LECTURE 4

Sturm-Liouville Eigenvalue Problems

Possibly one of the most useful facts in mathematics is that a symmetric matric has real eigenvalues and a set of eigenvectors that form an orthonormal basis. This property of symmetric matrices has a wide-ranging generalization to the spectral properties of self-adjoint operators in a Hilbert space, of which the Sturm-Liouville ordinary differential operators are fundamental examples.

Sturm-Liouville equations arise throughout applied mathematics. For example, they describe the vibrational modes of various systems, such as the vibrations of a string or the energy eigenfunctions of a quantum mechanical oscillator, in which case the eigenvalues correspond to the resonant frequencies of vibration or energy levels. It was, in part, the idea that the discrete energy levels observed in atomic systems could be obtained as the eigenvalues of a differential operator which led Schrödinger to propose his wave equation.

Sturm-Liouville problems arise directly as eigenvalue problems in one space dimension. They also commonly arise from linear PDEs in several space dimensions when the equations are separable in some coordinate system, such as cylindrical or spherical coordinates.

The general form of the Sturm-Liouville equation is an ODE for $u(x)$ of the form

$$-(pu')' + qu = \lambda ru. \tag{4.1}$$

Here, $p(x)$, $q(x)$ are coefficient functions, $r(x)$ is a weighting function (equal to one in the simplest case) and λ is an eigenvalue, or spectral, parameter. The ODE is supplemented by appropriate self-adjoint boundary conditions.

The simplest example of a Sturm-Liouville operator is the constant-coefficient second-derivative operator, whose eigenfunctions are trigonometric functions. Many other important special functions, such as Airy functions and Bessel functions, are associated with variable-coefficient Sturm-Liouville operators.

Just as we may expand a vector with respect to the eigenvectors of a symmetric matrix, we may expand functions in terms of the eigenfunctions of a regular Sturm-Liouville operator; the expansion of periodic functions in Fourier series is an example.

One feature that occurs for Sturm-Liouville operators, which does not occur for matrices, is the possibility of an absolutely continuous (or, for short, continuous) spectrum. Instead of eigenfunction expansions, we then then get integral transforms, of which the Fourier transform is an example.

Other, more complicated spectral phenomena can also occur. For example, eigenvalues embedded in a continuous spectrum, singular continuous spectrum, and pure point spectrum consisting of eigenvalues that are dense in an interval (see Section 4.6 on the Anderson localization of waves in random media for an example).

1. Vibrating strings

Consider the vibrations of a string such as a violin string. We label material points on the string by a Lagrangian coordinate $a \in \mathbb{R}$; for example, we can define a as the distance of the point from some fixed point in a given reference configuration of the string. We denote the position of the material point a on the string at time t by $\vec{r}(a,t)$.

Let $\rho_0(a)$ denote the mass-density of the string in the reference configuration, meaning that the mass of the part of the string with $c \le a \le d$ is given by

$$\int_c^d \rho_0(a)\, da.$$

We assume that the mass of the string is conserved as it vibrates, in which case the density $\rho_0(a)$ in the reference configuration is independent of time.

We suppose that the only force exerted by one part of the string on another is a tension force tangent to the string. This assumption distinguishes a string from an elastic rod that resists bending. We also suppose, for simplicity, that no external forces act on the string.

The contact force $\vec{F}$ exerted by the part of the string with $b > a$ on the part with $b < a$ is then given by

$$\vec{F}(a,t) = T(a,t)\,\vec{t}(a,t)$$

where $T(a,t)$ is the tension in the string and

$$\vec{t} = \frac{\vec{r}_a}{|\vec{r}_a|}$$

is the unit tangent vector. We assume that $\vec{r}_a$ never vanishes. The part of the string with $b < a$ exerts an equal and opposite force $-\vec{F}$ on the part of the string with $b > a$.

Newton's second law, applied to the part of the string with $c \le a \le d$, gives

$$\frac{d}{dt}\int_c^d \rho_0(a)\vec{r}_t(a,t)\, da = \vec{F}(d,t) - \vec{F}(c,t).$$

For smooth solutions, we may rewrite this equation as

$$\int_c^d \left\{\rho_0(a)\vec{r}_{tt}(a,t) - \vec{F}_a(a,t)\right\}\, da = 0.$$

Since this holds for arbitrary intervals $[c,d]$, and since we assume that all functions are smooth, we conclude that

$$\rho_0(a)\vec{r}_{tt}(a,t) = \vec{F}_a(a,t).$$

This equation expresses conservation of momentum for motions of the string.

To close the equation, we require a constitutive relation that relates the tension in the string to the stretching of the string. The local extension of the string from its reference configuration is given by

$$e(a,t) = |\vec{r}_a(a,t)|.$$

We assume that

$$T(a,t) = f\left(e(a,t), a\right)$$

where $f(e,a)$ is a given function of the extension e and the material coordinate a.

It follows that the position-vector $\vec{r}(a,t)$ of the string satisfies the nonlinear wave equation

$$\rho_0(a)\vec{r}_{tt}(a,t) = \partial_a \left\{ f\left(|\vec{r}_a(a,t)|, a\right) \frac{\vec{r}_a(a,t)}{|\vec{r}_a(a,t)|} \right\}. \tag{4.2}$$

1.1. Equilibrium solutions

A function $\vec{r} = \vec{r}_0(a)$ is an exact, time-independent solution of (4.2) if

$$\frac{d}{da} \left\{ f\left(|\vec{r}_{0a}|, a\right) \frac{\vec{r}_{0a}}{|\vec{r}_{0a}|} \right\} = 0. \tag{4.3}$$

We consider a solution such that the tangent vector of the string is in a constant direction, say the $\vec{i}$-direction.

We may then use as a material coordinate the distance a along the string in the equilibrium configuration, in which case

$$\vec{r}_0(a) = a\vec{i}. \tag{4.4}$$

Using (4.4) and the corresponding extension $e = 1$, in (4.3), we find that the tension

$$f\left(1, a\right) = T_0$$

is constant in equilibrium, as required by the balance of longitudinal forces.

1.2. Linearized equation

For small vibrations of the string about an equilibrium state, we may linearize the equations of motion. We look for solutions of the form

$$\vec{r}(a,t) = a\vec{i} + \vec{r}'(a,t), \tag{4.5}$$

where $\vec{r}'$ is a small perturbation of the equilibrium solution (4.4). We decompose $\vec{r}'$ into longitudinal and transverse components

$$\vec{r}'(a,t) = x'(a,t)\vec{i} + \vec{r}^{\perp}(a,t),$$

where $\vec{i} \cdot \vec{r}^{\perp} = 0$.

We use (4.5) in (4.2), with $e = 1 + x'_a + \ldots$, and Taylor expand the resulting equation with respect to $\vec{r}'$. This gives

$$\rho_0 \vec{r}'_{tt} = \partial_a \left\{ \left(T_0 + kx'_a\right)\left(1 - x'_a\right) \left[\left(1 + x'_a\right)\vec{i} + \vec{r}^{\perp}_a \right] \right\} + \ldots$$

where $k(a) = f_e\left(1, a\right)$. Linearizing the equation, and separating it into longitudinal and transverse components, we find that

$$\rho_0 x'_{tt} = \left(kx'_a\right)_a, \qquad \rho_0 \vec{r}^{\perp}_{tt} = T_0 \vec{r}^{\perp}_{aa}. \tag{4.6}$$

Thus we obtain decoupled equations for the longitudinal and transverse motions of the string.

The longitudinal displacement satisfies a one-dimensional wave equation of the form (3.56). The density is given by the density in the reference configuration, and the stiffness by the derivative of the tension with respect to the extension; the stiffness is positive, and the equation is a wave equation provided that the tension in the string increases when it is stretched. In general, both coefficients are functions of a, but for a uniform string they are constants.

Unlike the longitudinal mode, the stiffness constant T_0 for the transverse mode is necessarily constant. If $T_0 > 0$, meaning that the string is stretched, the transverse displacement satisfies a wave equation, but if $T_0 < 0$ it satisfies an elliptic

equation. As we explain in the following section, the initial value problem for such PDEs is subject to an extreme instability. This is consistent with our experience that one needs to stretch a string to pluck it.

1.3. Hadamard instability

As a short aside, we consider the instability of the initial value problem for an elliptic PDE, such as the one that arises above for transverse vibrations of a compressed elastic string. This type of instability arises in other physical problems, such as the Kelvin-Helmholtz instability of a vortex sheet in fluid mechanics.

The simplest case of the transverse equation in (4.6) with constant coefficients, normalized to $\rho_0 = 1$, $T_0 = -1$, and planar motions $x = a$ and $y = u(x,t)$, is the Laplace equation

$$u_{tt} = -u_{xx}. \tag{4.7}$$

Equation (4.7) has solutions

$$u(x,t) = Ae^{inx+|n|t} \tag{4.8}$$

for arbitrary $n \in \mathbb{R}$ and $A \in \mathbb{C}$. Since the equation is linear with real-coefficients, we may obtain real-valued solutions by taking the real or imaginary parts of any complex-valued solution, and we consider complex-valued solutions for convenience.

The solution in (4.8) has modulus $|u(x,t)| = |A|e^{|k|t}$. Thus, these solutions grow exponentially in time with arbitrarily large rates. (The solutions proportional to $e^{inx-|n|t}$ grow arbitrarily fast backward in time.)

This behavior is a consequence of the invariance of (4.8) under the rescalings $x \mapsto \lambda$, $t \mapsto \lambda t$. This scale-invariance implies that if there is one solution with bounded initial data and a nonzero growth rate, then we can obtain solutions with arbitrarily fast growth rates by rescaling the initial data.

As a result, solutions do not depend continuously on the initial data in any norm that involves only finitely many derivatives, and the resulting initial value problem for (4.7) is ill-posed with respect to such norms. For example, if

$$\|u\|_K(t) = \max_{0\leq k\leq K} \sup_{x\in\mathbb{R}} \left|\partial_x^k u(x,t)\right|$$

and

$$u_n(x,t) = e^{-|n|^{1/2}} \left\{e^{inx-nt} + e^{inx+nt}\right\},$$

then for every $K \in \mathbb{N}$ we have

$$\|u_n\|_K(0) \to 0 \qquad \text{as } n \to \infty,$$

but

$$|u_n(x,t)| \to \infty \qquad \text{as } n \to \infty \text{ if } t \neq 0.$$

This failure of continuous dependence leads to a loss of existence of solutions. For example, the Fourier series

$$f(x) = \sum_{k=-\infty}^{\infty} e^{-|k|^{1/2}} e^{ikx}$$

converges to a C^∞-function, but there is no solution of (4.7) with initial data

$$u(x,0) = f(x), \qquad u_t(x,0) = 0$$

in any time interval about 0, however short.

It is possible to obtain solutions of (4.7) for sufficiently 'good' initial data, such as analytic functions (which, from the Cauchy-Kovalewsky theorem, are given by locally convergent power series). Such assumptions, however, are almost always too restrictive in applications. The occurrence of Hadamard instability typically signals a failure of the model, and means that additional stabilizing effects must be included at sufficiently short length-scales.

2. The one-dimensional wave equation

Consider a uniform string with constant density ρ_0 and and constant stiffness k_0. Then, from (4.17), longitudinal vibrations of the string satisfy the one-dimensional wave equation

$$u_{tt} = c_0^2 u_{xx} \tag{4.9}$$

Planar transverse vibrations of a stretched string satisfy the same equation with $c_0^2 = T_0/\rho_0$.

2.1. The d'Alembert solution

The general solution of (4.9) is given by the d'Alembert solution

$$u(x,t) = F(x - c_0 t) + G(x + c_0 t) \tag{4.10}$$

where F, G are arbitrary functions. This solution represents a superposition of a right-moving traveling wave with profile F and a left-moving traveling wave with profile G.

