \langle v, w\rangle - \langle w, v\rangle + \|w\|^2$, and for the second we completed the square using $|c_n - z|^2 = |c_n|^2 - c_n\bar{z} - \overline{c_n}z + |z|^2$. The identity (14) is valid for any constants c_n, but to minimize it we take $c_n = \langle v, \varphi\rangle$, giving

$$\Big\| v - \sum_{n=0}^{N} c_n \varphi_n \Big\|^2 = \|v\|^2 - \sum_{n=0}^{N} |c_n|^2, \qquad \text{where } c_n = \langle v, \varphi_n\rangle.$$

This shows that $\sum_{n=0}^{\infty} |c_n|^2 \le \|v\|^2$ and in particular the sum converges. Hence the Cauchy convergence criterion is satisfied: for every $\varepsilon > 0$ there is M such that if $M \le N_1 \le N_2$ then $\|\sum_{n=N_1}^{N_2} c_n\varphi_n\|^2 = \sum_{n=N_1}^{N_2} |c_n|^2 < \varepsilon$, and it follows[3] that there is $w \in L^2(\mathbb{R})$ such that

[3] See e.g. Theorem 6.6 in [Fol] for the completeness of L^2.

$\lim_{N\to\infty}\left\|w-\sum_{n=0}^{N}c_n\varphi_n\right\|=0$. By the completeness of the eigenfunctions to finish the proof it is enough to show that $\langle w-v,\varphi_m\rangle=0$ for every m. For that we write

$$\langle w-v,\varphi_m\rangle=\Big\langle w-\sum_{n=0}^{N}c_n\varphi_n,\varphi_m\Big\rangle+\Big\langle\sum_{n=0}^{N}c_n\varphi_n-v,\varphi_m\Big\rangle, \tag{15}$$

and observe that the second inner product vanishes when $N\geq m$ because $\langle v,\varphi_m\rangle=c_m$ and the φ_n are orthonormal, while the first obeys[4]

$$\Big|\Big\langle w-\sum_{n=0}^{N}c_n\varphi_n,\varphi_m\Big\rangle\Big|\leq\Big\|w-\sum_{n=0}^{N}c_n\varphi_n\Big\|\to 0\qquad\text{as } N\to\infty,$$

and since the left hand side of (15) is independent of N it must be zero for all m.

For the converse, again use the fact that the Cauchy criterion is satisfied together with the completeness of L^2. □

We have shown that $L^2(\mathbb{R})$ has a *countable* complete orthonormal set, namely the φ_n, and this important property is called *separability.* Now we use this orthonormal set to solve the quantum harmonic oscillator problem.

THEOREM 2. *Let $f\in L^2(\mathbb{R})$, $c_n=\int f\varphi_n$, $E_n=2n+1$. Then*

$$u(x,t)=\sum_{n=0}^{\infty}c_ne^{-iE_nt}\varphi_n(x)$$

solves

$$i\partial_tu(x,t)=-\partial_x^2u(x,t)+x^2u(x,t),\qquad u(x,0)=f(x), \tag{16}$$

in the sense of distributions.

Proof. Put $u_N(x,t)=\sum_{n=0}^{N}c_ne^{i(2n+1)t}\varphi_n(x)$. Then $i\partial_tu_N(x,t)=-\partial_x^2u_N(x,t)+x^2u_N(x,t)$, and we want to take the limit as $N\to\infty$ of each term of this equation, justifying passing the limit through the ∂_t, ∂_x^2, and x^2 operators.

From Theorem 1 we know that $u_N\to u$ in L^2. To see that $u_N\to u$ in $\mathcal{S}'$ (i.e. in the sense of distributions), take $\varphi\in\mathcal{S}$, and apply Cauchy–Schwarz and the L^2 convergence theorem (12) to obtain

$$\Big|\int(u(x,t)-u_N(x,t))\varphi(x)dx\Big|\leq\|u(x,t)-u_N(x,t)\|\|\varphi\|\to 0,\qquad\text{as } N\to\infty. \tag{17}$$

We show that $x^2u_N\to x^2u$ in $\mathcal{S}'$ by applying (17) with $\varphi(x)$ replaced by $x^2\varphi(x)$, and then $\partial_x^2u_N\to\partial_x^2u$ in $\mathcal{S}'$ by applying (17) with φ replaced by φ''.

It remains to show that $\partial_tu_N\to\partial_tu$ in $\mathcal{S}'$. We use the fact that the coefficients $\langle\varphi,\varphi_n\rangle$ are rapidly decaying in n. More specifically, for any k, using $H=-\partial_x^2+x^2$ and $E_n=2n+1$, we have

$$|\langle\varphi,\varphi_n\rangle|=\Big|\int\varphi\varphi_n\Big|=E_n^{-k}\Big|\int\varphi H^k\varphi_n\Big|=E_n^{-k}\Big|\int(H^k\varphi)\varphi_n\Big|\leq E_n^{-k}\|H^k\varphi\|. \tag{18}$$

[4]This is the Cauchy–Schwarz inequality $|\langle f,\varphi_m\rangle|\leq\|f\|$, which follows from (14) in the form $\|f-c_m\varphi_m\|^2=\|f\|^2-|\langle f,\varphi_m\rangle|^2+|c_m-\langle f,\varphi_m\rangle|^2$. Indeed, putting $c_m=\langle f,\varphi_m\rangle$ and using $0\leq\|f-c_m\varphi_m\|^2$ gives $0\leq\|f\|^2-|\langle f,\varphi_m\rangle|^2$ which is equivalent to $|\langle f,\varphi_m\rangle|\leq\|f\|$.

We have

$$\int \partial_t u_N(x,t)\varphi(x)dx = -\sum_{n=0}^{N} iE_n c_n e^{-iE_n t}\langle \varphi, \varphi_n\rangle,$$

and so, by (18) with $k=3$, $\partial_t u_N$ converges in $\mathcal{S}'$ to $\sum_{n=0}^{\infty} iE_n c_n e^{-iE_n t}\varphi_n(x)$. On the other hand

$$\partial_t u[\varphi] = \partial_t \sum_{n=0}^{\infty} c_n e^{-iE_n t}\langle \varphi, \varphi_n\rangle = \lim_{h\to 0}\sum_{n=0}^{\infty} \frac{c_n}{h}(e^{-iE_n(t+h)} - e^{-iE_n t})\langle \varphi, \varphi_n\rangle$$

By $|e^{-iE_n h} - 1| = |\int_0^{E_n h} e^{-is}ds| \le E_n h$ and (18) with $k=3$ the terms of the sum are bounded by $|c_n|E_n|\langle \varphi, \varphi_n\rangle|$, and hence the sum is absolutely uniformly convergent and we may interchange the sum and limit to obtain

$$\partial_t u[\varphi] = -\sum_{n=0}^{\infty} iE_n c_n e^{-iE_n t}\langle \varphi, \varphi_n\rangle = \lim_{N\to\infty} \partial_t u_N[\varphi],$$

and hence $\partial_t u_N \to \partial_t u$ in $\mathcal{S}'$. $\square$

Exercise 4. Let f be the characteristic function of an interval, and plot (for example using `www.desmos.com`) the real and imaginary parts of $u_N(x,t)$, $i\partial_t u_N(x,t)$, and $\partial_x^2 u_N(x,t)$ for a few small values of t including $t=0$, for some value of N large enough that the neglected terms are reasonably small.

Exercise 5. Prove the analog of Theorem 2 for the wave equation

$$\partial_t^2 u(x,t) - \partial_x^2 u(x,t) + x^2 u(x,t) = 0, \qquad u(x,0) = f(x), \quad \partial_t u(x,0) = g(x),$$

where f and g are in L^2.

Exercise 6. Let I be an open interval containing 0, let $c_n\colon I \to \mathbb{C}$ be differentiable functions. Suppose that there are constants C and K such that $|c(t)| + |c'(t)| \le C(1+|n|)^K$ for all $t \in I$ and all n. Use (18) to prove that $\tilde{u}(x,t) = \sum_{n=0}^{\infty} c_n(t)\varphi_n(x)$ defines a distribution in x for every t. Use the method of proof of Theorem 2 to show that if $\tilde{u}(x,t)$ solves (16) in the sense of distributions, then $c_n(t) = c_n e^{-iE_n t}$, where $c_n = \langle f, \varphi_n\rangle$.

