Mathematical Methods in Physical Sciences

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1 Introduction

The majority of the fundamental processes of our natural world are described by differential equations. Some examples are the vibration of solids, the flow of fluids, the formation of crystals, the spread of infections, the diffusion of chemicals, the structure of molecules, etc. These examples are responsible for our interest in partial differential equations (PDE) such as Hamilton-Jacobi equation, Euler equation, Navier-Stokes equation, Diffusion equation, Wave equation and Korteweg-deVries equation. As the primary goal of the course, I discuss some of the above equations and explain some mathematical tools that are needed to solve them. I also use these equation as an excuse to introduce students to some basic questions in fluid mechanics and statistical physics.

As a warm-up for some of the challenging equations of the fluid mechanics such as Navier-Stokes equation, let us consider a diffusion equation

$$u_t = \alpha \Delta u, \tag{1.1}$$

where $u(x,t)$ represents the density function of a chemical substance in a motionless fluid. Alternatively, we may regard $u(x,t)$ as the temperature of a d dimentional body Ω. Here x is a point in the domain Ω, and t represents the time. From our interpretation, clearly (1.1) must be solved subject to initial and boundary conditions. Our experience with linear equations (such as ODEs) suggests expressing the solutions of (1.1) in terms of the eigenvalues and eigenfunctions of the operator Δ in the domain Ω. More specifically, we wish to express a solution as (a possibly infinite) linear combination of eigenfunctions. This leads to the Fourier expansion of a solution when Ω is a rectangular domain. We may express the solution as an integral operator that acts on the initial data, and has a kernel that can be expanded as an infinite series of weighted eigenfunctions. With the aid of this integral operator, we can solved the equation (1.1) when sources are added. In analogy with the linear ODES, we may formally write $u(x,t) = (e^{\alpha t \Delta} g)(x)$, where $g = u(x,0)$ is the initial data. Analogously the operator $(-\Delta)^{-1} = \int_0^\infty e^{t\Delta}\, dt$ is an integral operator with a kernel that is known as the Green's function of the domain Ω.

Our method of eigenfunction expansion of solutions can be used to treat any PDE of the form $u_t = \mathcal{L}u$ where $\mathcal{L}$ is a suitable operator. For example, $\mathcal{L}u = \alpha \Delta u + Vu$ would yield an important extension of (1.1), where $V(x)$ is a *potential* function. In the same manner the solutions to the Schrodinger equation

$$i\hbar \psi_t = -\frac{\hbar^2}{2m}\Delta\psi + V\psi, \tag{1.2}$$

can be represented.

The diffusion phenomenon occurs because the particles of the chemical substance are bombarded by the fluid molecules. One may attempt to write some differential equations for the motion of the particles, but such system of equations are impractical to solve because of the size of the system. Instead, we may use statistical mechanics to model the motion of typical particles. For (1.1), a Brownian motion describes the evolution of a typical particle statistically.

As our next model, we consider

$$u_t + |u_x|^2 + V = \alpha \Delta u, \tag{1.3}$$

which is an example of viscous Hamilton-Jacobi equation. When $\alpha = 0$, the equation (1.2) is a simple model of the growth of a crystal (with the graph of u representing the outer boundary of the crystal). When $\alpha > 0$, we may apply the so-called Hope-Cole transform to turn (1.3) to a variant of (1.1), namely

$$Z_t = \alpha \Delta Z + cVZ, \tag{1.4}$$

where $c = (2\alpha)^{-1}$. Kac found a probablistic representation for the solutions of (1.2) that has the same flavor as Feynman's path integral in quantum mechanics, and involves a killed Brownian motion when the potential V is nonnegative. Sending $\alpha \to 0$ in Feynman-Kac formula yields a variational representation of solutions of the corresponding (inviscid) Hamilton-Jacobi equation

$$u_t + |u_x|^2 + V = 0. \tag{1.5}$$

The equation (1.5) may be differentiated to yield inviscid Burgers equation

$$\rho_t + \rho \rho_x = f, \tag{1.6}$$

where $f = -V_x$ is the external force. Our variational formula for u can be used to represent ρ. An important feature of the equation is the occurrence of shock discontinuity and rarefaction waves. Regarding ρ as the mass density, we may regard (1.6) as a model for a simple fluid with a single conservation law. More generally, we will discuss the fundamental equations of fluid mechanics such as Euler and Navier-Stokes equations. When the fluid is incompressible, namely when the mass density is constant, we have a simpler PDE which is rich enough to exhibit turbulence. Euler equation is an hyperbolic system of conservation laws. We will briefly a systematic scheme for solving *Riemann Problem* for a system of conservation laws. The scheme will be examined for the equation of fluids and a PDE that is used in *chromatography*.