It follows that the solution of the Cauchy problem for (4.9) with initial data

$$u(x,0) = f(x), \qquad u_t(x,0) = g(x) \tag{4.11}$$

is given by (4.10) with

$$F(x) = \frac{1}{2} f(x) - \frac{1}{2c_0} \int_{x_0}^{x} g(\xi)\, d\xi, \qquad G(x) = \frac{1}{2} f(x) + \frac{1}{2c_0} \int_{x_0}^{x} g(\xi)\, d\xi.$$

Here, x_0 is an arbitrary constant; changing x_0 does not change the solution, it simply transforms $F(x) \mapsto F(x) + c$, $G(x) \mapsto G(x) - c$ for some constant c.

2.2. Normal modes

Next, consider a boundary value problem (BVP) for (4.9) in $0 \le x \le L$ with boundary conditions

$$u(0,t) = 0, \qquad u(L,t) = 0. \tag{4.12}$$

This BVP describes the vibration of a uniform string of length L that is pinned at its endpoints.

We look for separable solutions of the form

$$u(x,t) = \varphi(x) e^{-i\omega t} \tag{4.13}$$

where ω is a constant frequency and $\varphi(x)$ is a function of the spatial variable only. The real and imaginary parts of a complex-valued solution of a linear equation with real coefficients are also solutions, so we may recover the real-valued solutions from these complex-valued solutions.

The function $u(x,t)$ in (4.13) satisfies (4.9), (4.12) if $\varphi(x)$ satisfies

$$\varphi'' + k^2 \varphi = 0, \qquad \varphi(0) = 0, \quad \varphi(L) = 0$$

where the prime denotes a derivative with respect to x, and

$$k^2 = \frac{\omega^2}{c_0^2}.$$

The spectral problem

$$-\varphi'' = \lambda\varphi, \qquad \varphi(0) = 0, \quad \varphi(L) = 0$$

has a point spectrum consisting entirely of eigenvalues

$$\lambda_n = \frac{\pi^2 n^2}{L^2} \qquad \text{for } n = 1, 2, 3, \ldots. \tag{4.14}$$

Up to an arbitrary constant factor, the corresponding eigenfunctions $\varphi_n \in L^2[0, L]$ are given by

$$\varphi_n(x) = \sin\left(\frac{n\pi x}{L}\right). \tag{4.15}$$

These eigenfunctions are orthogonal with respect to the $L^2[0, L]$-inner product

$$\langle f, g\rangle = \int_0^L f(x)g(x)\,dx,$$

where $f, g : [0, L] \to \mathbb{R}$ are square-integrable functions. Explicitly, for any $m, n \in \mathbb{N}$

$$\int_0^L \sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right)\,dx = \begin{cases} L/2 & \text{if } n = m, \\ 0 & \text{if } n \neq m. \end{cases}$$

An arbitrary function $f \in L^2[0, L]$ may be expanded with respect to these eigenfunctions in a Fourier sine series as

$$f(x) = \sum_{n=1}^{\infty} a_n \sin n\pi x,$$

where, by orthogonality,

$$a_n = \frac{2}{L}\int_0^L f(x)\sin n\pi x\,dx.$$

The series converges to f in the L^2-norm, meaning that

$$\left\| f(x) - \sum_{n=1}^{N} a_n \sin n\pi x \right\| = \left(\int_0^L \left| f(x) - \sum_{n=1}^{N} a_n \sin n\pi x \right|^2 dx \right)^{1/2} \to 0 \qquad \text{as } N \to \infty.$$

We say that the eigenfunctions are a basis of $L^2[0, L]$, and form a complete set.

The solutions for k corresponding to (4.14) are

$$k_n = \frac{n\pi}{L} \qquad \text{for } n = 1, 2, 3, \ldots,$$

The separable solutions of (4.9), (4.12) associated with (4.15) are therefore

$$\sin(k_n x)\, e^{-ic_0 k_n t}, \qquad \sin(k_n x)\, e^{ic_0 k_n t}.$$

The real part of these solutions is

$$u(x, t) = \sin(k_n x)\cos\left(c_0 k_n t\right). \tag{4.16}$$

This is a standing-wave solution with profile proportional to $\sin\left(k_n x\right)$ that oscillates periodically in time with frequency $\omega_n = c_0 n$. The n^{th} mode has $n/2$ periods of the sine that fit between the two pinned endpoints at $x = 0$, $x = L$.

The frequencies of these solutions are $\omega_n = c_0 k_n$. When expressed in terms of the properties of the string, the lowest, or fundamental, frequency for transverse modes is

$$\omega_1 = \sqrt{\frac{T_0}{\rho_0 L^2}}.$$

Thus, for example, increasing the tension in a string increases the fundamental frequency of its transverse vibrations, and heavier, longer strings have a lower fundamental frequency than lighter, shorter ones.

The solution (4.16) may be written as

$$u(x,t) = \frac{1}{2}\sin\left[n\pi\left(x - c_0 t\right)\right] + \frac{1}{2}\sin\left[n\pi\left(x + c_0 t\right)\right],$$

which shows that the standing wave arise from the interference between two traveling waves propagating in opposite directions.

Since the PDE and the boundary conditions (4.9), (4.12) are linear, we can superpose the separated, time-periodic solutions to get the general real-valued solution

$$u(x,t) = \sum_{n=1}^{\infty} \sin(n\pi x)\left\{A_n e^{ic_0 nt} + \bar{A}_n e^{-ic_0 nt}\right\}$$

where $A_n \in \mathbb{C}$ is an arbitrary constant for each $n \in \mathbb{N}$.

We may write this solution in real form as

$$u(x,t) = \sum_{n=1}^{\infty} \sin(n\pi x)\left\{a_n \cos\left(c_0 nt\right) + b_n \sin\left(c_0 nt\right)\right\}$$

where $A_n = (a_n + ib_n)/2$. Imposing the initial condition (4.11), we find that

$$a_n = 2\int_0^1 f(x)\sin(n\pi x)\,dx, \qquad b_n = \frac{2}{nc_0}\int_0^1 g(x)\sin(n\pi x)\,dx.$$

This solution can again be written as a superposition of right-moving and right-moving traveling waves.

Similar solutions can be obtained for Neumann boundary conditions

$$\varphi'(0) = 0, \qquad \varphi'(L) = 0$$

leading to Fourier cosine series, and periodic boundary conditions

$$\varphi(0) = \varphi(L), \qquad \varphi'(0) = \varphi'(L)$$

leading to Fourier series.

2.3. The Fourier transform

On the real line, the spectral problem

$$-\varphi'' = \lambda\varphi$$

has a continuous spectrum $0 \le \lambda < \infty$, with bounded solutions that do not lie in $L^2(\mathbb{R})$; they are linear combinations of $e^{\pm i\sqrt{\lambda}x}$. Since $k^2 = \lambda$ and $\omega^2 = c_0^2 k^2$, we get a continuous set of solutions of the wave equation, proportional to

$$u(x,t) = e^{ikx - ic_0 kt}, \qquad u(x,t) = e^{ikx + ic_0 kt}$$

where $k \in \mathbb{R}$. The general superposition of these solutions is

$$u(x,t) = \int \left\{\hat{F}(k)e^{ik(x-c_0 t)} + \hat{G}(k)e^{ik(x+c_0 t)}\right\} dk$$

where $\hat{F}, \hat{G} : \mathbb{R} \to \mathbb{C}$ are arbitrary functions. The solution $u(x,t)$ is real-valued if $\hat{F}(-k) = \hat{F}^*(k)$ and $\hat{G}(-k) = \hat{G}^*(k)$ This solution is the Fourier transform of the d'Alembert solution (4.10).

This solution exhibits an important feature of the wave equation, namely that it is nondispersive. Fourier modes with different wavenumbers k propagate with the same velocity c_0 (or $-c_0$). As a result, The Fourier modes stay together as the solution evolves in time, and the solution is a superposition of traveling wave solutions with arbitrary wave-profiles that propagate at velocities c_0 (or $-c_0$) without changing their shape.

This behavior contrast with the behavior of linear dispersive waves, where the velocity of the Fourier modes depends on their wavenumbers. In this case, the Fourier modes making up the initial data separate, or disperse, as the solution evolves, leading to an extended oscillatory wavetrain.

2.4. Nonuniform strings

Let us return to the one-dimensional wave equation

$$\rho_0 u_{tt} = (k u_x)_x \tag{4.17}$$

for the longitudinal displacement $u(x,t)$ of a string of length L with mass-density $\rho_0(x)$ and stiffness $k(x)$, both of which we assume are smooth, strictly positive functions on $0 \le x \le L$. Suppose, for definiteness, that $u(x,t)$ satisfies the homogeneous Dirichlet condition (4.12) at the endpoints of the string.

Looking for separable time-periodic solutions of (4.17) and (4.12) of the form (4.13), we get the BVP

$$\begin{aligned} -(k\varphi')' &= \lambda \rho_0 \varphi, \\ \varphi(0) = 0, &\qquad \varphi(L) = 0, \end{aligned}$$

where $\lambda = \omega^2$. This equation has the form of a Sturm-Liouville eigenvalue problem (4.1) with $p = k$, $q = 0$, and $r = \rho_0$. Values of ω for which this BVP has nonzero solutions correspond to resonant frequencies of oscillation of the string. Unlike the uniform case, we cannot solve this eigenvalue problem explicitly for general coefficient functions ρ_0, k.

The qualitative behavior is, however, the same. There is an infinite sequence of simple positive eigenvalues $\lambda_1 < \lambda_2 < \lambda_3 < \dots$. The corresponding eigenfunctions $\{\varphi_1, \varphi_2, \varphi_3, \dots\}$ are orthogonal with respect to the weighted inner-product

$$\langle f, g \rangle = \int_0^L \rho_0(x) f(x) g(x)\, dx,$$

and form a complete set in $L^2[0,L]$. Moreover, like the sine-functions in the uniform case, the n^{th} eigenfunction has $(n-1)$ zeros in the interval $0 < x < L$. This is an example of a general oscillation property possessed by Sturm-Liouville eigenfunctions, and it means that eigenfunctions with higher eigenvalues oscillate more rapidly than ones with lower eigenvalues.

2.5. The Helmholtz equation

Analogous results apply in higher space dimensions, although the resulting eigenvalue problems are more difficult to analyze because they involve PDEs instead of ODEs.

Consider the wave equation in n space-dimensions,

$$u_{tt} = c_0^2 \Delta u.$$

We look for time-periodic solutions of the form

$$u(x,t) = \varphi(x) e^{-i\omega t}$$

where the frequency ω is constant. We find that φ satisfies the *Helmholtz* equation

$$-\Delta\varphi = \lambda\varphi, \tag{4.18}$$

where $\lambda = k^2$, and the wavenumber k is given by

$$k = \frac{\omega}{c_0}.$$

Consider solutions of (4.18) on a smooth, bounded domain $\Omega \subset \mathbb{R}^n$, subject to homogeneous Dirichlet boundary conditions

$$\varphi(x) = 0 \qquad \text{for } x \in \partial\Omega \tag{4.19}$$

Equations (4.18)–(4.19) are an eigenvalue problem for the Laplace equation on Ω.

It is possible to show that the eigenvalues form an infinite increasing sequence $0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \dots$. If λ_n is an eigenvalue, then $\omega_n = c_0\sqrt{\lambda_n}$ is a resonant frequency of the wave equation. For example, if $n = 2$, we may think of the resonant frequencies of a drum, and if $n = 3$, we may think of the resonant frequencies of sound waves in a container.

Mark Kac [**29**] asked the question: "Can one hear the shape of a drum?" In other words, is it possible to deduce the shape of a planar domain $\Omega \subset \mathbb{R}^2$ given the sequence of Dirichlet eigenvalues $\{\lambda_n\}$ for the Laplacian on Ω.