For every t, we denote the operator taking f to u at time t in Theorem 2 by e^{-iHt}. By Theorem 1, this a unitary operator (i.e. an isometry) on $L^2(\mathbb{R}^d)$, meaning $\|e^{-iHt}f\| = \|f\|$ for any f. More generally given any function $a\colon \mathbb{R} \to \mathbb{C}$, we define

$$a(H)f = \sum_{n=0}^{\infty} c_n a(E_n)\varphi_n(x), \qquad \text{where } c_n = \int f\varphi_n. \tag{19}$$

We also write this as

$$a(H) = \sum_{n=0}^{\infty} a(E_n)(\varphi_n \otimes \varphi_n), \tag{20}$$

where we use the notation $(u \otimes v)f = u\langle f, v\rangle$. Observe that $(\varphi_n \otimes \varphi_n)$ is the orthogonal projection onto the eigenspace with eigenvalue E_n.

A mapping from functions of a real (or complex) variable to functions of an operator is called a *functional calculus*. If a is the constant function 1, then $a(H) = I$ is the identity operator I and the equation $I = \sum_{n=0}^{\infty}(\varphi_n \otimes \varphi_n)$ is the *resolution of the identity* corresponding to H; it is just the decomposition of L^2 into the eigenspaces of H. In terms of Dirac's bra and ket notation we write $1 = \sum_{n=0}^{\infty} |\varphi_n\rangle\langle\varphi_n|$.

If a is bounded then, by Theorem 1, $a(H)$ maps $L^2 \to L^2$ and we have

$$\|a(H)\|_{L^2\to L^2} = \sup_n |a(E_n)|, \tag{21}$$

where we use the definition of the operator norm

$$\|a(H)\|_{L^2\to L^2} = \sup_{f\in L^2\colon \|f\|=1} \|a(H)f\|_{L^2}.$$

In words, we say that $a(H)$ is then a bounded operator on L^2, with operator norm given by the least upper bound of the magnitudes of its values on the eigenvalues. For example, $\|e^{-itH}\|_{L^2\to L^2} = 1$ for all t.

Exercise 7. Use (19) and the definition of supremum to verify (21).

Exercise 8. In the setting of Exercise 5, what two operators are the analogs of e^{-iHt}? What can you say about their norms?

If a is not bounded, we still use the same definition, even though the mapping properties of a are more complicated. Observe that, as we showed in Theorem 2, if a is the identity function ($a(x) = x$) then defining Hf by (19) is equivalent to defining Hf in the sense of distributions, and more generally if a is a polynomial then (19) agrees with the definition of $a(H)f$ in the sense of distributions.

The d-dimensional solution is built directly out of the 1-dimensional one. Let

$$H = -\Delta + |x|^2,$$

and consider a multiindex $\alpha = (\alpha_1, \cdots, \alpha_d)$, a d-tuple of nonnegative integers. Put $|\alpha| = \alpha_1 + \cdots + \alpha_d$. Then put

$$u_\alpha(x) = u_{\alpha_1}(x_1)\dots u_{\alpha_d}(x_d),$$

which gives

$$Hu_\alpha = E_\alpha u_\alpha, \qquad E_\alpha = 2|\alpha| + d. \tag{22}$$

Exercise 9. Let $\varphi_\alpha = u_\alpha/\|u_\alpha\|$. Prove that the φ_α are an orthonormal basis for $L^2(\mathbb{R}^d)$; i.e. they are an orthonormal set such that if $v \in L^2$ is orthogonal to every φ_α then $v = 0$.

Exercise 10. Let k be a nonnegative integer. Find the multiplicity of k as an eigenvalue of H, as a function of d and k, at least for some small values of d and/or k; this is the dimension of the space of $u \in L^2(\mathbb{R}^d)$ such that $Hu = ku$.

Exercise 11. The operator H commutes with rotations: if M is any orthogonal matrix on $\mathbb{R}^d$ and we define $R_M u(x) = u(Mx)$, then $R_M H = HR_M$. Find a joint basis of eigenfunctions for H and R_M, for at least one choice of M. The easiest one is $Mx = -x$. Other relatively simple examples include reflections around a hyperplane and rotations about an axis. For any family of mutually commuting rotations there is a joint eigenbasis for all of them. When $d = 2$, you can use polar coordinates to handle rotations having $e^{in\theta}$ as an eigenfunction for any n: $Me^{in\theta} = e^{in(\theta+\alpha)} = e^{in\alpha}e^{in\theta}$; the higher-dimensional analogs of this lead to the theory of *spherical* *harmonics*. The spherical harmonics are the eigenfunctions of $\Delta_{\mathbb{S}^{d-1}}$, the Laplacian on the unit sphere (see Exercise 1).

Exercise 12. Find the eigenvalues of $\Delta_{\mathbb{S}^{d-1}}$ for $d = 2$ (see Exercise 1), for the Hilbert space $L^2([0, 2\pi])$. Find two bases for each eigenspace, one consisting of complex exponentials and one consisting of real-valued functions.

Exercise 13. The operator H also commutes with the Fourier transform. Use this to find the eigenvalues of the Fourier transform and a corresponding basis of eigenfunctions.

Another important characterization of the eigenvalues and eigenfunctions is as follows: for $z \in \mathbb{C} \setminus \{d,\, d+2,\, d+4, \dots\}$, define the *resolvent* $(H-z)^{-1} \colon L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ by the eigenbasis functional calculus (19) or (20) with $a(x) = (x-z)^{-1}$. The resolvent has many nice properties. For one it is bounded on L^2, even though H is not. For another (as we will discuss in more detail in Section 2) it depends holomorphically on z.[5]

Exercise 14. Check that $z \mapsto \langle (H-z)^{-1} f, g\rangle$ is holomorphic by term-by-term differentiation of the series defining it, or by expanding each $(E_\alpha - z)^{-1}$ in that series into a geometric series.

To characterize the eigenfunctions using the resolvent, we write it out as follows. For any nonnegative integer k, by the eigenbasis functional calculus (20) we have

$$\begin{aligned}(H-z)^{-1} &= \sum_{\alpha}^{\infty} (E_\alpha - z)^{-1} (\varphi_\alpha \otimes \varphi_\alpha) \\ &= \frac{-1}{z - z_k} \sum_{|\alpha| = k} (\varphi_\alpha \otimes \varphi_\alpha) + B_k(z),\end{aligned}$$

where $z_k = 2k + d$ and $B_k(z)$ is a holomorphic family of operators near z_k. Thus the residue of $(H-z)^{-1}$ at z_k is $-\Pi_{z_k}$, i.e. minus the projection onto the eigenspace with eigenvalue z_k. With the convention that $\Pi_w = 0$ when $w \in \mathbb{C}$ is not a point of the spectrum of H, by the residue theorem we thus have

$$\Pi_w = \frac{i}{2\pi} \int_{C_w} (H-z)^{-1} dz,$$

where C_w is piecewise smooth simple closed curve[6] in the complex plane enclosing w and no points of the spectrum of H besides w. More generally if C is the boundary of a region $D \subset \mathbb{C}$, then $\frac{i}{2\pi} \int_C (H-z)^{-1} dz$ is the projection onto the eigenspaces whose eigenvalues lie within D.

For more complicated operators than the harmonic oscillator, it is often easier and better to work with the resolvent than with the eigenvectors and eigenvalues. Among other things, the eigenvectors do not always form a complete set (see for example Exercise 16 below).

[5]This means $z \mapsto \langle (H-z)^{-1} f, g\rangle$ is holomorphic for any f and g in L^2. See Section 4.2.2 of [Bor], especially Theorem 4.8, for more on this.

[6]See Section 1.6 of [Fis] for more on such curves.

2. The Resolvent. Let H be a differential operator on $\mathbb{R}^d$, and let $z \in \mathbb{C}$. Suppose that, for every $f \in L^2(\mathbb{R}^d)$, there is a unique $u \in L^2(\mathbb{R}^d)$ such that $(H - z)u = f$, and moreover that there is a constant C (depending on H and z but not on f and u) such that $\|u\|_{L^2(\mathbb{R}^d)} \le C\|f\|_{L^2(\mathbb{R}^d)}$. Then we note the operator mapping f to u by $(H - z)^{-1}f$. This operator is called the *resolvent*. The best possible constant C is denoted $\|(H - z)^{-1}\|_{L^2 \to L^2}$.