As we mentioned before, we use differential equations to model many phenomena in nature. If a phenomenon of interest exhibit certain symmetries, we expect to have the same symmetry for the corresponding differential equation. We can take advantage symmetries in two ways: finding conservation laws for our equation, and constructing self-similar solutions. A former can be done in a systematic way; a theorem of Nother gives us a recipe for constructing a conservation law associated with a symmetry of the underlying equation. As an example, consider Hamiltonian ODEs of classical mechanics:

$$\dot{q} = H_p(q,p,t), \qquad \dot{p} = -H_p(q,p,t). \tag{1.7}$$

Here $q \in \mathbb{R}^d$ represents the positions, $p \in \mathbb{R}^d$ represents the momenta, and H is the total energy, and is known as the Hamiltonian function. It turns out that if there is *enough* conserved quantities, namely d many conservation laws, then the equation (1.7) is *completely integrable*. Newton discovered that the two body problem (like Newton's equation for the motion of the sun and earth) is completely integrable. This is no longer the case for the N body problem when $N > 2$. It turns our that some nonlinear PDEs are infinite dimensional examples of completely integrable systems. As an example, we will discuss Korteweg-de Vries (KdV) equation

$$V_t - 6VV_x + V_{xxx} = 0, \tag{1.8}$$

which models the motion of waves along a canal. Indeed this PDE is completely integrable, and possess very stable traveling wave solutions known as *solitons*. The PDE (1.8) is closely related to the Schrodinger operator

$$\mathcal{L}\psi = -\psi'' + V\psi,$$

where the potential V is a solution of (1.8). The equation (1.8) can be written as a Lax equation

$$\mathcal{L}_t = [\mathcal{P}, \mathcal{L}], \tag{1.9}$$

for a suitable operator $\mathcal{L}$. The pair of $(\mathcal{P},)$ is an example of a *Lax pair* that would allow us to use the spectral data associated with $\mathcal{L}$ to completely integrate the equation (1.8).

Burgers formulated (1.6) as a toy model for turbulence. Euler equation is a system of conservation laws governing inviscid fluids. Writing

$$\rho : \mathbb{R}^d \times [0,T] \to \mathbb{R}, \qquad u = (u^1, \dots, u^d) : \mathbb{R}^d \times [0,T] \to \mathbb{R}^d, \qquad e : \mathbb{R}^d \times [0,T] \to \mathbb{R},$$

for the density, velocity and internal energy, Euler equation reads as

$$\begin{aligned} &\rho_t + \nabla \cdot (\rho u) = 0, \\ &u_t + \nabla(\rho u \otimes u) + \nabla P(\rho, e) = 0, \\ &(\rho E)_t + \nabla \cdot \big((E + P(\rho, e))u\big) = 0, \end{aligned} \tag{1.10}$$

where $P(\rho, e)$ is the pressure, and $E = \frac{1}{2}|u|^2 + e$ is the total energy. (In the middle equation, ∇ is regarded as a row vector.) When ρ is constant, the first two equations can be written as

$$u_t + (u \cdot \nabla)u + \nabla P = 0, \qquad \nabla \cdot u = 0. \tag{1.11}$$

Here we are using the fact that the j-th component of the vector $\nabla(u \otimes u)$ is given by

$$\sum_i (u^i u^j)_{x_i} = (\nabla \cdot u) u^j + \sum_i u^i u^j_{x_i} = (u \cdot \nabla) u^j.$$

Note that in (1.10), the pressure is given as a function of (ρ, e). However (1.11) is a system of $d+1$ equations of $d+1$ unknowns $u^1, \ldots, u^d, P$.