The sequence of eigenvalues contains a considerable amount of geometrical information. For example, according to Weyl's formula, in n space-dimensions the volume V (or area if $n = 2$) of the domain is given by

$$V = \lim_{R\to\infty} \frac{(2\pi)^n N(R)}{R^{n/2}}$$

where $N(R)$ denotes the number of eigenvalues of the Dirichlet Laplacian that are less than R.

More generally, one can ask a similar question about the whether or not the eigenvalues of the Laplace-Beltrami operator on a Riemannian manifold determine the manifold up to an isometry. Milnor (1964) gave examples of two non-isometric sixteen dimensional tori whose Laplace-Betrami operators have the same eigenvalues. The two-dimensional question remained open until 1992, when Gordon, Webb, and Wolpert constructed two non-isometric plane domains whose Dirichlet Laplacians have the same eigenvalues.

Related inverse spectral problems that involve the reconstruction of the coefficients of a differential operator from appropriate spectral data are important in connection with the theory of completely integrable nonlinear PDEs, such as the KdV equation.

3. Quantum mechanics

> I was in Bristol at the time I started on Heisenberg's theory. I had returned home for the last part of the summer vacation, and I went back to Cambridge at the beginning of October, 1925, and resumed my previous style of life, intensive thinking on the

> problems during the week and relaxing on Sunday, going for a long walk in the country alone. It was during one of these Sunday walks in October, when I was thinking very much about this $uv - vu$, in spite of my intention to relax, that I thought about Poisson brackets.[1]

There is no systematic derivation of quantum mechanics from classical mechanics. (If there were, presumably quantum mechanics would have been discovered by the founders of classical mechanics.) There is, however, a close correspondence between the two theories. One way to understand the correspondence is through path integrals, which leads to the Lagrangian formulation of classical mechanics. Here, we will discuss an alternative, Hamiltonian, approach.

3.1. The correspondence principle

In the Hamiltonian formulation of classical mechanics, observables (such as the energy) are functions defined on the phase space of the system. In the Heisenberg formulation of quantum mechanics, observables are self-adjoint operators acting on a complex Hilbert space. The possible values of a quantum mechanical observable are the elements of its spectrum, and an eigenvector of an observable is a state with a definite value of the observable equal to the associated eigenvalue. The quantum and classical theories correspond in the sense that the commutators of quantum-mechanical operators agree with the canonical Poisson brackets of the corresponding classical functions multiplied by $i\hbar$.

To write this requirement explicitly, we let $\hat{F}$ denote the quantum mechanical operator corresponding to the classical observable F. Then for any pair of classical observables F, G we require that

$$\widehat{\{F,G\}} = \frac{1}{i\hbar}\left[\hat{F},\hat{G}\right].$$

Here, $\{F,G\}$ is the canonical Poisson bracket of F, G, and

$$\left[\hat{F},\hat{G}\right] = \hat{F}\hat{G} - \hat{G}\hat{F}$$

is the commutator of the operators $\hat{F}$, $\hat{G}$. This prescription is dimensionally consistent, since the canonical bracket involves a derivative with respect to momentum and position, which has the dimension of action.

Thus, roughly speaking, the prescription in passing from classical to quantum mechanics is to replace Poisson brackets by commutators divided by $i\hbar$. This prescription is not entirely unambiguous when it leads to products of non-commuting operators, since all such ordering information is lost in the passage from quantum to classical mechanics.

The classical Hamiltonian equations for the evolution of a function F with respect to a Hamiltonian H is

$$F_t = \{F,H\}.$$

Thus, the corresponding quantum mechanical equation is

$$i\hbar\hat{F}_t = \left[\hat{F},\hat{H}\right].$$

[1] P. A. M. Dirac, Varenna lectures, 1972. Dirac apparently had to wait until Monday so he could look up Poisson brackets in the library, such was the speed of transmission of information at the time.

This operator equation has the solution

$$\hat{F}(t) = e^{-i\hat{H}t/\hbar}\hat{F}_0 e^{i\hat{H}t/\hbar}. \tag{4.20}$$

The Hamiltonian $\hat{H}$ is self adjoint, so

$$\left(e^{-i\hat{H}t/\hbar}\right)^* = e^{i\hat{H}^*t/\hbar} = e^{i\hat{H}t/\hbar} = \left(e^{-i\hat{H}t/\hbar}\right)^{-1},$$

meaning that the evolution operator $e^{-i\hat{H}t/\hbar}$ is unitary.

In this 'Heisenberg picture' the operators evolve in time and act on a fixed vector ψ_0 in an underlying Hilbert space $\mathcal{H}$. The measurable quantities associated with an observable $\hat{F}$ are inner products of the form

$$\left\langle \varphi_0, \hat{F}(t)\psi_0 \right\rangle$$

where $\varphi_0, \psi_0 \in \mathcal{H}$, and $\langle \cdot, \cdot \rangle$ denotes the inner product in $\mathcal{H}$.

3.2. The Schrödinger equation

To obtain the 'Schrödinger picture,' from the 'Heisenberg picture,' we transfer the time-evolution from the operators to the states. That is, given a fixed vector $\psi_0 \in \mathcal{H}$, we define

$$\psi(t) = e^{i\hat{H}t/\hbar}\psi_0. \tag{4.21}$$

Then, if φ_0, ψ_0 are any two vectors in $\mathcal{H}$, with corresponding time-dependent states $\psi(t)$, $\varphi(t)$, we have from (4.20)

$$\left\langle \varphi_0, \hat{F}(t)\psi_0 \right\rangle = \left\langle \varphi(t), \hat{F}_0\psi(t) \right\rangle.$$

Moreover, since conjugation preserves commutators, the operators $\hat{F}(t)$ and $\hat{F}_0$ satisfy the same commutation relations. Thus, both 'pictures' lead to the same result.

The Schrödinger state vector $\psi(t)$ in (4.21) satisfies the evolution equation

$$i\hbar\psi_t = H\psi.$$

This equation is the Schrödinger equation for a nonrelativistic quantum mechanical system.

Now consider the canonical Hamiltonian formulation of a classical mechanical system with conjugate position and momentum variables,

$$\vec{x} = (x_1, x_2, \ldots, x_n), \qquad \vec{p} = (p_1, p_2, \ldots, p_n).$$

Their Poisson brackets are given by

$$\{x_j, x_k\} = 0, \qquad \{p_j, p_k\} = 0, \qquad \{x_j, p_k\} = \delta_{jk}.$$

We represent these operators as operators acting on functions in $L^2(\mathbb{R}^n)$. We define the position operator $\hat{x}$ as a multiplication operator, and the momentum operator $\hat{p}$ as a gradient:

$$\hat{x} = \vec{x}, \quad \hat{x}_j = x_j; \qquad \hat{p} = -i\hbar\nabla, \quad \hat{p}_k = -i\hbar\frac{\partial}{\partial x_k}.$$

We have

$$[\hat{x}_j, \hat{x}_k] = 0, \qquad [\hat{p}_j, \hat{p}_k] = 0, \qquad [\hat{x}_j, \hat{p}_k] = i\hbar\delta_{jk},$$

in correspondence with the Poisson brackets of the classical position and momentum functions.

We again consider a particle of mass m moving in n-space dimensions in a potential V. of the particles. The kinetic energy operator $T = \hat{p}^2/(2m)$ is given by

$$T = -\frac{\hbar^2}{2m}\Delta,$$

where we now drop the 'hats' on operators. The potential energy operator V is multiplication by $V(\vec{x})$. The Hamiltonian operator $H = T + V$ is therefore

$$H = -\frac{\hbar^2}{2m}\Delta + V(\vec{x}).$$

We describe the state of a quantum-mechanical particle by a complex-valued wavefunction $\psi(\vec{x}, t)$, where $|\psi|^2(\vec{x}, t)$ is the spatial probability density for the location of the particle at time t.

The time-dependent Schrödinger equation in this case is the linear PDE

$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\Delta\psi + V(\vec{x})\psi. \tag{4.22}$$

3.3. Energy eigenfunctions

> In this paper I wish to consider, first, the simple case of the hydrogen atom (no-relativistic and unperturbed), and show that the customary quantum conditions can be replaced by another postulate, in which the notion of "whole numbers," merely as such, is not introduced. Rather, when integrality does appear, it arises in the same natural way as it does in the case of the *node numbers* of a vibrating string. The new conception is capable of generalization, and strikes, I believe, very deeply at the nature of the quantum rules.[2]

Separable solutions of (4.22) of the form

$$\psi(\vec{x}, t) = \varphi(\vec{x})\, e^{-iEt/\hbar}$$

correspond to energy eigenstates with energy E. The function $\varphi(\vec{x})$ satisfies the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\Delta\varphi + V(\vec{x})\varphi = E\varphi.$$

This equation may be supplemented with suitable boundary conditions. For example, if the particle is confined to a bounded domain $\Omega \subset \mathbb{R}^n$, we impose $\varphi = 0$ on $\partial\Omega$ Eigenvalues correspond to the energy levels of bound states, while continuous spectrum corresponds to scattered states.

4. The one-dimensional Schrödinger equation

For a single quantum-mechanical particle of mass m moving in one space dimension in a potential $V(x)$, the time-dependent Shrödinger equation (4.22) is

$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\psi_{xx} + V(x)\psi. \tag{4.23}$$

Looking for separable solutions

$$\psi(x, t) = \varphi(x)\, e^{-iEt/\hbar},$$

[2]E. Schrodinger, translated from *Annalen der Physic***79** (1926).

we find that $\varphi(x)$ satisfies the ODE

$$-\frac{\hbar^2}{2m}\varphi'' + V(x)\,\varphi = E\varphi. \tag{4.24}$$

After normalization, this a Sturm-Liouville equation (4.1) of the form

$$-u'' + qu = \lambda u.$$

The coefficient q is proportional to the potential V and the eigenvalue parameter λ in proportional to the energy E.

4.1. A free particle in a box

Consider a particle that is confined to a finite 'box' of length L, but is otherwise free to move. Formally, this corresponds to a potential

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < L, \\ \infty & \text{otherwise.} \end{cases}$$

Since the probability of finding the particle outside the box $0 \le x \le L$ is zero, continuity of the wavefunction implies that it vanishes at the endpoints, and the spatial profile $\varphi(x)$ of an energy eigenfunction with energy E satisfies the BVP

$$-\frac{\hbar^2}{2m}\varphi'' = E\varphi, \qquad \varphi(0) = 0, \qquad \varphi(L) = 0.$$

This has exactly the same form as the eigenvalue problem arising from the vibration of a uniform string. In particular, the energy levels are

$$E_n = \frac{1}{2m}\left(\frac{n\hbar\pi}{L}\right)^2, \qquad n = 1, 2, 3, \ldots.$$

4.2. Motion in a constant force

Consider a particle that is confined to a half-line $x > 0$ and acted on by a constant force $-F$ directed toward the origin, so that $F > 0$. The corresponding potential is $V(x) = Fx$, and the energy eigenfunction with energy E satisfies the BVP

$$\begin{aligned} -\frac{\hbar^2}{2m}\varphi'' + Fx\varphi &= E\varphi, \\ \varphi(0) &= 0, \\ \varphi(x) &\to 0 \qquad \text{as } x \to \infty. \end{aligned}$$

This problem may be solved in terms of Airy functions $\mathrm{Ai}(x)$, discussed below. Its spectrum consists of eigenvalues, which may be expressed in terms of the zeros of $\mathrm{Ai}(x)$.

Classically, a particle of energy E would repeatedly bounce elastically off the wall at $x = 0$ to a distance $a = E/F$. In quantum mechanics, the wavefunction of the particle is localized near the wall.

4.3. The simple harmonic oscillator

> I remember that when someone had started to teach me about creation and annihilation operators, that this operator creates an electron, I said, "how do you create an electron? It disagrees with the conservation of charge", and in that way, I blocked my mind from learning a very practical scheme of calculation. [3]

[3] Richard P. Feynman, Nobel Lecture, December 11, 1965.