Exercise 15. Check that for the harmonic oscillator $H = -\Delta + |x|^2$ this definition of the resolvent $(-\Delta + |x|^2 - z)^{-1}$ agrees with the one from Section 1. Compute $\|(-\Delta + |x|^2 - z)^{-1}\|_{L^2 \to L^2}$ in terms of the distance from z to the set of eigenvalues $\{d, d + 2, d + 4, \dots\}$.

The range of the resolvent is denoted $\mathcal{D}$, the *domain* of H as an unbounded operator on $L^2(\mathbb{R}^d)$. It can be difficult to compute $\mathcal{D}$, but we always know that $Hu \in L^2$ for all $u \in \mathcal{D}$ (because $Hu = zu + f$) and this is enough for many purposes. We now prove that $\mathcal{D}$ does not depend on z.

Theorem 3. *Suppose $H - z_1$ is bijective $\mathcal{D}_1 \to L^2(\mathbb{R}^d)$ and $H - z_2$ is bijective $\mathcal{D}_2 \to L^2(\mathbb{R}^d)$. Then $\mathcal{D}_1 = \mathcal{D}_2$.*

Proof. We factor the difference:

$$\begin{aligned}(H - z_1)^{-1} - (H - z_2)^{-1} &= ((H - z_1)^{-1}(H - z_2) - I)(H - z_2)^{-1} \\ &= (H - z_1)^{-1}(H - z_2 - (H - z_1))(H - z_2)^{-1}\end{aligned}$$

The right hand side maps L^2 into $\mathcal{D}_1$, and the first term on the left does too. Hence $(H - z_2)^{-1}$ maps L^2 into $\mathcal{D}_1$. That shows $\mathcal{D}_2 \subset \mathcal{D}_1$. By symmetry, $\mathcal{D}_1 \subset \mathcal{D}_2$. $\square$

The set of values of z where the resolvent is defined is called the *resolvent set*, and its complement (the set where the resolvent is not defined) is called the *spectrum*. The spectrum includes the set of all L^2 eigenvalues: these are the z for which $H - z$ is not injective.[7] For the harmonic oscillator the set of L^2 eigenvalues equals the spectrum, but for other problems the spectrum can include more, as in the following example.

Example 1. Consider the free Laplacian $H = -\Delta$. Given $f \in L^2(\mathbb{R}^d)$ and $z \in \mathbb{C}$ we can solve $(-\Delta - z)u = f$ for u if and only if we can solve $(|\xi|^2 - z)\hat{u} = \hat{f}$, i.e. z is in the resolvent set if and only if the mapping $\hat{f} \mapsto (|\xi|^2 - z)^{-1}\hat{f}$ is bounded on L^2, i.e. if and only if the function $\xi \mapsto (|\xi|^2 - z)^{-1}$ is bounded. That shows that the spectrum of $-\Delta$ is given by $[0, \infty)$. This kind

[7] If V is a finite-dimensional vector space, then a linear map $A \colon V \to V$ is injective if and only if it is surjective (and hence if and only if it is invertible). This is sometimes called the fundamental theorem of linear algebra: see Corollary 1.3.7 of [Tay]. For infinite dimensional spaces this is not so. For example, consider the left and right shift operators on sequences, given by $L(a_1, a_2, \dots) = (a_2, a_3, \dots)$ and $R(a_1, a_2, \dots) = (0, a_1, a_2, \dots)$. Then L is surjective but not injective, and R is injective but not surjective. Moreover $LR = I$, so L is a left inverse for R and R is a right inverse for L. But L has no left inverse and R has no right inverse.

If you are interested in going deeper into these issues, do the following exercise. Consider L and R as bounded operators on $\ell^2(\mathbb{N})$, the Hilbert space of sequences $a_1, a_2, \dots$ such that $\sum |a_n|^2$ converges, with norm given by $\sqrt{\sum |a_n|^2}$. Compute the spectrum of R, and for each point z of the spectrum see if you can determine whether $R - z$ is injective, surjective, both, or neither. Then do the same for L. (For some points of the spectrum this is easier than for others.)

of spectrum is called *continuous* spectrum, in contrast to the *discrete* spectrum of the harmonic oscillator which is given by $\{d, d+2, d+4, \dots\}$; see Figure 1.

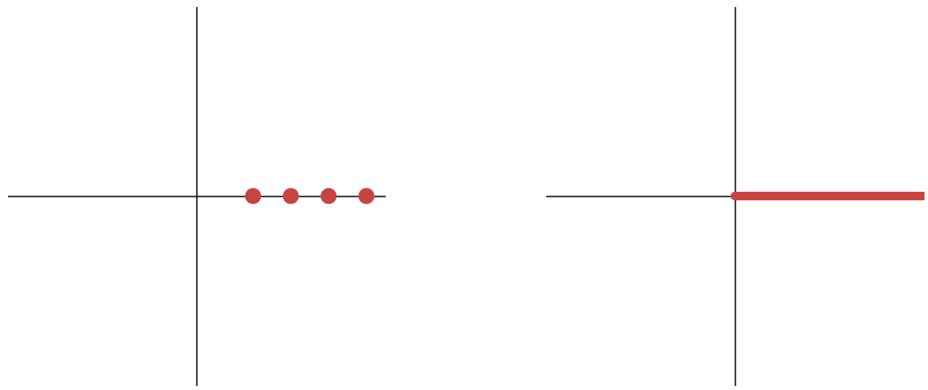

FIGURE 1. The spectra of the harmonic oscillator $-\Delta + |x|^2$ and of the free Laplacian $-\Delta$.

For more general operators the spectrum can have a more complicated structure than for the simple examples of the free Laplacian and the harmonic oscillator, but we will see that typically it consists of some combination of continuous and discrete components.

EXERCISE 16. Use Fourier transformation to prove that the domain $\mathcal{D}$ of the free Laplacian $-\Delta$ equals the Sobolev space $H^2(\mathbb{R}^d)$,[8] and that $(-\Delta - z)\colon H^2(\mathbb{R}^d) \to L^2(\mathbb{R}^2)$ is injective for all $z \in \mathbb{C}$; i.e. $-\Delta$ has no L^2 eigenvalues.

EXERCISE 17. In (19) and (20) we gave a formula for $a(-\frac{d^2}{dx^2} + x^2)$ as a superposition of terms parametrized by the spectrum of the harmonic oscillator. For the free Laplacian we have a formula which is in many ways analogous given by the Fourier integral

$$a(-\Delta) f(x) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{ix\xi} a(|\xi|^2) \int_{\mathbb{R}^d} e^{-iy\xi} f(y)\, dy\, d\xi.$$

Bring this formula to a form more closely analogous to (19) in the case $d = 1$ by manipulating it to find functions $e_1(x, \rho)$ and $e_2(x, \rho)$ such that

$$a(-\tfrac{d^2}{dx^2}) f(x) = \int_0^\infty a(\rho) \Big(\Big[\int_{\mathbb{R}} f(y) \overline{e_1(y, \rho)}\, dy \Big] e_1(x, \rho) + \Big[\int_{\mathbb{R}} f(y) \overline{e_2(y, \rho)}\, dy \Big] e_2(x, \rho) \Big) d\rho.$$

Because of the two terms e_1 and e_2 one sometimes says that the spectrum of $-\frac{d^2}{dx^2}$ is $[0, \infty)$ with multiplicity 2. Note the analogy with the corresponding formula for the d-dimensional harmonic oscillator

$$a(-\Delta + |x|^2) f(x) = \sum_{n=0}^\infty a(2n + d) \sum_{\alpha\colon |\alpha| = n} \Big[\int f(y) \varphi_\alpha(y)\, dy \Big] \varphi_\alpha(x);$$

here the spectrum is made up of the eigenvalues $\{d, d+2, d+4, \dots\}$ and the multiplicity of the eigenvalue $d + 2n$ is equal to the number of multiindices α such that $|\alpha| = n$. See also Exercises 9 and 10 and the paragraph preceding them.

[8] See Section 6 of [FW].