2 Laplace Operator

In this chapter, we mostly focus on the spectral properties of the Laplace operator. This in turn can be used to solve the diffusion equation (1.4), and the Schrodinger equation (1.2). As we mentioned in the introduction, the equations (1.2) or (1.4) must be solved subject to an initial condition $u(x,0) = g$ (or in the case of (1.2), we require $\psi(x,0) = g(x)$). Additionally we need a boundary condition that comes in three flavors: Given a function $h : \partial\Omega \times [0,T] \to \mathbb{R}$,

(i) *(Dirichlet Condition)* $u(x,t) = h(x,t)$ for $(x,t) \in \partial\Omega \times [0,T]$.

(ii) *(Neumann Condition)* $\frac{\partial u}{\partial n}(x,t) := u_x(x,t) \cdot n(x) = h(x,t)$ for $(x,t) \in \partial\Omega \times [0,T]$, where $n(x)$ is the outer unit normal at x.

(iii) *(Robin Condition)* $a(x)u(x,t) + \frac{\partial u}{\partial n}(x,t) = h(x,t)$ for $(x,t) \in \partial\Omega \times [0,T]$. Here $a : \partial\Omega \to \mathbb{R}$ is a given function.

When $h = 0$, we say that we have a *homogeneous boundary condition.* Physically speaking, a homogeneous boundary condition means that we have closed system in the case of the diffusion equation (or the body Ω is insulated along the boundary $\partial\Omega$ in the case of the heat equation). It turns out that when we boundary condition is not homogeneous, we can replace it with a homogeneous boundary condition for the price of producing an external force. As we will see later in this chapter, the external force can be taken care of with a trick known as the *Duhammel Principle.*

We now assume that we have a homogeneous boundary condition. This is a very convenient assumption because the set of solution with homogeneous is a vector space i.e., it is closed under addition and scalar multiplication. This makes the equation (**??**) or (1.2) particularly tractable because we can build new solutions from a family of solutions by taking linear combinations.

As the first step, let use ignore the initial condition, and search for special solution of say (1.1) of the form

$$u(x,t) = X(x)T(t).$$

Substituting this into (1.1) yields

$$\frac{T'(t)}{\alpha T(t)} = \frac{\Delta X(x)}{X(x)}.$$

This is possible only if both sides are equal to a constant, say $-\lambda$. From this we learn that if there exists a function $X(x)$ and a constant λ such that

$$-\Delta X(x) = \lambda X(x), \tag{2.1}$$

then

$$u(x,t) = e^{-\alpha\lambda t} X(x),$$

satisfies (1.1). The same idea works when we have a potential $V(x)$ which is independent of t, or if we consider the Schrodinger equation. In the latter case, if we have a function $\phi : \Omega \to \mathbb{R}$, and a constant $\mu \in \mathbb{R}$ such that

$$\mathcal{H}\phi = -\frac{\hbar^2}{2m}\Delta\phi + V\phi = \mu\phi,$$

then

$$\psi(x,t) = \exp\left(\frac{1}{i\hbar}\mu t\right)\phi(x), \tag{2.2}$$

is a solution of (1.2).

To get a feel for the equation (2.1), let us discuss a concrete example.

Example 2.1 Assume that Ω is a rectangular domain of the form

$$\Omega = \prod_{j=1}^{d}(0,\ell_j),$$

with $\ell_1,\ldots,\ell_j > 0$. In this case we may *separate variables* and search for an eigenfunction of the form

$$X(x_1,\ldots,x_d) = \prod_{j=1}^{d} X_j(x_j),$$

where $X_j : [0,\ell_j] \to \mathbb{R}$, for $j = 1,\ldots,d$. Note that if X satisfies (2.1), then

$$-\sum_{j=1}^{d}\frac{X''(x_j)}{X(x_j)} = \lambda.$$

This is possible only if there are constants $\ell_1,\ldots,\ell_d$ such that $\ell_1 + \cdots + \ell_d = \ell$, and