The quadratic potential $V(x) = \frac{1}{2}kx^2$ corresponds to a simple harmonic oscillator. In that case, the energy eigenstates satisfy

$$-\frac{\hbar^2}{2m}\varphi'' + \frac{1}{2}kx^2\varphi = E\varphi. \tag{4.25}$$

We consider this eigenvalue problem on the infinite domain $-\infty < x < \infty$, and look for solutions $\varphi \in L^2(\mathbb{R})$ that decay as $|x| \to \infty$.

Although this problem is posed on the whole real line, its spectrum consists entirely of eigenvalues. This is because it involves an 'oscillator-type' potential, meaning that $V(x) \to +\infty$ as $|x| \to \infty$, so a particle with finite energy is confined to a bounded region with high probability.

Despite the fact that the ODE in (4.25) has variable coefficients, the eigenvalue problem is explicitly solvable in terms of elementary Hermite functions. From the perspective of Feynman path integrals, this is explained by the fact that the corresponding path integral is an oscillatory Gaussian integral, which can be evaluated exactly.

We will solve the problem by the introduction of creation and annihilation, or 'ladder,' operators, which map an eigenfunction to the succeeding, or preceding, eigenfunction. The creation operator adds a quantum of energy to the oscillator, while the annihilation operator removes quantum of energy.

We write (4.25) in operator form as

$$H\varphi = E\varphi \tag{4.26}$$

where the Hamiltonian operator H is given by

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2. \tag{4.27}$$

We may write H as

$$H = \frac{1}{2m}p^2 + \frac{1}{2}kx^2,$$

where p denotes the momentum operator

$$p = -i\hbar\frac{d}{dx}.$$

Let

$$\omega_0 = \sqrt{\frac{k}{m}}$$

denote the frequency of the corresponding classical simple harmonic oscillator. We define the *annihilation operator* a and the adjoint *creation operator* a^* by

$$a = \sqrt{\frac{k}{2\hbar\omega_0}}\left(x + \frac{ip}{m\omega_0}\right) = \sqrt{\frac{\hbar}{2m\omega_0}}\frac{d}{dx} + \sqrt{\frac{k}{2\hbar\omega_0}}x$$
$$a^* = \sqrt{\frac{k}{2\hbar\omega_0}}\left(x - \frac{ip}{m\omega_0}\right) = -\sqrt{\frac{\hbar}{2m\omega_0}}\frac{d}{dx} + \sqrt{\frac{k}{2\hbar\omega_0}}x,$$

The annihilation and creation operators are dimensionless, and satisfy the commutation relation

$$[a, a^*] = 1.$$

We may express the Hamiltonian in (4.27) in terms of a, a^* as

$$H = \hbar\omega_0\left(aa^* - \frac{1}{2}\right) = \hbar\omega_0\left(a^*a + \frac{1}{2}\right). \tag{4.28}$$

It follows from these equations that

$$[H, a^*] = \hbar\omega_0 a^*, \qquad [H, a] = -\hbar\omega_0 a.$$

Now suppose that φ is an eigenfunction of H, with energy eigenvalue E, so that $H\varphi = E\varphi$. Let $\tilde{\varphi} = a^*\varphi$. Then we find that

$$H\tilde{\varphi} = Ha^*\varphi = a^*H\varphi + [H, a^*]\,\varphi = Ea^*\varphi + \hbar\omega_0 a^*\varphi = \tilde{E}\tilde{\varphi},$$

where $\tilde{E} = E + \hbar\omega_0$. There are no non-zero functions $\varphi \in L^2(\mathbb{R})$ such that $a^*\varphi = 0$, and a^* maps L^2 functions to L^2 functions. Therefore a^* maps an eigenfunction of H with eigenvalue E to one with eigenvalue $E + \hbar\omega_0$.

To start the 'ladder' of eigenfunctions, we observe from (4.28) that if $a\varphi = 0$, then $H\varphi = \frac{1}{2}\hbar\omega_0$. The condition $a\varphi = 0$ corresponds to the ODE

$$\varphi' + \frac{m\omega_0 x}{\hbar}\varphi = 0,$$

which has the L^2-solution

$$\varphi_0(x) = \exp\left(-\frac{m\omega_0 x^2}{2\hbar}\right).$$

It then follows that the n^{th}-eigenfunction φ_n has the form

$$\varphi_n = c_n\,(a^*)^n\,\varphi_0 \tag{4.29}$$

where c_n is any convenient normalization coefficient. The corresponding energy eigenvalues are

$$E_n = \hbar\omega_0\left(n + \frac{1}{2}\right) \qquad \text{where } n = 0, 1, 2, \ldots.$$

The 'ground state' of the oscillator, with $n = 0$, has nonzero energy $\hbar\omega_0/2$. The fact that the energy of the oscillating particle cannot be reduced completely to zero contrasts with the behavior of the corresponding classical oscillator. It may be interpreted as a consequence of the uncertainty principle that the position and momentum of a quantum-mechanical particle cannot both specified simultaneously. As a result, if the particle is located at the point $x = 0$, where the potential energy attains its minimum value of zero, it would necessarily have nonzero momentum and therefore nonzero kinetic energy.

The energy of the n^{th} level is equal to the energy of the ground state plus n 'quanta' of energy $\hbar\omega_0$. This quantization of energy also contrasts with classical mechanics, where the particle can posses any energy $0 \le E < \infty$.

Each derivative in $(a^*)^n$ of the Gaussian φ_0 in (4.29) brings down a factor of x. Thus, the eigenfunctions φ_n have the form of a polynomial of degree n, called a Hermite polynomial, multiplied by the same Gaussian factor. Explicitly, we have

$$\varphi_n(x) = e^{-\alpha^2 x^2/2} H_n(\alpha x), \qquad n = 0, 1, 2, \ldots$$

where the n^{th} Hermite polynomial $H_n(x)$ is defined in (4.31), and

$$\alpha = \sqrt{\frac{m\omega_0}{\hbar}}.$$

The lengthscale α^{-1} is a characteristic lengthscale over which the wavefunction of the ground state of the oscillator varies.

4.4. The Hermite functions

The Hermite functions $\varphi_n(x)$, where $n = 0, 1, 2, \dots$, are eigenfunctions of the Sturm-Liouville equation on $-\infty < x < \infty$

$$-\varphi'' + x^2\varphi = \lambda\varphi. \tag{4.30}$$

The corresponding eigenvalues $\lambda = \lambda_n$ are given by

$$\lambda_n = 2n + 1.$$

Thus, the spectrum σ of (4.30) consists entirely of eigenvalues.

The Hermite functions have the form

$$\varphi_n(x) = e^{-x^2/2} H_n(x),$$

where the Hermite polynomials $H_n(x)$ are given by Rodriguez' formula

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right). \tag{4.31}$$

We see from this formula that H_n is a polynomial of degree n. Thus, the Hermite functions decay exponentially as $|x| \to \infty$.

First, we show that $\{\varphi_n \mid n = 0, 1, 2, \dots\}$ form an orthogonal set in $L^2(\mathbb{R})$ with respect to the standard inner product

$$\langle f, g\rangle = \int_{-\infty}^{\infty} f(x)g(x)\,dx.$$

It is sufficient to show that φ_n is orthogonal to $e^{-x^2/2}x^m$ for every $0 \le m \le n-1$, since then φ_n is orthogonal to every function of the form $e^{-x^2/2}p_m$ where p_m is a polynomial of degree $m \le n-1$, and hence in particular to φ_m.

Integrating by parts m-times, and using the fact that $e^{-x^2/2}p(x) \to 0$ as $|x| \to \infty$ for every polynomial p, we compute that

$$\begin{aligned}
\left\langle e^{-x^2/2}x^m, \varphi_n \right\rangle &= (-1)^n \int_{-\infty}^{\infty} x^m \frac{d^n}{dx^n}\left(e^{-x^2}\right) dx \\
&= (-1)^{m+n} m! \int_{-\infty}^{\infty} \frac{d^{n-m}}{dx^{n-m}}\left(e^{-x^2}\right) dx \\
&= (-1)^{m+n} m! \left[\frac{d^{n-m-1}}{dx^{n-m-1}}\left(e^{-x^2}\right)\right]_{-\infty}^{\infty} \\
&= 0,
\end{aligned}$$

which proves the result.

Next, we prove that the Hermite polynomials satisfy the following recurrence relations:

$$H_{n+1} = 2xH_n - 2nH_{n-1}, \tag{4.32}$$

$$\frac{dH_n}{dx} = 2nH_{n-1}. \tag{4.33}$$

First, carrying out one differentiation and using the Leibnitz formula for the nth derivative of a product, we get

$$\begin{aligned}
\frac{d^{n+1}}{dx^{n+1}}\left(e^{-x^2}\right) &= \frac{d^n}{dx^n}\left(-2xe^{-x^2}\right) \\
&= -2x\frac{d^n}{dx^n}\left(e^{-x^2}\right) - 2n\frac{d^{n-1}}{dx^{n-1}}\left(e^{-x^2}\right).
\end{aligned}$$

Multiplying this equation by $(-1)^{n+1}e^{x^2}$ and using the definition of the Hermite polynomials, we get (4.32).

Second, using the definition of the Hermite polynomials and the product rule, we get

$$\begin{aligned}\frac{dH_n}{dx} &= (-1)^n \frac{d}{dx}\left[e^{x^2}\frac{d^n}{dx^n}\left(e^{-x^2}\right)\right] \\ &= (-1)^n e^{x^2}\frac{d^{n+1}}{dx^{n+1}}\left(e^{-x^2}\right) + (-1)^n 2x e^{x^2}\frac{d^n}{dx^n}\left(e^{-x^2}\right) \\ &= -H_{n+1} + 2xH_n.\end{aligned}$$

Using (4.32) to eliminate H_{n+1} from this equation, we get (4.33).

To show that the Hermite functions are eigenfunctions of the operator

$$H = -\frac{d^2}{dx^2} + x^2$$

in (4.30), we define annihilation and creation operators

$$a = \frac{d}{dx} + x, \qquad a^* = -\frac{d}{dx} + x, \qquad H = aa^* - 1.$$

Using (4.32)–(4.33), we compute that

$$\begin{aligned}a\varphi_n &= \left(\frac{d}{dx} + x\right)\left(e^{-x^2/2}H_n\right) = e^{-x^2/2}\frac{dH_n}{dx} = 2n\varphi_{n-1}, \\ a^*\varphi_n &= \left(-\frac{d}{dx} + x\right)\left(e^{-x^2/2}H_n\right) = e^{-x^2/2}\left(-\frac{dH_n}{dx} + 2xH_n\right) = \varphi_{n+1}.\end{aligned}$$

It follows that

$$H\varphi_n = (aa^* - 1)\,\varphi_n = a\varphi_{n+1} - \varphi_n = (2n+1)\,\varphi_n,$$

which proves the result.

It is interesting to note that the Hermite functions are eigenfunctions of the Fourier transform. With a convenient normalization, the Fourier transform

$$\mathcal{F} : L^2(\mathbb{R}) \to L^2(\mathbb{R}), \qquad \mathcal{F} : f \mapsto \hat{f}$$

is an isometry on $L^2(\mathbb{R})$. A function f and its Fourier transform $\hat{f}$ are related by

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \hat{f}(k)e^{ikx}\,dk, \qquad \hat{f}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-ikx}\,dx.$$

Then, using (4.31) in the definition of the Fourier transform, we find that

$$\mathcal{F}[\varphi_n] = (-i)^n\varphi_n.$$

For example, if $n = 0$, this is the familiar fact that the Fourier transform of the Gaussian $e^{-x^2/2}$ is the same Gaussian $e^{-k^2/2}$. As with any unitary map, the spectrum of the Fourier transform lies on the unit circle. It consists of four eigenvalues $1, i, -1, -i$, each of which has infinite multiplicity.