Exercise 18. Prove that, in the notation of (20), (22), and Exercise 9, the domain $\mathcal{D}$ of the harmonic oscillator $H = -\Delta + |x|^2$ equals the set of $f \in L^2(\mathbb{R}^d)$ such that $\sum_\alpha |E_\alpha|^2 |\langle f, \varphi_\alpha \rangle|^2$ converges.

We now prove that the resolvent has the further important property of being holomorphic. This means that it can be expanded into a power series in z near each point where it is defined.

Theorem 4. *Given any w in the resolvent set of H, there is a disk D centered at w, disjoint from the spectrum of H, such that $(H - z)^{-1}$ is given by a convergent power series in D.*

Proof. Given $z \in \mathbb{C}$, we try to invert $(H - z)$ by using $(H - w)^{-1}$ as an approximate inverse. (An approximate inverse is sometimes called *parametrix.*) Write

$$(H - z)(H - w)^{-1} = I - (z - w)(H - w)^{-1}.$$

Let D be the set of z such that $|z - w| < 1/\|(H - w)^{-1}\|_{L^2 \to L^2}$. Then for $z \in D$ we can solve for $(H-z)^{-1}$ by a geometric series, since $\sum_{n=0}^\infty A^n$ converges to $(I-A)^{-1}$ when $\|A\| < 1$. That proves $\sum_{n=0}^\infty C_n(z - w)^n$ with $C_n = (H - w)^{-n-1}$ is a right inverse for $(H - z)$. The same calculation for $(H - w)^{-1}(H - z)$ shows it is a left inverse, and hence $H - z$ is invertible with

$$(H - z)^{-1} = \sum_{n=0}^\infty C_n(z - w)^n, \qquad C_n = (H - w)^{-n-1},$$

for all $z \in D$, as desired. □

Note that by Theorem 4, the resolvent set is open and the spectrum is closed.

Exercise 19. Use the method of proof of Theorems 3 and 4 to show that $\frac{d}{dz}(H-z)^{-1} = (H-z)^{-2}$.

3. Decaying potentials. In this section we will conisder Schrödinger operators $H = -\Delta + V$, where $V(x) \to 0$ as $|x| \to \infty$. We start by assuming that V is bounded, but later relax this assumption so as to be able to handle the Coulomb potential, as discussed in Exercise 1 above and in the paragraph preceding it.

Our first important milestone in the study of H is the construction of the resolvent $(H - z)^{-1}$ for certain values of z.

Theorem 5. *Let $H = -\Delta + V$, where $V = V(x)$ is a bounded function on $\mathbb{R}^d$. Then the resolvent set of H is not empty.*

Proof. We follow the approach of the proof of Theorem 4. Given $z \in \mathbb{C}$, we try to invert $(H - z)$ by using $(-\Delta - z)^{-1}$ as an approximate inverse. Write

$$(H - z)(-\Delta - z)^{-1} = I + V(-\Delta - z)^{-1}.$$

If $\|V(-\Delta - z)^{-1}\|_{L^2 \to L^2} < 1$, then we can use a geometric series to write

$$(H - z)(-\Delta - z)^{-1} \sum_{n=0}^\infty (-1)^n (V(-\Delta - z)^{-1})^n = I,$$

and thereby obtain a right inverse for $H - z$. We will check that this works for z far enough away from the positive real axis. Our first step is observing that

$$\|V(-\Delta - z)^{-1}\|_{L^2\to L^2} \le \|V\|_{L^2\to L^2}\|(-\Delta - z)^{-1}\|_{L^2\to L^2}.$$

Next we have

$$\|V\|_{L^2\to L^2} \le \sup|V|,$$

because

$$\int |Vu|^2 \le \sup|V|^2 \int |u|^2.$$

Thus it is enough to have

$$\|(-\Delta - z)^{-1}\|_{L^2\to L^2} < 1/\sup|V|.$$

To control $\|(-\Delta - z)^{-1}\|_{L^2\to L^2}$ we recall Plancherel's theorem: $\|u\|_{L^2} = (2\pi)^{-d/2}\|\hat{u}\|_{L^2}$. Thus we have

$$\|u\| = (2\pi)^{-d/2}\|\hat{u}\| = (2\pi)^{-d/2}\|(|\xi|^2 - z)^{-1}\hat{f}\| \le \sup_\xi(|\xi|^2 - z)^{-1}(2\pi)^{-d/2}\|\hat{f}\| = \sup_\xi(|\xi|^2 - z)^{-1}\|f\|,$$

and so we get that $\|(-\Delta - z)^{-1}\|_{L^2\to L^2}$ goes to 0 for $z \ll -1$. In particular if z is real and sufficiently negative, then z is in the resolvent set. □

Thus we have constructed $(H - z)^{-1}$ when $H = -\Delta + V$ with V a bounded function on $\mathbb{R}^d$, when $z \ll -1$. Using the exercise below, the construction extends to all values of z in a domain given by the exterior of the shaded region in Figure 2.

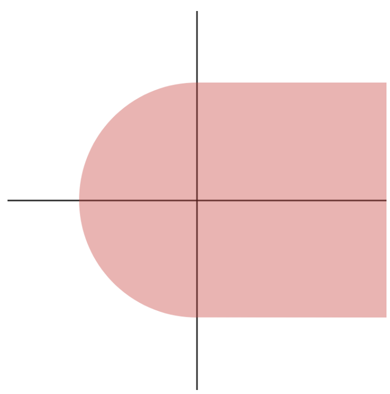

FIGURE 2. When V is a bounded function on $\mathbb{R}^d$, the construction of the resolvent $(H - z)^{-1}$ by geometric series succeeds in the exterior of the shaded region.

EXERCISE 20. Given a bounded function V, find the set of $z \in \mathbb{C}$ such that

$$\sup_{\xi\in\mathbb{R}^d}\left|\frac{1}{|\xi|^2 - z}\right| < \frac{1}{\sup|V|}.$$

Hint: Consider separately the cases $\operatorname{Re} z \le 0$ and $\operatorname{Re} z \ge 0$.

Exercise 21. In the course of the proof of Theorem 5 we showed that $\|V\|_{L^2\to L^2} \le \sup|V|$. Show that, if V is continuous and $\sup|V|$ is attained, then $\|V\|_{L^2\to L^2} \ge \sup|V|$. One way to do this is to compute $\lim_{n\to\infty}\int|Vu_n|^2$ for $u_n(x) = \pi^{-d/4}n^{d/2}e^{-n^2|x-x_n|^2/2}$, where x_n is a sequence in $\mathbb{R}^d$ converging to a point x^* such that $|V(x^*)| = \sup|V|$. If you know the definition, you can also show that $\|V\|_{L^2\to L^2}$ equals the essential supremum of $|V|$, in the case where V is bounded and measurable but not necessarily continuous.

We will now show that if additionally $V(x)\to 0$ as $|x|\to\infty$, then $(H-z)^{-1}$ extends meromorphically to $\mathbb{C}\setminus[0,\infty)$ with poles where H has L^2 eigenvalues. Note that any such eigenvalues must be on the real axis if V is real, because if $Hu = Eu$ then

$$E\int|u|^2 = \int(-\Delta u + Vu)\bar{u} = \int(\overline{-\Delta u + Vu})u = \bar{E}\int|u|^2,$$

and also in that case $E \ge \inf V$ because

$$E\int|u|^2 = \int(-\Delta u + Vu)\bar{u} = \int|\nabla u|^2 + V|u|^2 \ge \int V|u|^2 \ge (\inf V)\int|u|^2.$$

Exercise 22. Let $V\colon\mathbb{R}^d\to\mathbb{C}$ be bounded, and let $A\subset\mathbb{C}$ be the range of V. What can you say about the locations of possible L^2 eigenvalues of H, in terms of A?.

The above follows from the following:

Theorem 6. *Let $V = V(x)$ be a bounded function on $\mathbb{R}^d$ such that $V(x)\to 0$ as $|x|\to\infty$. Then $(I+V(x)(-\Delta-z)^{-1})^{-1}\colon L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)$ is a meromorphic family of operators on $z\in\mathbb{C}\setminus[0,\infty)$ and $I+V(x)(-\Delta-z)^{-1}$ has L^2 eigenvalues at any poles.*

Recall that a *meromorphic* function is a quotient of holomorphic functions, for example a rational function or $z\mapsto\tan z$. In anaolgy with our definition of a holomorophic family of operators, we say that a family $z\mapsto K(z)$ of operators is *meromorphic* if $z\mapsto\langle f, K(z)g\rangle$ is meromorphic for each f and g.