$$\frac{X''(x_j)}{X(x_j)} = \lambda_j, \tag{2.3}$$

for $j = 1,\ldots,d$. For the sake of definiteness, let us assume a homogeneous Dirichlet boundary condition i.e., $X_j(0) = X_j(\ell_j) = 0$. Then (2.3) has a non-trivial unique solution only if $\ell_j = k_j^2 > 0$, and the solution is

$$X_j(x_j) = \sin\frac{\pi k_j x_j}{\ell_j}.$$

In summary, given positive integers $k_1,\ldots,k_d$, the function

$$X(x_1,\ldots,x_d) = \prod_{j=1}^{d}\sin\frac{\pi k_j x_j}{\ell_j},$$

is an eigenfunction associated with the eigenvalue

$$\lambda = \pi^2 \sum_{j=1}^{d} \left(\frac{k_j}{\ell_j} \right)^2 . \tag{2.4}$$

The spectrum of Δ consists of λ of the above form, and, as it turns out, there is no other eigenvalue. When $d = 1$, all eigenvalues are simple (of multiplicity 1). This is no longer the case when $d \geq 2$. For example when $d = 2$, and $\ell_1 = \ell_2 = \pi$, then the list of eigenvalues is $2, 5, 5, 8, 10, 10, \ldots$. Note that the eigenvalue 5 is of multiplicity 2 because there are two ways to write 5 as a sum of two squares, namely $1^2 + 2^2$, and $2^2 + 1^2$.

In the case of homogeneous Neumann boundary condition, the eigenvalues are still of the form (2.4), except that our condition on the integer k_j is $k_j \geq 0$. The corresponding eigenfunctions are

$$\hat{X}(x_1, \ldots, x_d) = \prod_{j=1}^{d} \cos \frac{\pi k_j x_j}{\ell_j}.$$

The lowest eigenvalue is 0, associated with the eigenfunction 1. The list of eigenvalues is $0, 1, 1, 2, 4, 4, 5, 8, 9, 9, \ldots$. $\square$

Except for some simple domains, it is not possible to find the eigenvalues and eigenfunctions explicitly. However for every bounded domain with nice boundary, we can show that the set of eigenvalues is always discrete and all the multiplicities are finite. The modern proof of these facts for the Laplace operator (or more generally any *elliptic operator*) involves the *Fredholm Theory* of *compact operators*, and can be found in Evans [E]. On account of this general and important fact, we may write $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n \leq \ldots$ (with multiplicities) for the (ordered) set of eigenvalues. The corresponding (non-trivial) eigenfunctions are denoted by $w_1, w_2, \ldots, w_n, \ldots$. From our previous discussions we deduce that for any set of constants $c_1, c_2, \ldots,$ the function

$$u(x,t) := \sum_{n=1}^{\infty} c_n e^{-\alpha \lambda_n t} w_n(x),$$

is a solution provided that the sum converges in C^2-sense. This solution would satisfy our initial condition if

$$g(x) = \sum_{n=1}^{\infty} c_n w_n(x). \tag{2.5}$$

In order to succeed in our task, we need to examine the following problem. Given an initial data g, can we find constants c_n such that (2.5)?

Before tackling this question, we need to explore some basic properties of eigenvalues and eigenfunctions.

Definition 2.1(i) We write $\mathcal{C}^k$ for the space of functions $h : \Omega \to \mathbb{R}$ such that $h \in C^k$, and one of our homogeneous boundary conditions is satisfied. When needed we display the type of boundary condition we have in our notation for $\mathcal{C}^k$. More specifically, we write C_D^k (respectively C_N^k) for $\mathcal{C}^k$ when we have a homogeneous Dirichlet (respectively Neumann) boundary condition. Similarly, we write $\mathcal{C}_R^k$ for $\mathcal{C}^k$ when we have a homogeneous Robin boundary condition.