One way to understand why the eigenfunctions of (4.30) are also eigenfunctions of the Fourier transform is to observe that the transforms of a derivative and a product with x are given by

$$\mathcal{F}[f'(x)] = ik\hat{f}(k), \qquad \mathcal{F}[xf(x)] = i\hat{f}'(k).$$

Thus, the operations of differentiation and multiplication by the independent variable exchange places under the Fourier transform. As a result, the operator

$$-\frac{d^2}{dx^2} + x^2 \mapsto k^2 - \frac{d^2}{dk^2}$$

maps to itself. Hence, if φ is an eigenfunction, then $\hat{\varphi}$ is also an eigenfunction.

4.5. Periodic potentials

> When I started to think about it, I felt that the main problem was to explain how the electrons could sneak by all the ions in the metal...By straight Fourier analysis I found to my delight that the wave differed from the plane wave of free electrons only by a periodic modulation.[4]

A simple model for the motion of a conduction electron in a crystal lattice consists of the time-independent Schrödinger equation with a potential that varies periodically in space. This potential describes the effect of the forces due to the ions in the crystal lattice and the other electrons in the crystal on the motion of the electron.

Let us consider the one-dimensional version of this problem. The wavefunction of the electron then satisfies the one-dimensional Schrödinger equation in which the potential $V(x)$ is a periodic function. Suppose that the period is a, so that $V(x+a) = V(x)$. Then, after making the change of variables

$$u(x) = \varphi\left(\frac{x}{a}\right), \qquad q(x) = \frac{2ma^2}{\hbar} V\left(\frac{x}{a}\right), \qquad \lambda = \frac{2mE}{\hbar^2},$$

the normalized wavefunction u and energy parameter λ satisfy

$$-u'' + q\,(x)\,u = \lambda u, \tag{4.34}$$

where $q(x+1) = q(x)$. We will consider (4.34) on the real line $-\infty < x < \infty$ with a general 1-periodic potential q which we assume is continuous.

A specific example of such an equation (with the period of the coefficient q normalized to π rather than 1) is the Mathieu equation

$$-u'' + 2k\cos(2x)u = \lambda u, \tag{4.35}$$

where k is a real parameter. Its solutions, called Mathieu functions, have been studied extensively.

A simpler example to analyze is a 'delta-comb' potential

$$q(x) = Q \sum_{n=-\infty}^{\infty} \delta(x-n),$$

corresponding to a periodic array of δ-potentials at integer lattice points. This equation may be solved explicitly by matching solutions $e^{\pm kx}$ of the 'free' equation with $q = 0$ and $\lambda = k^2$ across the points $x = n$, where u' jumps by Q. Alternatively, one may consider periodic, piecewise constant potentials (the 'Kronig-Penney' model).

As we will see, the spectrum of (4.34) is absolutely continuous, and consists of the union of closed intervals, or 'bands,' separated by 'gaps'. When λ lies inside a band, the equation has bounded, non-square integrable, solutions; when λ lies inside a gap, all nonzero solutions are unbounded, and grow exponentially either at $-\infty$ or ∞.

---

[4] Felix Bloch, quoted in [**31**].

The existence of these bands and gaps has significant implications for the conductivity properties of crystals. Electrons whose energy lies in one of the bands can move freely through the crystal, while electrons whose energy lies in one of the gaps cannot move large distances. A crystal behaves like an insulator if its non-empty energy bands are completely filled with electrons, while it conducts electricity if, like a metal, it has energy bands that are only partially filled (say between 10 and 90 percent). Semiconductors typically have a full valence band, but a small band gap energies E_g of the same order as the thermal energy $k_B T$. As a result, electrons can be thermally excited from the valence band to an empty conduction band. The excited electrons, and the 'holes' they leave behind in the valence band, then conduct electricity (see [**31**] for a detailed discussion).

To study the spectrum of (4.34), we use Floquet theory, which applies to linear ODEs with periodic coefficients. Floquet theory is also used to study the stability of time-periodic solutions of ODEs.

The periodicity of the coefficient $q(x)$ does not imply that solutions are periodic, but it does imply that if $u(x)$ is a solution, then so is $u(x+1)$. For example, the ODE $u'' + u = 0$ trivially has 1-periodic coefficients, since they are constant. The solutions $\cos x$, $\sin x$ are not 1-periodic, but $\sin(x+1) = \sin 1 \cos x + \cos 1 \sin x$ is a solution.

Suppose that, for a given value of λ, the functions $u_1(x;\lambda)$, $u_2(x;\lambda)$ form a fundamental pair of solutions for (4.34). It follows that there are constants $a_{ij}(\lambda)$, $1 \le i, j \le 2$, such that

$$\begin{aligned} u_1(x+1;\lambda) &= a_{11}(\lambda) u_1(x;\lambda) + a_{12}(\lambda) u_2(x;\lambda), \\ u_2(x+1;\lambda) &= a_{21}(\lambda) u_1(x;\lambda) + a_{22}(\lambda) u_2(x;\lambda). \end{aligned}$$

Let

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}.$$

If $\rho \in \mathbb{C}$ is an eigenvalue of A with left eigenvector (c_1, c_2) and $v = c_1 u_1 + c_2 u_2$, then it follows that

$$v(x+n;\lambda) = \rho^n(\lambda) v(x,\lambda) \qquad \text{for every } n \in \mathbb{Z}.$$

This solution is bounded if $|\rho| = 1$, otherwise it grows exponentially either as $x \to -\infty$ (if $|\rho| < 1$) or as $x \to +\infty$ (if $|\rho| > 1$). We call the eigenvalues of A *Floquet multipliers*.

The Wronskian $u_1 u_2' - u_2 u_1'$ is a nonzero constant (since its derivative vanishes and u_1, u_2 are independent). It follows that the matrix A has determinant one, so the characteristic equation of A has the form

$$\det(A - \rho I) = \rho^2 - D\rho + 1,$$

where $D(\lambda) = \operatorname{tr} A(\lambda)$. The value of $D(\lambda)$ does not depend in the choice of the fundamental pair of solutions, since the use of another pair leads to a matrix that is similar to A and has the same trace.

If $|D| > 2$, then A has two real eigenvalues ρ_1, ρ_2, one with $|\rho_1| < 1$ and the other with $|\rho_2| > 1$. Thus, the corresponding fundamental solution are unbounded, and (4.34) has no non-zero bounded solutions.

If $|D| < 2$, then A has two complex-conjugate eigenvalues. Since the product of the eigenvalues is equal to 1, the eigenvalues have modulus equal to one, say

$\rho_1 = e^{i\alpha}$, $\rho_2 = e^{-i\alpha}$. We may then write the corresponding pair of fundamental solutions as

$$v_1(x;\lambda) = e^{i\alpha(\lambda)x} p_1(x;\lambda), \qquad v_2(x;\lambda) = e^{-i\alpha(\lambda)x} p_2(x;\lambda),$$

where $p_1(x;\lambda)$, $p_2(x;\lambda)$ are 1-periodic functions of x. These functions, called Bloch waves, are bounded but not square-integrable, so they are not eigenfunctions.

The function $D(\lambda)$ is a continuous function of λ, and the spectrum σ of (4.34) is real and closed. It follows that the spectrum is given by

$$\sigma = \{\lambda \in \mathbb{R} : |D(\lambda)| \leq 2\}.$$

To describe the spectrum in more detail, we need to analyze the function $D(\lambda)$. We will not carry out a general analysis here but we will describe the result (see [**16**] for more information).

As motivation, it is useful to consider the, almost trivial, explicitly solvable case $q(x) = 0$ from the perspective of Floquet theory. In that case (4.34) is

$$-u'' = \lambda u.$$

If $\lambda < 0$, a fundamental pair of solutions of the ODE is

$$u_1(x;\lambda) = e^{-\sqrt{-\lambda}x}, \qquad u_2(x;\lambda) = e^{\sqrt{-\lambda}x}.$$

Thus,

$$u_1(x+1;\lambda) = e^{-\sqrt{-\lambda}} u_1(x;\lambda), \qquad u_2(x+1;\lambda) = e^{\sqrt{-\lambda}} u_2(x;\lambda),$$

and $A(\lambda)$ is a diagonal matrix with trace

$$D(\lambda) = 2\cosh\sqrt{-\lambda}.$$

If $\lambda > 0$, a fundamental pair of solutions of the ODE is

$$u_1(x;\lambda) = \cos\left(\sqrt{\lambda}x\right), \qquad u_2(x;\lambda) = \sin\left(\sqrt{\lambda}x\right),$$

and

$$u_1(x+1;\lambda) = \cos\left(\sqrt{\lambda}\right) u_1(x;\lambda) - \sin\left(\sqrt{\lambda}\right) u_2(x;\lambda),$$
$$u_2(x+1;\lambda) = \sin\left(\sqrt{\lambda}\right) u_1(x;\lambda) + \cos\left(\sqrt{\lambda}\right) u_2(x;\lambda),$$

so

$$D(\lambda) = 2\cos\sqrt{\lambda}.$$

Thus, $|D(\lambda)| \leq 2$ for $0 \leq \lambda < \infty$, corresponding to continuous spectrum. Also note that $D(\lambda) = 2$ at $\lambda = (2m)^2\pi^2$, where the equation has a two-dimensional space of 1-periodic solutions, and $D(\lambda) = -2$ at $\lambda = (2m+1)^2\pi^2$, where the equation has a two-dimensional space of 2-periodic solutions.

For nonzero periodic potentials, the behavior of $D(\lambda)$ is similar, except that its local maximum values are, in general, greater than 2, and its local minimum values, are in general, less than -2. This leads to a structure with bands of continuous spectrum separated by gaps.

Specifically, given a periodic potential $q(x)$, we introduce two auxiliary eigenvalue problems. The first eigenvalue problem on $0 \leq x \leq 1$ is for 1-periodic solutions of (4.34),

$$-u'' + q(x)\,u = \lambda u,$$
$$u(0) = u(1), \qquad u'(0) = u'(1).$$

This is a regular Sturm-Liouville eigenvalue problem, and its spectrum consists of an infinite sequence of real eigenvalues

$$\lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \dots$$

such that $\lambda_n \to \infty$ as $n \to \infty$. Here, if there are any eigenvalues of multiplicity two (meaning that it has two linearly independent eigenfunctions), we include them twice in the sequence.

The second the eigenvalue problem on $0 \leq x \leq 1$ is for semi-periodic solutions of (4.34), which satisfy

$$\begin{aligned} -u'' + q(x)\,u &= \mu u, \\ u(0) = -u(1), &\qquad u'(0) = -u'(1). \end{aligned}$$

The spectrum of this eigenvalue problem also consists of an infinite sequence of real eigenvalues

$$\mu_0 \leq \mu_1 \leq \mu_2 \leq \dots$$

such that $\mu_n \to \infty$ as $n \to \infty$, where again any eigenvalue of multiplicity two appears twice. The corresponding eigenfunctions extend to 2-periodic functions on $\mathbb{R}$.

One can prove that [**16**]:

(a) $\lambda_0 < \mu_0 \leq \mu_1 < \lambda_1 \leq \lambda_2 < \mu_2 \leq \mu_3 < \lambda_3 \leq \lambda_4 < \dots$;

(b) $D(\lambda)$ decreases from 2 to -2 in the intervals $[\lambda_{2m}, \mu_{2m}]$;

(c) $D(\lambda)$ increases from -2 to 2 in the intervals $[\mu_{2m+1}, \lambda_{2m+1}]$;

(d) $D(\lambda) > 2$ in the intervals $(-\infty, \lambda_0)$ and $(\lambda_{2m+1}, \lambda_{2m+2})$;

(e) $D(\lambda) < -2$ in the intervals (μ_{2m}, μ_{2m+1}).