Theorem 6 is a consequence of Theorems 7 and 8.

Theorem 7. *Let $V = V(x)$ be a bounded function on $\mathbb{R}^d$ such that $V(x)\to 0$ as $|x|\to\infty$. Then $V(x)(-\Delta-z)^{-1}$ is a* compact *operator on $L^2(\mathbb{R}^d)$ for each $z\in\mathbb{C}\setminus[0,\infty)$. This means that for any such z and any $\varepsilon>0$ there is a finite rank operator F such that $\|V(x)(-\Delta-z)^{-1}-F\|_{L^2\to L^2}<\varepsilon$.*

Recall that the *rank* of an operator is the dimension of its range, and so a finite rank operator is one which has a finite-dimensional range. The basic example is the tensor product $u\mapsto(f\otimes g)u = f\langle u,g\rangle$, which is the same thing as the orthogonal projection onto the span of φ when $f=g=\varphi$ is a unit vector. The finite rank operators and compact operators are both subspaces of $L^2(\mathbb{R}^d)$, with the latter being the closure of former.

Theorem 8. *Let $z\mapsto K(z)$ be a holomorphic family of compact operators on $L^2(\mathbb{R}^d)$ (or more generally on any separable Hilbert space) for $z\in\Omega$, where $\Omega\subset\mathbb{C}$ is a connected open set. If $I-K(z_0)$ is invertible for any $z_0\in\mathbb{C}$, then $(I-K(z))^{-1}$ (which exists in a neighborhood of z_0 by Theorem 4) extends to a meromorphic family of operators for $z\in\Omega$. Moreover any $z\in\Omega$ is a pole of $(I-K(z))^{-1}$ if and only if $I-K(z)$ has nullspace in $L^2(\mathbb{R}^d)$.*

Theorem 8 is called the *analytic Fredholm theorem.*

Proof of Theorem 8. Let $D \subset \Omega$ be a disk such that $\|K(z) - K(z')\| < 1/2$ for any z and z' in D. Suppose there is $z' \in D$ such that $I - K(z')$ is invertible, and pick a finite rank F such that $\|K(z') - F\| < 1/2$, so that $z \mapsto (I - K(z) + F)^{-1}$ is holomorphic for $z \in D$. Then

$$(I - K(z))(I - K(z) + F)^{-1} = I - G(z), \qquad \text{where } G(z) = F(I - K(z) + F)^{-1}.$$

Thus $I - K(z)$ is invertible if and only if $I - G(z)$ is, i.e. if and only if $u - G(z)u = f$ has a unique solution for every f. Since $G(z)$ has finite rank, we see that any solution u must be close to f, and so we substitute $u = f + v$. Then solving $u - G(z)u = f$ is equivalent to solving

$$v = G(z)(f + v). \tag{23}$$

Any solution v must be in the range of F, i.e. of the form $v = \sum_{n=1}^N c_n(z)\varphi_n$, where $\{\varphi_1, \dots, \varphi_N\}$ is an orthonormal basis of the range of F. Inserting this into (23) and pairing both sides with φ_m gives

$$\begin{aligned} c_m(z) &= \Big\langle G(z)\Big(f + \textstyle\sum_{n=1}^N c_n(z)\varphi_n\Big), \varphi_n\Big\rangle \\ &= \langle G(z)f, \varphi_m\rangle + \textstyle\sum_{n=1}^N \langle G(z)\varphi_n, \varphi_m\rangle c_n(z), \end{aligned} \qquad \text{for } m = 1, \dots N. \tag{24}$$

By assumption, this system of N linear equations in N unknowns is solvable for at least one value of z (namely $z = z'$). Hence, by Cramer's formula from linear algebra, it defines a meromorphic function $z \mapsto c_n(z)$ for each n, for $z \in D$. Moreover, poles occur precisely at values of z for which the system (24) has a nontrivial solution with $f = 0$, i.e. at values of z for which $u - G(z)u = 0$ has a nontrivial solution, i.e. at values of z for which $I - K(z)$ has nullspace in $L^2(\mathbb{R}^d)$. This proves the result for $z \in D$. By connectedness, the result follows for $z \in \Omega$: see Exercise 23. $\square$

EXERCISE 23. Fill in the details of the connectedness argument mentioned in the last sentence of the proof of Theorem 8. One way to do this is to consider an arbitrary point $z_1 \in \Omega$, and a path from z_0 to z_1, and then define a sequence of finitely many overlapping disks covering the path, each of which is small enough that $\|K(z) - K(z')\| < 1/2$ for any z and z' in the disk. See Figure 3.

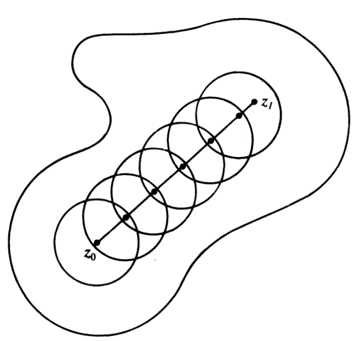

FIGURE 3. A possible sequence of disks as in the connectedness argument in the proof of Theorem 8. Adapted from Figure 2.11 of [Fis].

Theorem 7 follows from the following more general result.

Theorem 9. *Let f and g be bounded functions $\mathbb{R}^d \to \mathbb{C}$ which tend to 0 as $|x|$ tends to infinity. Let $f(x)$ be the operator $u(x) \mapsto f(x)u(x)$ and let $g(-i\partial_x)$ be the operator $u \mapsto (2\pi)^{-d}\int e^{ix\xi}g(\xi)\hat{u}(\xi)d\xi$. Then the compositions*

$$f(x)g(-i\partial_x) \qquad \text{and} \qquad g(-i\partial_x)f(x)$$

are both compact operators $L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$.

Proof. 1. The adjoint of a finite rank operator is finite rank, and so the adjoint of a compact operator is compact, and hence it is enough to consider $f(x)g(-i\partial_x)$.

2. We now show that it is enough to consider f and g compactly supported (i.e. identically zero outside of some ball). To do this let $f_R(x) = \mathbf{1}_{[0,R]}(|x|)f(x)$ and $g_R(\xi) = \mathbf{1}_{[0,R]}(|\xi|)g(\xi)$, where $\mathbf{1}_{[0,R]}$ is the function which is 1 on $[0,R]$ and 0 elsewhere. Then we have

$$\|f(x)g(-i\partial_x) - f_R(x)g_R(-i\partial_x)\| \le \|f(x)(g(-i\partial_x) - g_R(-i\partial_x))\| + \|(f(x) - f_R(x))g_R(-i\partial_x)\|,$$

where the norms are $L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$. Next we have

$$\|(f(x) - f_R(x))g_R(-i\partial_x)\| \le \|f(x) - f_R(x)\|\|g_R(-i\partial_x)\| \le \sup|f - f_R|\sup|g_R|,$$

and $\sup|f - f_R| \to 0$ and $\sup|g_R| \to \sup|g|$ as $R \to \infty$. Consequently, assuming we have solved the problem for f and g compactly supported, given $\varepsilon > 0$ take R large enough that $\|f(x)g(-i\partial_x) - f_R(x)g_R(-i\partial_x)\| < \varepsilon/2$, and then take a finite rank F such that $\|f_R(x)g_R(-i\partial_x) - F\| < \varepsilon/2$, and it follows that $\|f(x)g(-i\partial_x) - F\| < \varepsilon$.