Thus, the spectrum σ of (4.34) is given by

$$\sigma = \bigcup_{m=0}^{\infty} [\lambda_{2m}, \mu_{2m}] \cup [\mu_{2m+1}, \lambda_{2m+1}]\,.$$

It is purely absolutely continuous, and consists of an infinite sequence of 'bands,' or 'stability intervals,' separated by 'gaps,' or 'instability intervals,' $(\lambda_{2m+1}, \lambda_{2m+2})$ or (μ_{2m}, μ_{2m+1}).

In the case when $\lambda_{2m+1} = \lambda_{2m+2}$, or $\mu_{2m} = \mu_{2m+1}$, is a double eigenvalue of the auxiliary eigenvalue problem, the corresponding 'gap' disappears. For instance, all of the gaps disappear if $q = 0$. On the other hand, for the Mathieu equation (4.35) with $k \neq 0$, every gap has nonzero width, which tends to zero rapidly as $m \to \infty$.

An interesting special class of potentials are the 'finite-gap' potentials, in which $\lambda_{2m+1} = \lambda_{2m+2}$ and $\mu_{2m} = \mu_{2m+1}$ for all but finitely many m. An example of an n-gap potentials is the Lamé equation

$$-u'' + n(n+1)\wp(x)u = \lambda u$$

where the elliptic function $\wp$ is the Weierstrass 'p'-function. These results are of interest in the theory of completely integrable systems, in connection with the use of the inverse scattering transform for spatially-periodic solutions the KdV equation.

Generalizations of these results apply to the time-independent Schrödinger equation with a periodic potential in higher space dimensions, including the existence of Bloch waves. The analysis there is more complicated, and there are

many more possible lattice symmetries in two and three space dimensions than the single periodic lattice in one space dimension.

4.6. Anderson localization

The spectrum of the one-dimensional, time-independent Schrödinger equation on the real line with a continuous periodic potential is always absolutely continuous. For values of λ in the spectrum, the ODE has bounded solutions which do not decay at infinity.

Anderson (1958) observed that random stationary potentials, such as ones that model a disordered medium, can have a dense point spectrum with associated, exponentially decaying eigenfunctions. This phenomenon is called *Anderson localization.*

As an example, consider a Schrödinger equation of the form

$$-u'' + \left(\sum_{n \in \mathbb{Z}} Q_n(\omega) f(x-n) \right) u = \lambda u \qquad -\infty < x < \infty, \tag{4.36}$$

where $f(x)$ is a given potential function, which is the same at different lattice points n, and the amplitudes $Q_n(\omega)$ are independent identically distributed random variables.

Then, under suitable assumptions (for example, $f(x) \geq 0$ has support in $[0,1]$, so the supports of f do not overlap, and the Q_n are independent random variables uniformly distributed on $[0,1]$) the spectrum of (4.36) is, almost surely, the interval $0 \leq \lambda < \infty$. Moreover, it is pure point spectrum, meaning that there are countably many eigenvalues which are dense in $[0,\infty)$ (similar to the way in which the rational numbers are dense in the real numbers).

Localization has also been studied and observed in classical waves, such as waves in an elastic medium.

5. The Airy equation

The eigenvalue equation for Airy's equation is

$$-u'' + xu = \lambda u.$$

In this case, we can remove the spectral parameter λ by a translation $x \mapsto x - \lambda$, so we set $\lambda = 0$ to get

$$-u'' + xu = 0. \tag{4.37}$$

(The Airy operator on the real line has continuous spectrum $\mathbb{R}$, with bounded solutions given by translations of the Airy function described below.)

The coefficient of the lower order term in (4.37) changes sign at $x = 0$. As a result, one might expect that the qualitative behavior of its solutions changes from oscillatory (like $u'' + u = 0$) when x is large and negative to exponential (like $u'' - u = 0$) when x is large and positive. This is indeed the case, and the Airy functions are, perhaps, the most fundamental functions that describe a continuous transition from oscillatory to exponential behavior as a real variable changes.

One of the most familiar example of this phenomenon occurs at the bright caustics one can observe in light reflections. Airy functions describe the high-frequency light wave-field near a smooth convex caustic that separates the illuminated region from the shadow region. Similar problems arise in semi-classical quantum mechanics, where the wavefunction of a particle is oscillatory in classically allowed regions,

and exponential in classically forbidden regions. The Airy functions describe the transition between these two regimes. The fact that the Airy functions have an exponentially decaying tail is what allows a quantum mechanical particle to 'tunnel' through a classically impassible potential barrier. Here, we will describe an application of Airy functions to the propagation of linear dispersive waves.

First, we summarize some properties of the Airy functions. A standard fundamental pair of solutions of (4.37) is denoted by $\mathrm{Ai}(x)$ and $\mathrm{Bi}(x)$. The solution Ai is determined uniquely, up to a normalization constant, by the condition that it decays exponentially as $x \to \infty$. The function Bi is a second, independent solution of (4.37), which grows exponentially as $x \to \infty$. This property does not determine Bi up to normalization, since we could add to it any multiple of Ai without altering this asymptotic behavior.

These solutions may be defined by their initial values at $x = 0$:

$$\mathrm{Ai}(0) = \alpha, \quad \mathrm{Ai}'(0) = -\beta, \qquad \mathrm{Bi}(0) = \sqrt{3}\alpha, \quad \mathrm{Bi}'(0) = \sqrt{3}\beta.$$

Here, the constants $\alpha \approx 0.355$, $\beta \approx 0.259$ are defined by

$$\alpha = \frac{1}{3^{2/3}\Gamma(2/3)}, \qquad \beta = \frac{1}{3^{1/3}\Gamma(1/3)}$$

where the Gamma-function Γ is defined by

$$\Gamma(x) = \int_0^\infty e^{-t} t^{x-1}\, dt, \qquad \text{for } x > 0,$$

An integration by parts shows that $\Gamma(n) = (n-1)!$ for $n \in \mathbb{N}$, so the Gamma-function may be regarded as an extension of the factorial to non-integers.

In order to properly understand the behavior of the Airy functions it is necessary to consider them in the complex plane. For $z \in \mathbb{C}$, using a Fourier-Laplace transform, we write

$$u(z) = \int_C e^{z\xi} f(\xi)\, d\xi \tag{4.38}$$

where C is a suitable contour and $f : C \to \mathbb{C}$ is a function.

Then, assuming we can differentiate under the integral sign and integrate by parts, we find that

$$-\frac{d^2u}{dz^2} + zu = \int_C e^{z\xi} \left(\xi^2 f + \frac{df}{d\xi} \right) d\xi.$$

Thus, $u(z)$ is a solution of the Airy equation if $f(\xi)$ satisfies

$$f' + \xi^2 f = 0.$$

The simplification here is that, since $u(z)$ is multiplied by the first power of z in the original equation, we get a first-order ODE for $f(\xi)$, which is easy to solve. Up to a constant factor, the solution is

$$f(\xi) = e^{-\xi^3/3}.$$

Suppose that the contour C is given parametrically as $\xi = \xi(t)$ with $-\infty < t < \infty$. In order to ensure convergence of the contour integral in (4.38), we require that $\xi(t) \sim te^{2\pi ik/3}$ for some $k = -1, 0, 1$ as $t \to \infty$, in which case $\xi^3(t) \sim t^3$, and $\xi(t) \sim -te^{2\pi ik/3}$ for some $k = -1, 0, 1$ as $t \to -\infty$, in which case $\xi^3(t) \sim -t^3$.

Up to orientation, this gives three types of contours C_1, C_2, C_3. We define

$$E_k(z) = \frac{1}{\pi i} \int_{C_k} e^{z\xi - \xi^3/3}\, d\xi.$$

Then, since the integrand has no singularities in $\mathbb{C}$ and $C_1 + C_2 + C_3$ is a closed curve (after being deformed away from infinity), Cauchy's theorem implies that

$$E_1(z) + E_2(z) + E_3(z) = 0$$

Also

$$E_2(z) = -\overline{E_2}(z).$$

One can show that the Airy functions are defined so that

$$E_3(z) = \mathrm{Ai}(z) + i\,\mathrm{Bi}(z).$$

These functions are entire (that is, analytic in all of $\mathbb{C}$), with an essential singularity at ∞.

Deforming the contours C_3 to the real axis, we may derive a Fourier representation of the Airy functions as oscillatory integrals

$$\begin{aligned}
\mathrm{Ai}(x) &= \frac{1}{\pi} \int_0^\infty \cos\left(\frac{1}{3}t^3 + xt\right)\, dt, \\
\mathrm{Bi}(x) &= \frac{1}{\pi} \int_0^\infty \left[e^{-t^3/3+xt} + \sin\left(\frac{1}{3}t^3 + xt\right)\right]\, dt
\end{aligned}$$

Note that, in comparison with the Fresnel integral, the oscillatory integrals for the Airy functions have two stationary phase points at $t = \pm\sqrt{-x}$ when $x < 0$ and no stationary phase points when $x > 0$. This explains their transition from oscillatory to exponential behavior.

Using the method of steepest descent, one can show that the Airy functions have the asymptotic behaviors

$$\begin{aligned}
\mathrm{Ai}(x) &\sim \frac{\sin\left(2|x|^{3/2}/3 + \pi/4\right)}{\sqrt{\pi}|x|^{1/4}} && \text{as } x \to -\infty, \\
\mathrm{Bi}(x) &\sim \frac{\cos\left(2|x|^{3/2}/3 + \pi/4\right)}{\sqrt{\pi}|x|^{1/4}} && \text{as } x \to -\infty, \\
\mathrm{Ai}(x) &\sim \frac{\exp\left(-2x^{3/2}/2\right)}{2\sqrt{\pi}x^{1/4}} && \text{as } x \to \infty, \\
\mathrm{Bi}(x) &\sim \frac{\exp\left(2x^{3/2}/3\right)}{2\sqrt{\pi}x^{1/4}} && \text{as } x \to \infty.
\end{aligned}$$

6. Dispersive wave propagation

An important application of the method of stationary phase, discussed briefly in Section 14.2, concerns the long-time, or large-distance, behavior of linear dispersive waves. Kelvin (1887) originally developed the method for this purpose, following earlier work by Cauchy, Stokes, and Riemann. He used it to study the pattern of dispersive water waves generated by a ship in steady motion, and showed that at large distances from the ship the waves form a wedge with a half-angle of $\sin^{-1}(1/3)$, or approximately 19.5°.

Here, we will illustrate this method by using it to study the linearized Korteweg-de Vries (KdV), or Airy equation. We will then show how Airy functions arise

when two stationary phase point coalesce, leading to a transition from oscillatory to exponential behavior.

Consider the following initial value problem (IVP) for the linearized KdV equation

$$\begin{aligned} u_t &= u_{xxx}, \\ u(x,0) &= f(x). \end{aligned}$$

This equation provides an asymptotic description of linear, unidirectional, weakly dispersive long waves. It was first derived for shallow water waves. In the following section we give a derivation of the KdV equation for ion-acoustic waves in a plasma.

We assume for simplicity that the initial data $f : \mathbb{R} \to \mathbb{R}$ is a Schwarz function, meaning that it is smooth and decays, together with all its derivatives, faster than any polynomial as $|x| \to \infty$.

Let $\widehat{u}(k,t)$ denote the Fourier transform of $u(x,t)$ with respect to x,

$$\begin{aligned} u(x,t) &= \int_{-\infty}^{\infty} \widehat{u}(k,t) e^{ikx}\, dk, \\ \widehat{u}(k,t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} u(x,t) e^{-ikx}\, dx. \end{aligned}$$

Then $\widehat{u}(k,t)$ satisfies

$$\begin{aligned} \widehat{u}_t + ik^3 \widehat{u} &= 0, \\ \widehat{u}(k,0) &= \widehat{f}(k). \end{aligned}$$

The solution of this equation is

$$\widehat{u}(k,t) = \widehat{f}(k) e^{-i\omega(k)t},$$

where

$$\omega(k) = k^3.$$

The function $\omega : \mathbb{R} \to \mathbb{R}$ gives the (angular) frequency $\omega(k)$ of a wave with wavenumber k, and is called the *dispersion relation* of the KdV equation.

Inverting the Fourier transform, we find that the solution is given by

$$u(x,t) = \int_{-\infty}^{\infty} \widehat{f}(k) e^{ikx - i\omega(k)t}\, dk.$$

Using the convolution theorem, we can write this solution as

$$u(x,t) = f * g(x,t), \tag{4.39}$$

where the star denotes convolution with respect to x, and

$$g(x,t) = \frac{1}{(3t)^{1/3}} \operatorname{Ai}\left(-\frac{x}{(3t)^{1/3}} \right)$$

is the Green's function of the Airy equation.

This Green's function may also be found directly by looking for similarity solutions

$$g(x,t) = \frac{1}{t^m} G\left(\frac{x}{t^n} \right)$$

of the linearized KdV equation such that

$$\int_{-\infty}^{\infty} g(x,t)\, dx \to 1 \qquad \text{as } t \to 0.$$

We consider the asymptotic behavior of the solution (4.39) as $t \to \infty$ with $x/t = v$ fixed. This limit corresponds to the large-time limit in a reference frame moving with velocity v.

Thus, we want to find the behavior as $t \to \infty$ of

$$u(vt,t) = \int_{-\infty}^{\infty} \widehat{f}(k) e^{i\varphi(k,v)t}\, dk, \tag{4.40}$$

where

$$\varphi(k,v) = kv - \omega(k).$$

The stationary phase points satisfy $\varphi_k = 0$, or

$$v = \omega'(k).$$

The solutions are the wavenumbers k whose group velocity $\omega'(k)$ is equal to v. It follows that

$$3k^2 = v.$$

If $v < 0$, then there are no stationary phase points, and $u(vt,t) = o(t^{-n})$ as $t \to \infty$ for any $n \in \mathbb{N}$.

If $v > 0$, then there are two nondegenerate stationary phase points at $k = \pm k_0(v)$, where

$$k_0(v) = \sqrt{\frac{v}{3}}.$$

These two points contribute complex conjugate terms, and the method of stationary phase implies that

$$u(vt,t) \sim \sqrt{\frac{2\pi}{|\omega''(k_0)|t}}\, \widehat{f}(k_0) e^{i\varphi(k_0,v)t - i\pi/4} + \text{c.c.} \qquad \text{as } t \to \infty.$$

The energy in the wave-packet therefore propagates at the group velocity $C = \omega'(k)$,

$$C = 3k^2,$$

rather than the phase velocity $c = \omega/k$,

$$c = k^2.$$

The solution decays at a rate of $t^{-1/2}$, in accordance with the linear growth in t of the length of the wavetrain and the conservation of energy,

$$\int_{-\infty}^{\infty} u^2(x,t)\, dt = \text{constant}.$$

The two stationary phase points coalesce when $v = 0$, and then there is a single degenerate stationary phase point. To find the asymptotic behavior of the solution when v is small, we make the change of variables

$$k = \frac{\xi}{(3t)^{1/3}}$$

in the Fourier integral solution (4.40). This gives

$$u(x,t) = \frac{1}{(3t)^{1/3}} \int_{-\infty}^{\infty} \widehat{f}\left(\frac{\xi}{(3t)^{1/3}}\right) e^{-i\left(\xi w + \frac{1}{3}\xi^3\right)}\, d\xi,$$

where

$$w = -\frac{t^{2/3} v}{3^{1/3}}.$$

It follows that as $t \to \infty$ with $t^{2/3}v$ fixed,

$$u(x,t) \sim \frac{2\pi}{(3t)^{1/3}} \widehat{f}(0)\, \mathrm{Ai}\left(-\frac{t^{2/3}v}{3^{1/3}}\right).$$

Thus the transition between oscillatory and exponential behavior is described by an Airy function. Since $v = x/t$, the width of the transition layer is of the order $t^{1/3}$ in x, and the solution in this region is of the order $t^{-1/3}$. Thus it decays more slowly and is larger than the solution elsewhere.

7. Derivation of the KdV equation for ion-acoustic waves

The Korteweg-de Vries (KdV) equation is the following nonlinear PDE for $u(x,t)$:

$$u_t + uu_x + u_{xxx} = 0. \tag{4.41}$$

This equation was first derived by Korteweg and de Vries (1895) for shallow water waves, and it is a generic asymptotic equation that describes weakly nonlinear waves with weak long-wave dispersion.

The term u_t is the rate of change of the wave profile u in a reference frame moving with the linearized phase velocity of the wave. The term uu_x is an advective nonlinearity, and u_{xxx} is a linear dispersive term.

Water waves are described by a relatively complicated system of equations which involve a free boundary. Here, we derive the KdV equation from a simpler system of PDEs that describes ion acoustic waves in a plasma. This derivation illustrates the universal nature of the KdV equation, which applies to any wave motion with weak advective nonlinearity and weak long wave dispersion. Specifically, the linearized dispersion relation $\omega = \omega(k)$ between frequency ω and wavenumber k should have a Taylor expansion as $k \to 0$ of the form $\omega = c_0 k + \alpha k^3 + \dots$.

7.1. Plasmas

A plasma is an ionized fluid consisting of positively charged ions and negatively charged electrons which interact through the electro-magnetic field they generate. Plasmas support waves analogous to sound waves in a simple compressible fluid, but as a result of the existence of ion and electron oscillations in plasmas, these waves are dispersive.

Here, we use a simple 'two-fluid' model of a plasma in which the ions and electrons are treated as separate fluids. More detailed models use a kinetic description of the plasma. The full system of equations follows from the fluid equations for the motion of the ions and electrons, and Maxwell's equations for the electro-magnetic field generated by the charged fluids. We will consider relatively low frequency waves that involve the motion of the ions, and we assume that there are no magnetic fields. After simplification and nondimensionalization, we get the equations summarized in (4.47) below.

Let n^i, n^e denote the number density of the ions and electrons, respectively, u^i, u^e their velocities, p^i, p^e their pressures, and E the electric field.

In one space dimension, the equations of conservation of mass and momentum for the ion fluid are

$$\begin{aligned} &n^i_t + (n^i u^i)_x = 0, \\ &m^i n^i \left(u^i_t + u^i u_{ix}\right) + p^i_x = e n^i E. \end{aligned}$$

Here, m^i is the mass of an ion and e is its charge. For simplicity, we assume that this is the same as the charge of an electron.

We suppose that the ion-fluid is 'cold', meaning that we neglect its pressure. Setting $p^i = 0$, we get

$$\begin{aligned} &n^i_t + (n^i u^i)_x = 0, \\ &m^i \left(u^i_t + u^i u_{ix}\right) = eE. \end{aligned}$$

The equations of conservation of mass and momentum for the electron fluid are

$$\begin{aligned} &n^e_t + (n^e u^e)_x = 0, \\ &m^e n^e \left(u^e_t + u^e u^e_x\right) + p^e_x = -e n^e E, \end{aligned}$$

where m^e is the mass of an electron and $-e$ is its charge. The electrons are much lighter than the ions, so we neglect their inertia. Setting $m^e = 0$, we get

$$p^e_x = -e n^e E. \tag{4.42}$$

As we will see, this equation provides an equation for the electron density n^e. The electron velocity u^e is then determined from the equation of conservation of mass. It is uncoupled from the remaining variables, so we do not need to consider it further.

We assume an isothermal equation of state for the electron fluid, meaning that

$$p^e = kTn^e, \tag{4.43}$$

where k is Boltzmann's constant and T is the temperature. Using (4.43) in (4.42) and writing $E = -\varphi_x$ in terms of an electrostatic potential φ, we get

$$kTn^e_x = en^e\varphi_x.$$

This equation implies that n^e is given in terms of φ by

$$n^e = n_0 \exp\left(\frac{e\varphi}{kT}\right), \tag{4.44}$$

where the constant n_0 is the electron number density at $\varphi = 0$.

Maxwell's equation for the electrostatic field E generated by a charge density σ is $\epsilon_0 \nabla \cdot E = \sigma$, where ϵ_0 is a dielectric constant. This equation implies that

$$\epsilon_0 E_x = e(n^i - n^e). \tag{4.45}$$

In terms of the potential φ, equation (4.45) becomes

$$-\varphi_{xx} = \frac{e}{\epsilon_0}\left(n^i - n^e\right). \tag{4.46}$$

We may then use (4.44) to eliminate n^e from (4.46).

Dropping the i-superscript on the ion-variables (n^i, u^i), we may write the final system of equations for (n, u, φ) as

$$\begin{aligned} &n_t + (nu)_x = 0, \\ &u_t + uu_x + \frac{e}{m}\varphi_x = 0, \\ &-\varphi_{xx} + \frac{en_0}{\epsilon_0}\exp\left(\frac{e\varphi}{kT}\right) = \frac{e}{\epsilon_0}n. \end{aligned}$$

This system consists of a pair of evolution equations for (n, u) coupled with a semi-linear elliptic equation for φ.

To nondimensionalize these equations, we introduce the the Debye length λ_0 and the ion-acoustic sound speed c_0, defined by

$$\lambda_0^2 = \frac{\epsilon_0 kT}{n_0 e^2}, \qquad c_0^2 = \frac{kT}{m}.$$

These parameters vary by orders of magnitudes for plasmas in different conditions. For example, a dense laboratory plasma may have $n_0 \approx 10^{20}\,\mathrm{m}^{-3}$, $T \approx 60,000\,\mathrm{K}$ and $\lambda_0 \approx 10^{-6}\,\mathrm{m}$; the solar wind near the earth has $n_0 \approx 10^{7}\,\mathrm{m}^{-3}$, $T \approx 120,000\,\mathrm{K}$, and $\lambda_0 \approx 10\,\mathrm{m}$.

Introducing dimensionless variables

$$\bar{x} = \frac{x}{\lambda_0}, \quad \bar{t} = \frac{c_0 t}{\lambda_0}, \quad \bar{n} = \frac{n}{n_0}, \quad \bar{u} = \frac{u}{c_0}, \quad \bar{\varphi} = \frac{e\varphi}{kT},$$

and dropping the 'bars', we get the nondimensionalized equations

$$\begin{aligned} &n_t + (nu)_x = 0, \\ &u_t + uu_x + \varphi_x = 0, \\ &-\varphi_{xx} + e^{\varphi} = n. \end{aligned} \tag{4.47}$$

7.2. Linearized equations

First, we derive the linearized dispersion relation of ion acoustic waves. Linearizing the system (4.47) about $n = 1$, $\varphi = 0$ and $u = 0$, we get

$$\begin{aligned} &n_t + u_x = 0, \\ &u_t + \varphi_x = 0, \\ &-\varphi_{xx} + \varphi = n, \end{aligned}$$

where n now denotes the perturbation in the number density about 1.

We seek Fourier solutions

$$n(x,t) = \hat{n} e^{ikx - i\omega t}, \quad u(x,t) = \hat{u} e^{ikx - i\omega t}, \quad \varphi(x,t) = \hat{\varphi} e^{ikx - i\omega t}.$$

From the last equation, we find that

$$\hat{\varphi} = \frac{\hat{n}}{1 + k^2}.$$

From the first and second equations, after eliminating $\hat{\varphi}$, we get

$$\begin{pmatrix} -i\omega & ik \\ ik/(1+k^2) & -i\omega \end{pmatrix} \begin{pmatrix} \hat{n} \\ \hat{u} \end{pmatrix} = 0$$

This linear system has a non-zero solution if the determinant of the matrix is zero, which implies that (ω, k) satisfies the dispersion relation

$$\omega^2 = \frac{k^2}{1 + k^2}.$$

The corresponding null-vector is

$$\begin{pmatrix} \hat{n} \\ \hat{u} \end{pmatrix} = \hat{a} \begin{pmatrix} k \\ \omega \end{pmatrix},$$

where $\hat{a}$ is an arbitrary constant.