3. Now suppose f and g are compactly supported and write

$$f(x)g(-i\partial_x)u(x) = \frac{1}{(2\pi)^d}\int\int f(x)e^{i(x-y)\xi}g(\xi)u(y)\,dy\,d\xi = \int K(x,y)u(y)\,dy,$$

where

$$K(x,y) = \frac{1}{(2\pi)^d}f(x)\hat{g}(y-x).$$

The function K is called the *integral kernel* of the operator $f(x)g(-i\partial_x)$. Observe that $K \in L^2(\mathbb{R}^{2d})$ because

$$\|K\|^2_{L^2(\mathbb{R}^{2d})} = \frac{1}{(2\pi)^{2d}}\int\int|f(x)|^2|\hat{g}(y-x)|^2dy\,dx = \frac{1}{(2\pi)^{2d}}\int|f(x)|^2dx\int|\hat{g}(\tilde{y})|^2d\tilde{y} < +\infty.$$

Next write $K(x,y)$ as a linear combination of the harmonic oscillator eigenfunctions $\varphi_\alpha(x)\varphi_\beta(y)$ by applying Theorem 1, but with $L^2(\mathbb{R})$ replaced by $L^2(\mathbb{R}^{2d})$, with $f(x)$ replaced by $K(x,y)$, and with the $\varphi_n(x)$ replaced by $\varphi_\alpha(x)\varphi_\beta(y)$, where

$$\varphi_\alpha(x) = \frac{u_\alpha(x)}{\|u_\alpha\|_{L^2(\mathbb{R}^d)}}, \qquad u_\alpha(x) = H_{\alpha_1}(x_1)\cdots H_{\alpha_d}(x_d)e^{-|x|^2/2},$$

and the H_n are the Hermite polynomials as in (11) and (22). Thus

$$K(x,y) = \sum_{\alpha,\beta\in\mathbb{N}_0^d} c_{\alpha\beta}\,\varphi_\alpha(x)\varphi_\beta(y).$$

Define the finite rank approximations

$$F_Nu(x) = \int K_N(x,y)u(y)dy, \qquad K_N(x,y) = \sum_{|\alpha|+|\beta|\le N} c_{\alpha\beta}\,\varphi_\alpha(x)\varphi_\beta(y).$$

Note that each F_N has finite rank because its rank is contained in the span of the φ_α with $|\alpha| \le N$, so it is enough to show that

$$\|u\|_{L^2(\mathbb{R}^d)}^{-1}\Big\| \int K(x,y)u(y)dy - \int K_N(x,y)u(y)dy\Big\|_{L^2(\mathbb{R}^d)} \to 0, \qquad \text{as } N \to \infty.$$

For that we put $\tilde{K} = K - K_N$ and write, using the Cauchy–Schwarz inequality,

$$\Big\| \int \tilde{K}(x,y)u(y)dy\Big\|^2_{L^2(\mathbb{R}^d)} = \int \Big| \int \tilde{K}(x,y)u(y)dy\Big|^2 dx \le \|\tilde{K}\|_{L^2(\mathbb{R}^{2d})}\|u\|^2_{L^2(\mathbb{R}^d)}.$$

But, by the Pythagoren theorem (13), we have

$$\|\tilde{K}\|_{L^2(\mathbb{R}^{2d})} = \sum_{|\alpha|+|\beta|>N} |c_{\alpha\beta}|^2,$$

which tends to 0 as $N \to \infty$, as desired. □

That concludes the proof that the spectrum of $-\Delta + V$ is discrete in $\mathbb{C} \setminus [0,\infty)$ when V is bounded and $V(x) \to 0$ as $|x| \to \infty$. It is not necessary to assume that V is bounded. We will prove that if $d \le 3$, then the same conclusion holds under the assumption that $V(x) \to 0$ as $|x| \to \infty$ and that there is $R > 0$ such that $V\mathbf{1}_{|x|\le R} \in L^2(\mathbb{R}^d)$, where $\mathbf{1}_{|x|\le R}$ is the function which is 1 when $|x| \le R$ and 0 otherwise. This includes the case of the Coulomb potential $V(x) = -Z/|x|$ in $\mathbb{R}^3$.

By the above reasoning, it is enough to show that $V\mathbf{1}_{|x|\le R}(-\Delta - z)^{-1}$ is a compact operator $L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$, and that $\|V\mathbf{1}_{|x|\le R}(-\Delta - z)^{-1}\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \to 0$ as $z \to -\infty$. For the latter we write

$$\|V\mathbf{1}_{|x|\le R}(-\Delta - z)^{-1}u\|_{L^2(\mathbb{R}^d)} \le \|V\mathbf{1}_{|x|\le R}\|_{L^2(\mathbb{R}^d)} \sup|(-\Delta - z)^{-1}u|,$$

and

$$\sup|(-\Delta - z)^{-1}u| \le \frac{1}{(2\pi)^d}\int \frac{|\hat{u}(\xi)|}{||\xi|^2 - z|}d\xi \le \frac{1}{(2\pi)^{d/2}}\|u\|_{L^2}\Big(\int ||\xi|^2 - z|^{-2}d\xi\Big)^{1/2},$$

and observe that $d \le 3$ implies that $\int ||\xi|^2 - z|^{-2}d\xi \to 0$ as $z \to -\infty$ (substitute $\eta = \xi/\sqrt{-z}$).

To prove that $V\mathbf{1}_{|x|\le R}(-\Delta - z)^{-1}$ is compact, by Theorem 9 it is enough to show that $\|V\mathbf{1}_{|x|\le R}(-\Delta - z)^{-1} - \tilde{V}_M(-\Delta - z)^{-1}\|_{L^2\to L^2} \to 0$ as $M \to \infty$, where $\tilde{V}_M$ is that function which equals V when $|x| \le R$ and $|V(x)| \le M$ and which equals 0 otherwise. For that we write

$$\|V\mathbf{1}_{|x|\le R}(-\Delta - z)^{-1}u - \tilde{V}_M(-\Delta - z)^{-1}u\|_{L^2(\mathbb{R}^d)} \le \|V\mathbf{1}_{|x|\le R} - \tilde{V}_M\|_{L^2(\mathbb{R}^d)} \sup|(-\Delta - z)^{-1}u|,$$

and observe that

$$\|V\mathbf{1}_{|x|\le R} - \tilde{V}_M\|_{L^2(\mathbb{R}^d)} \to 0,$$

as $M \to \infty$, by the dominated convergence theorem.

4. Propagation of singularities and propagation of regularity. Let c be a positive constant and let I be an interval. A distributional solution to the one-dimensional free wave equation $(\partial_{x_0}^2 - c^2\partial_{x_1}^2)w(x_0,x_1) = 0$ is $w(x_0,x_1) = \mathbf{1}_I(x_1 - cx_0) + \delta(x_1 + cx_0)$. This distribution is not smooth, but its singularities have a special structure. The first term is smooth in the direction $(1,c)$ and the second term is smooth in the direction $(1,-c)$. This structure can be generalized to wave equations of arbitrary dimension and with variable coefficients. To do this introduce definitions which allow us to describe singularities of distributions more generally and precisely. We begin with the following example.

EXAMPLE 2. Define $u \in \mathcal{S}'(\mathbb{R}^2)$ by $u(x_0,x_1) = \varphi(x_1)\delta(x_0)$, where $\varphi \in \mathcal{S}(\mathbb{R})$. Then $\hat{u}(\xi_0,\xi_1) = \hat{\varphi}(\xi_1)$. To find the values of s for which $u \in H^s(\mathbb{R}^2)$ we write

$$\int_{\mathbb{R}^2} (1+|\xi|^2)^s|\hat{\varphi}(\xi_1)|^2 d\xi = \int_{\mathbb{R}}\int_{\mathbb{R}} (1+\xi_0^2+\xi_1^2)^s d\xi_0 |\hat{\varphi}(\xi_1)|^2 d\xi_1.$$

The inner integral converges if and only if $s < -1/2$ and we can simplify it by putting $\xi_0 = (1+\xi_1^2)^{1/2}\eta$, $d\xi_0 = (1+\xi_1^2)^{1/2}d\eta$. That gives

$$\int_{\mathbb{R}}\int_{\mathbb{R}} (1+\xi_0^2+\xi_1^2)^s d\xi_0 |\hat{\varphi}(\xi_1)|^2 d\xi_1 = \int (1+\eta^2)^s d\eta \int (1+\xi_1^2)^{s+1/2}|\hat{\varphi}(\xi_1)|^2 d\xi_1.$$

The ξ_1 integral converges because $\varphi \in \mathcal{S}$, and hence we see that $u \in H^s(\mathbb{R}^2)$ if and only if $s < -1/2$.