The phase velocity $c = \omega/k$ of these waves is given

$$c = \frac{1}{(1 + k^2)^{1/2}},$$

so that $c \to 1$ as $k \to 0$ and $c \to 0$ as $k \to \infty$.

The group velocity $C = d\omega/dk$ is given by

$$C = \frac{1}{(1+k^2)^{3/2}}.$$

For these waves, the group veclocity is smaller than the phase velocity for all $k > 0$.

In the long-wave limit $k \to 0$, we get the leading order approximation $\omega = k$, corresponding to non-dispersive sound waves with phase speed $\omega/k = 1$. In the original dimensional variables, this speed is the ion-acoustic speed c_0, and the condition for long-wave dispersion to be weak is that $k\lambda_0 \ll 1$, meaning that the wavelength is much larger than the Debye length. In these long waves, the electrons oscillate with the ions, and the fluid behaves essentially like a single fluid. The inertia of the wave is provided by the ions and the restoring pressure force by the electrons.

By contrast, in the short-wave limit $k \to \infty$, we get waves with constant frequency $\omega = 1$, corresponding in dimensional terms to the ion plasma frequency $\omega_0 = c_0/\lambda_0$. In these short waves, the ions oscillate in an essentially fixed background of electrons.

For water waves, the condition for weak long-wave dispersion is that the wavelength is much larger than the depth of the fluid. Such waves are called 'shallow water waves.'

At the next order in k, we find that

$$\omega = k - \frac{1}{2}k^3 + O(k^5) \qquad \text{as } k \to 0. \tag{4.48}$$

The $O(k^3)$ correction corresponds to weak KdV-type long-wave dispersion.

For very long waves, we may neglect φ_{xx} in comparison with e^{φ} in (4.47), which gives $n = e^{\varphi}$ and $n_x = n\varphi_x$. In that case, (n, u) satisfy the isothermal compressible Euler equations

$$\begin{aligned} &n_t + (nu)_x = 0, \\ &n\,(u_t + uu_x) + n_x = 0. \end{aligned}$$

These equations form a nondispersive hyperbolic system. (The analogous system for water waves is the shallow water equations.) In general, solutions form shocks, but then the long-wave approximation breaks down and it is no longer self-consistent.

A weakly nonlinear expansion of these long wave equations, which is a limiting case of the KdV expansion given below,

$$\begin{pmatrix} n \\ u \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \epsilon a(x - t, \epsilon t) \begin{pmatrix} 1 \\ 1 \end{pmatrix} + O(\epsilon^2),$$

leads to an inviscid Burgers equation for $a(\xi, \tau)$,

$$a_\tau + aa_\xi = 0.$$

In the next section, we apply a similar expansion to (4.47) and include the effect of weak long wave dispersion, leading to a KdV equation.

7.3. KdV expansion

We can see from the KdV equation (4.41) what orders of magnitude of the wave amplitude and the spatial and temporal scales lead to a balance between weak nonlinearity and long-wave dispersion. We need u to have the same order of magnitude

as ∂_x^2 and ∂_t to have the same order of magnitude as ∂_x^3. Thus, we want

$$u = O(\epsilon), \qquad \partial_x = O(\epsilon^{1/2}), \qquad \partial_t = O(\epsilon^{3/2})$$

where ϵ is a small positive parameter. We could, of course, replace ϵ by ϵ^2, or some other small parameter, provided that we retain the same relative scalings. Here, the time-derivative ∂_t is taken in a reference frame moving with the linearized wave velocity.

This scaling argument suggests that we seek an asymptotic solution of (4.47), depending on a small parameter ϵ of the form

$$\begin{aligned} n &= n\left(\epsilon^{1/2}(x-\lambda t), \epsilon^{3/2}t; \epsilon\right), \\ u &= u\left(\epsilon^{1/2}(x-\lambda t), \epsilon^{3/2}t; \epsilon\right), \\ \varphi &= \varphi\left(\epsilon^{1/2}(x-\lambda t), \epsilon^{3/2}t; \epsilon\right). \end{aligned}$$

We will determine the wave velocity λ as part of the solution. The parameter ϵ does not appear explicitly in the PDE (4.47), but it could appear in the initial conditions, for example.

We introduce multiple-scale variables

$$\xi = \epsilon^{1/2}(x-\lambda t), \qquad \tau = \epsilon^{3/2}t.$$

According to the chain rule, we may expand the original space-time derivatives as

$$\partial_x = \epsilon^{1/2}\partial_\xi, \qquad \partial_t = -\epsilon^{1/2}\lambda\partial_\xi + \epsilon^{3/2}\partial_\tau.$$

After including the small parameter ϵ explicitly in the new variables, we assume that derivatives with respect to ξ, τ are of the order 1 as $\epsilon \to 0^+$, which is not the case for derivatives with respect to the original variables x, t.

It follows that $n(\xi,\tau;\epsilon)$, $u(\xi,\tau;\epsilon)$, $\varphi(\xi,\tau;\epsilon)$ satisfy

$$\begin{aligned} &(nu)_\xi - \lambda n_\xi + \epsilon n_\tau = 0, \\ &\varphi_\xi - \lambda u_\xi + u u_\xi + \epsilon u_\tau = 0, \\ &e^\varphi - \epsilon\varphi_{\xi\xi} = n. \end{aligned} \tag{4.49}$$

We look for an asymptotic solution of (4.49) of the form

$$\begin{aligned} n &= 1 + \epsilon n_1 + \epsilon^2 n_2 + \epsilon^3 n_3 + O(\epsilon^4), \\ u &= \epsilon u_1 + \epsilon^2 u_2 + \epsilon^3 u_3 + O(\epsilon^4), \\ \varphi &= \epsilon\varphi_1 + \epsilon^2\varphi_2 + \epsilon^3\varphi_3 + O(\epsilon^4). \end{aligned}$$

Using these expansions in (4.49), Taylor expanding the result with respect to ϵ, and equating coefficients of ϵ, we find that

$$\begin{aligned} &u_{1\xi} - \lambda n_{1\xi} = 0, \\ &\varphi_{1\xi} - \lambda u_{1\xi} = 0, \\ &\varphi_1 - n_1 = 0. \end{aligned} \tag{4.50}$$

Equating coefficients of ϵ^2, we find that

$$\begin{aligned} &u_{2\xi} - \lambda n_{2\xi} + n_{1\tau} + (n_1 u_1)_\xi = 0, \\ &\varphi_{2\xi} - \lambda u_{2\xi} + u_{1\tau} + u_1 u_{1\xi} = 0, \\ &\varphi_2 - n_2 + \frac{1}{2}\varphi_1^2 - \varphi_{1\xi\xi} = 0. \end{aligned} \tag{4.51}$$

Eliminating φ_1 from (4.50), we get a homogeneous linear system for (n_1, u_1),

$$\begin{pmatrix} -\lambda & 1 \\ 1 & -\lambda \end{pmatrix} \begin{pmatrix} n_1 \\ u_1 \end{pmatrix}_\xi = 0.$$

This system has a nontrivial solution if $\lambda^2 = 1$. We suppose that $\lambda = 1$ for definiteness, corresponding to a right-moving wave. Then

$$\begin{pmatrix} n_1 \\ u_1 \end{pmatrix} = a(\xi,\tau) \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \varphi_1 = a(\xi,\tau), \tag{4.52}$$

where $a(\xi, \tau)$ is an arbitrary scalar-valued function.

At the next order, after setting $\lambda = 1$ and eliminating φ_2 in (4.51), we obtain a nonhomogeneous linear system for (n_2, u_2),

$$\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} n_2 \\ u_2 \end{pmatrix}_\xi + \begin{pmatrix} n_{1\tau} + (n_1 u_1)_\xi \\ u_{1\tau} + u_1 u_{1\xi} - \varphi_1\varphi_{1\xi} + \varphi_{1\xi\xi\xi} \end{pmatrix} = 0. \tag{4.53}$$

This system is solvable for (n_2, u_2) if and only if the nonhomogeneous term is orthogonal to the null-vector $(1, 1)$. Using (4.52), we find that this condition implies that $a(\xi, \tau)$ satisfies a KdV equation

$$a_\tau + a a_\xi + \frac{1}{2} a_{\xi\xi\xi} = 0. \tag{4.54}$$

Note that the linearized dispersion relation of this equation agrees with the long wave expansion (4.48) of the linearized dispersion relation of the original system.

If a satisfies (4.54), then we may solve (4.53) for (n_2, u_2). The solution is the sum of a solution of the nonhomogeneous equations and an arbitrary multiple

$$a_2(\xi,\tau) \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

of the solution of the homogeneous problem.

We may compute higher-order terms in the asymptotic solution in a similar way. At the order ϵ^k, we obtain a nonhomogeneous linear equation for (n_k, u_k) of the form

$$\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} n_k \\ u_k \end{pmatrix}_\xi + \begin{pmatrix} f_{k-1} \\ g_{k-1} \end{pmatrix} = 0,$$

where f_{k-1}, g_{k-1} depend only on (n_1, u_1),..., (n_{k-1}, u_{k-1}), and φ_k may be expressed explicitly in terms of $n_1, \ldots, n_k$. The condition that this equation is solvable for (n_k, u_k) is $f_{k-1} + g_{k-1} = 0$, and this condition is satisfied if a_{k-1} satisfies a suitable equation. The solution for (n_k, u_k) then involves an arbitrary function of integration a_k. An equation for a_k follows from the solvability condition for the order $(k + 1)$-equations.

In summary, the leading-order asymptotic solution of (4.47) as $\epsilon \to 0^+$ is

$$\begin{pmatrix} n \\ u \\ \varphi \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + \epsilon a\left(\epsilon^{1/2}(x-t), \epsilon^{3/2} t\right) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + O(\epsilon^2),$$

where $a(\xi, \tau)$ satisfies the KdV equation (4.54). We expect that this asymptotic solution is valid for long times of the order $\tau = O(1)$ or $t = O(\epsilon^{-3/2})$.

8. Other Sturm-Liouville problems

Finally, we summarize a few other Sturm-Liouville equations and some of their applications. See [**2**] for a much more extensive list and an interesting collection of recent reviews on the subject.

8.1. Bessel's equation

This equation arises in solving the Laplace and Helmholtz equations by separation of variables in cylindrical polar coordinates:

$$-u'' + \left(\nu^2 - \frac{1}{4}\right)\frac{1}{x^2}u = \lambda u \qquad 0 < x < \infty$$

where $0 \leq \nu < \infty$ is a parameter. One pair of solutions is

$$x^{1/2}J_\nu\left(\sqrt{\lambda}x\right), \qquad x^{1/2}Y_\nu\left(\sqrt{\lambda}x\right)$$

where J_ν, Y_ν are Bessel functions of the order ν.

8.2. Legendre equations

The Legendre and associated Legendre equations arise in solving the Laplace equation in spherical polar coordinates, and give an expression for the spherical harmonic functions. The Legendre equation is

$$-\left[\left(1-x^2\right)u'\right]' + \frac{1}{4}u = \lambda u \qquad -1 < x < 1$$

The associated Legendre equation is

$$-\left[\left(1-x^2\right)u'\right]' + \frac{\mu^2}{1-x^2}u = \lambda u \qquad -1 < x < 1.$$

8.3. Laguerre equations

The Laguerre polynomials arise in solutions of the three-dimensional Schrödinger equation with an inverse-square potential, and in Gaussian integration. The Laguerre equation is

$$-\left(x^{\alpha+1}e^{-x}u'\right)' = \lambda x^\alpha e^{-x}u \qquad 0 < x < \infty,$$

where $-\infty < \alpha < \infty$.