Observe that we only used the decay given by the condition $s < -1/2$ in the ξ_0 direction, as in the ξ_1 direction we had ample decay coming from the fact that $\varphi \in \mathcal{S}$. This is a reflection of the fact that u_0 is regular in the ξ_1 direction and singular in the ξ_0 direction. Moreover, $u(x) = 0$ when $x_0 \neq 0$ and is thus completely regular there. To capture this information we will introduce the notion of being in H^s in a particular direction $\xi/|\xi|$ at a particular point x, or more shortly being in H^s at $(x,\xi/|\xi|)$. The notion requires a few preliminary definitions, and before stating it we mention that in this example we will get that $u \in H^s$ at $(x,\xi/|\xi|)$ for all s if $x_0 \neq 0$ or if $\xi_0 = 0$, and $u \in H^s$ at $(x,\xi/|\xi|)$ for $s < -1/2$ if $x_0 = 0$ and $\xi_1 = 0$.

EXERCISE 24. Determine for which values of s is $u \in H^s(\mathbb{R}^2)$ for one or more of the following functions: a) $u(x) = \delta(x_0)\varphi(x_1)$, where $\varphi \in H^r(\mathbb{R})$ for some given real r, b) $u(x) = \delta(x_0)\mathbf{1}_I(x_1)$, where I is a bounded interval, c) $u(x) = \mathbf{1}_I(x_0)\mathbf{1}_J(x_1)$, where I and J are bounded intervals, d) $u(x) = \varphi_0(x_0)\varphi_1(x_1)$, where each $\varphi_j \in H^{r_j}(\mathbb{R})$ for some given real r_j.

A function $a \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ is called a *symbol* of order m if its partial derivatives obey the bounds

$$|\partial_x^\alpha \partial_\xi^\beta a(x,\xi)| \le C_{\alpha,\beta}|\xi|^{m-|\beta|},$$

for ξ large. To each such symbol we associate a *pseudodifferential operator* A, called the *right quantization* of a, given by

$$Au(x) = \frac{1}{(2\pi)^d}\int\int e^{i(x-y)\cdot\xi}a(y,\xi)u(y)\,dy\,d\xi.$$

An important example is the classical Hamiltonian $a(x,\xi) = |\xi|^2 + V(x)$, whose quantization is the Schrödinger operator $-\Delta + V(x)$. More generally, if $a \in S^m$ is a polynomial of degree m in the ξ variable, then its quantization is a differential operator of order m.

Exercise 25. Find a symbol a such that $A = \sum_{j=0}^3 \partial_{x_j}^j$. For which m is $a \in S^m$?

Exercise 26. Find a symbol a such that $A = \partial_{x_0}^3 \partial_{x_1}^4 + e^{-x_0^1 - x_1^2} \partial_{x_0} \partial_{x_1}$. For which m is $a \in S^m$?

The major mapping property of these pseudodifferential operators is the following:

Theorem 10. *If $a \in S^m$, then A is a bounded operator from H^k to H^{k-m} for every k.*

We will discuss the proof Theorem 10 later, but for now note the following simpler cases:

(1) If $a(x,\xi) = a(\xi)$ is independent of x then A is called a Fourier multiplier. This is bounded $H^k \to H^{k-m}$ because $|a(\xi)| \le C(1+|\xi|^2)^{m/2}$ and hence

$$\|Au\|_{H^{k-m}}^2 = \int |(1+|\xi|^2)^{(k-m)/2} a(\xi) \hat{u}(\xi)|^2 d\xi \le C \int |(1+|\xi|^2)^{k/2} \hat{u}(\xi)|^2 d\xi = C\|u\|_{H^k}^2.$$

(2) If $a(x,\xi) = a(x)$ is independent of ξ then A is the multiplier $u(x) \mapsto a(x)u(x)$. This is bounded $L^2 \to L^2$ because $\int |au|^2 \le \sup |a|^2 \int |u|^2$. If k is an integer, we can prove boundedness $H^k \to H^k$ by arguing as follows: it is enough to show that if all partial derivatives of u up to order k are in L^2 then all partial derivatives of au up to order k are in L^2. This in turn follows from writing out using the product rule that

$$\int |\partial^\alpha(au)|^2 = \sum_{\gamma \le \alpha} \int |c_{\alpha,\gamma} \partial^{\alpha-\gamma} a \partial^\gamma u|^2 \le \sum_{\gamma \le \alpha} |c_{\alpha,\gamma}|^2 \sup |\partial^{\alpha-\gamma} a|^2 \int |\partial^\gamma u|^2.$$

In light of Theorem 10 we can say that $u \in H^k$ if and only if $Au \in L^2$ for all[9] $a \in S^k$. This motivates the following definitions:

Given $x' \in \mathbb{R}^d$, we say that $u \in H^k$ *at* x' if there is a neighborhood $U \subset \mathbb{R}^d$ of x' such that $Au \in L^2$ for all[10] $a \in S^k$ such that $a(x,\xi) = 0$ whenever $x \notin U$.

Example 3. Let u be as in Example 2. We can show that $u \in H^k$ for all k at all x' such that $x_0' \ne 0$ as follows. Let $U \subset \mathbb{R}^d$ be a neighborhood of x' such that $x_0 \ne 0$ for all x in U. Take $a \in S^k$ such that $a(x,\xi) = 0$ whenever $x \notin U$. Then $Au = 0$ just because $a(y,\xi)\delta(y_0) = a(0,y_2,\xi)\delta(y_0) = 0$.

Given $x' \in \mathbb{R}^d$ and $\xi' \in \mathbb{R}^d \setminus \{0\}$, we say that $u \in H^k$ *at* $(x', \xi'/|\xi'|)$ if there is a neighborhood $U \subset \mathbb{R}^d \times \mathbb{S}^{d-1}$ of $(x', \xi'/|\xi'|)$ such that $Au \in L^2$ for all[11] $a \in S^k$ such that $a(x,\xi) = 0$ whenever $(x, \xi/|\xi|) \notin U$.

Example 4. Let u be as in Example 2. We can show that $u \in H^k$ for all k at all $(x', \xi'/|\xi'|)$ such that either $x_0' \ne 0$ or such that $\xi_1' \ne 0$ as follows. If $x_0' \ne 0$, then let $U \subset \mathbb{R}^d \times \mathbb{S}^{d-1}$ be a neighborhood of $(x', \xi'/|\xi'|)$ such that $x_0 \ne 0$ for all $(x, \xi/|\xi|)$ in U. Then proceed as in Example 3. If $\xi_1' \ne 0$, then let $U \subset \mathbb{R}^d \times \mathbb{S}^{d-1}$ be a neighborhood of $(x', \xi'/|\xi'|)$ such that

$$\text{there is some constant } C \text{ such that } |\xi| \le C|\xi_1| \text{ whenever } (x, \xi/|\xi|) \text{ is in } U; \tag{25}$$

[9] Of course in practice, if we want to know whether $u \in H^k$, checking $Au \in L^2$ for every last $a \in S^k$ is overkill because by definition it is enough to check it for $a(x,\xi) = (1+|\xi|^2)^{k/2}$.

[10] As in the previous footnote, we will see later that it is enough to check $Au \in L^2$ for a single well-chosen a.

[11] Again, as in the previous two footnotes, we will see later that it is enough to check $Au \in L^2$ for a single well-chosen a.

to arrange this it is enough to ensure that $\overline{U}$ does not intersect the set where $\xi_1 = 0$. Take $a \in S^k$ such that $a(x,\xi) = 0$ whenever $(x, \xi/|\xi|) \notin U$. Then

$$\|Au\|_{L^2}^2 = \frac{1}{(2\pi)^d}\|\widehat{Au}\|_{L^2}^2 = \frac{1}{(2\pi)^d}\int\Big|\int e^{-iy\xi}a(y,\xi)u(y)\,dy\Big|^2 d\xi$$
$$= \frac{1}{(2\pi)^d}\int\Big|\int e^{-iy_1\xi_1}a(0,y_1,\xi)\varphi(y_1)\,dy_1\Big|^2 d\xi \stackrel{\text{def}}{=} \int F(\xi)\,d\xi,$$

where $F(\xi)$ is defined by the equation. F is well-defined (i.e. the integral defining it converges) and F is continuous because $\varphi \in \mathcal{S}$. To see that $\int F$ converges we write $\int F(\xi)d\xi = \int_{|\xi_1|\le 1} F(\xi)d\xi + \int_{|\xi_1|\ge 1} F(\xi)d\xi$, and observe that $\int_{|\xi_1|\le 1} F(\xi)d\xi$ converges because the region of integration and integrand are both bounded.

Thus it is enough to check that $\int_{|\xi_1|\ge 1} F(\xi)d\xi$ converges. We will prove this by proving that $|F(\xi)| \le C_1|\xi|^{-4}$. For that we integrate by parts repeatedly, writing

$$\int e^{-iy_1\xi_1}a(0,y_1,\xi)\varphi(y_1)\,dy_1 = \Big(\frac{i}{\xi_1}\Big)^{k+2}\int(\partial_{y_1}^{k+2}e^{-iy_1\xi_1})a(0,y_1,\xi)\varphi(y_1)\,dy_1$$
$$= \Big(\frac{-i}{\xi_1}\Big)^{k+2}\int e^{-iy_1\xi_1}\partial_{y_1}^{k+2}(a(0,y_1,\xi)\varphi(y_1))\,dy_1,$$

which shows that $|\int e^{-iy_1\xi_1}a(0,y_1,\xi)\varphi(y_1)\,dy_1| \le C_2|\xi|^k|\xi_1|^{-k-2} \le C_3|\xi|^{-2}$, where for the last inequality we used (25). This concludes the proof that, in this example, if $\xi_1' \neq 0$, then $u \in H^k$ for all k at $(x', \xi'/|\xi'|)$. In summary, if u is as in Example 2, then $u \in H^k$ for all k at all $(x', \xi'/|\xi'|)$ provided only that $(x', \xi'/|\xi'|)$ is not of the form $(0, x_1', \pm 1, 0)$.

Exercise 27. Let $u(x_0, x_1) = \delta(x_0)\mathbf{1}_I(x_1)$, where I is a bounded interval. For which $(x', \xi'/|\xi'|)$ can you show that $u \in H^k$ for all k at $(x', \xi'/|\xi'|)$?

Our definition of what it means for u to be in $H^k(\mathbb{R}^d)$ at a point $x \in \mathbb{R}^d$ is called a *local* regularity condition. Our definition of what it means for u to be in $H^k(\mathbb{R}^d)$ in a certain direction $\xi/|\xi|$ at a point $x \in \mathbb{R}^d$ is called a *microlocal* regularity condition. The term *microlocal analysis* refers to analysis in *phase space*, i.e. the space of $\mathbb{R}^d \times \mathbb{R}^d$ of positions $x \in \mathbb{R}^d$ and momenta $\xi \in \mathbb{R}^d$ taken together.

Our next result is a microlocal *elliptic* regularity result. We will define what it means for a symbol a to be elliptic at $(x, \xi/|\xi|)$, and show that if $Au = 0$ then $u \in H^k$ for all k at all $(x, \xi/|\xi|)$ at which a is elliptic.

This is a microlocal generalization of the classical result that if $\Delta u = 0$ then $u \in C^\infty$. One says that the Laplacian $\partial_{x_0}^2 + \partial_{x_1}^2$ is an *elliptic* differential operator and the D'Alembertian (i.e. the wave operator) $\partial_{x_0}^2 - \partial_{x_1}^2$ is a *hyperbolic*; this terminology predates symbols and pseudodifferential operators but in our language we can say this is because the level sets of the symbol of the Laplacian are ellipses and the level sets of the symbol of the D'Alembertian are hyperbolas. We will see however that the D'Alembertian is microlocally elliptic for almost every $(x, \xi/|\xi|)$, even though there is no sense in which it is locally elliptic for any x at all.

We say $a \in S^m$ is *elliptic* at $(x', \xi'/|\xi'|)$ if there are positive constants C and ε, and a neighborhood $U \subset \mathbb{R}^d \times \mathbb{S}^{d-1}$ of $(x', \xi'/|\xi'|)$, such that

$$|a(x, \xi)| \geq \varepsilon |\xi|^m,$$

when $(x, \xi/|\xi|) \in U$ and $|\xi| \geq C$. The set of points in $\mathbb{R}^d \times \mathbb{S}^{d-1}$ at which a is elliptic is denoted $\mathrm{ell}(a)$.

Example 5. The symbol $-|\xi|^2$ of the Laplacian $\partial_{x_0}^2 + \partial_{x_1}^2 + \cdots + \partial_{x_d}^2$ is elliptic at all $(x', \xi'/|\xi'|)$, and the symbol $-\xi_0^2 + \xi_1^2 + \cdots + \xi_d^2$ of the D'Alembertian $\partial_{x_0}^2 - \partial_{x_1}^2 - \cdots - \partial_{x_d}^2$ is elliptic at all $(x', \xi'/|\xi'|)$ such that $\xi_0^2 \neq \xi_1^2 + \cdots + \xi_d^2$.

Exercise 28. Let $c > 0$ be given. For which values of a is $u(x_0, x_1) = \delta(x_1 + ax_0)$ a solution to $(\partial_{x_0}^2 - c^2\partial_{x_1}^2)u(x_0, x_1) = 0$? Prove that, for every $(x', \xi'/|\xi'|)$, if $(\partial_{x_0}^2 - c^2\partial_{x_1}^2)$ is elliptic at $(x', \xi'/|\xi'|)$, then $u \in H^k$ for all k at $(x', \xi'/|\xi'|)$.

To each $a \in S^m$ which is compactly supported in x, we associate an *essential support* in terms of $(x', \xi'/|\xi'|)$, denoted by $\mathrm{ess\,supp}(a)$, and defined as follows: $(x', \xi'/|\xi'|)$ is not in the essential support if and only if there is a neighborhood $U \subset \mathbb{R}^d \times \mathbb{S}^{d-1}$ of $(x', \xi'/|\xi'|)$, such that the partial derivatives of a obey the bounds

$$|\partial_x^\alpha \partial_\xi^\beta a(x, \xi)| \leq C_{\alpha,\beta,N} |\xi|^{-N},$$

for $|\xi|$ large enough, when $(x, \xi/|\xi|) \in U$.

Theorem 11. *Let* $a \in S^m$ *and* $a' \in S^{m'}$ *be such that* a *is compactly supported in* x *and* $\mathrm{ess\,supp}\, a \subset \mathrm{ell}(a')$. *Then for any* k *and* N *there is* C *such that*

$$\|Au\|_{H^k} \leq C(\|A'u\|_{H^{k+m-m'}} + \|u\|_{H^{-N}}). \tag{26}$$

Further discussion and references. A broader presentation of spectral theory with applications to differential equations can be found in [Bor]. The introduction of that book describes the development of spectral theory, including the various mathematical and physical concepts that have gone into it (and come out of it). The proof of Theorem 8 is from Theorem VI.14 of [RS] and the proof of Theorem 9 is from Lemma 7.21 of [Tes].

The discussion of propagation of singularities and propagation of regularity is a minimalist version of Hörmander's propagation of singularities theorem for the wave equation. For a more complete presentation, see Section 8 of [Hin], and for still more see Section E.4 of [DZ] or Section 3.5 of the original paper of Hörmander [Hör].

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List of notation.

- $\hat{f}(\xi) = \int e^{-ix\xi} f(x)dx$ is the Fourier transform of f. See Section 3 of [FW].
- $\langle f, g\rangle = \int f\bar{g}$, and $f \otimes g$ is the operator mapping u to $f\langle u, g\rangle$.
- $B(a, R) = \{x \in \mathbb{R}^d \colon |x - a| < R\}$ is the open ball with center a and radius R.
- $C^k(\mathbb{R}^d)$ is the space of k-times continuously differentiable functions. This is sometimes abbreviated as C^k, and similar abbreviations are used for the spaces below.
- $H^s(\mathbb{R}^d)$ is the space of Sobolev functions. See Section 6 of [FW].
- $L^p(\mathbb{R}^d)$ is the Lebesgue space of measurable functions such that $\int |f|^p$ converges.
- $\mathcal{S}(\mathbb{R}^d)$ is the space of Schwartz functions. See Section 2 of [FW].
- $\mathcal{S}'(\mathbb{R}^d)$ is the space of tempered distributions. See Section 2 of [FW].