(ii) We define an inner product (and its corresponding norm) by

$$\langle h_1, h_2 \rangle = \int_\Omega h_1(x) h_2(x)\ dx, \qquad \|h\| := \langle h, h \rangle^{1/2}.$$

We write $h_1 \perp h_2$, when $\langle h_1, h_2 \rangle = 0$. □

Recall that by the Divergence Theorem,

$$\int_\Omega div\ F\ dx = \int_{\partial\Omega} F \cdot n\ dS, \tag{2.6}$$

where dS denotes the surface integration on $\partial\Omega$. For two C^1 functions w and v, we may choose $F = w\nabla v$ to deduce

$$\int_\Omega w \Delta v\ dx = -\int_\Omega \nabla w \cdot \nabla v\ dx + \int_{\partial\Omega} w \frac{\partial v}{\partial n}\ dS. \tag{2.7}$$

Proposition 2.1 **(i)** *The operator $\Delta : \mathcal{C}^2 \to \mathcal{C}^0$ is symmetric.*

(ii) *For every $w \in \mathcal{C}_D^2 \cup \mathcal{C}_N^2$, we have $\langle \Delta w, w \rangle \le 0$. Similarly if $u \in \mathcal{C}_R^2$ with $a \ge 0$ in the Robin condition, then $\langle \Delta w, w \rangle \le 0$.*

(iii) *If $-\Delta v = \lambda v$, $-\Delta w = \mu w$, and $\mu \ne \lambda$, then $v \perp w$.*

Proof (i)-(ii) By (2.7),

$$v, w \in \mathcal{C}_D^2 \ \text{ or } \ v, w \in \mathcal{C}_N^2 \quad \Longrightarrow \quad \int_\Omega w \Delta v\ dx = -\int_\Omega \nabla w \cdot \nabla v\ dx, \tag{2.8}$$

$$v, w \in \mathcal{C}_R^2 \quad \Longrightarrow \quad \int_\Omega w \Delta v\ dx = -\int_\Omega \nabla w \cdot \nabla v\ dx - \int_{\partial\Omega} avw\ dS, \tag{2.9}$$

The operator Δ is symmetric because the right-hand side is symmetric. Moreover the right-hand side is non-positive when $v = w$.

(iii) By symmetry,

$$-\lambda \langle v, w \rangle = \langle \Delta v, w \rangle = \langle v, \Delta w \rangle = -\mu \langle v, w \rangle.$$

Hence $\langle v, w \rangle = 0$ because $\lambda \ne \mu$. □

Proposition 2.2 *The set of eignfunctions $\{w_n : n \in \mathbb{N}\}$ can be chosen to be an orthonormal set.*

Proof Note that the eigenspace

$$\mathcal{E}_n = \{w \in \mathcal{C}^2 : -\Delta w = \lambda_n w\},$$

is finite dimensional, and has an orthonormal basis. We are done, because $\mathcal{E}_n \perp \mathcal{E}_m$ whenever $\lambda_n \neq \lambda_m$. $\square$

Note that if (2.5) holds, with $\{w_n : n \in \mathbb{N}\}$ as in Proposition 2.2, we can take the inner product of both side with respect to w_m to deduce that $c_m = \langle g, w_m \rangle$. The expansion (2.5) can be written as

$$g = \sum_{n=1}^{\infty} \langle g, w_n \rangle w_n. \tag{2.10}$$

We say that the orthonormal set $\{w_n : n \in \mathbb{N}\}$ is complete if (2.10) holds for every $g \in L^2(\Omega)$, with the series on the right-hand side convergent with respect the L^2-norm, namely $\|\cdot\|$ of Definition 2.1. To prepare for the proof of the completeness, we first provide a variational expression for the eigenvalues in the case of Dirichlet or Neumann boundary condition. To motivate our formula, observe that if (2.10) holds, then

$$\begin{aligned}
\|g\|^2 &= \left\langle \sum_n c_n w_n, \sum_n c_n w_n \right\rangle = \sum_{n=1}^{\infty} c_n^2, \\
\|\nabla g\|^2 &= \left\langle \sum_n c_n \nabla w_n, \sum_n c_n \nabla w_n \right\rangle = \sum_{n,m} c_n c_m \langle \nabla w_n, \nabla w_m \rangle \\
&= -\sum_{n,m} c_n c_m \langle w_n, \Delta w_m \rangle = \sum_{n,m} c_n c_m \lambda_m \langle w_n, w_m \rangle = \sum_{n=1}^{\infty} c_n^2 \lambda_n.
\end{aligned}$$

From this, it is not hard to deduce that if (2.9) is valid for every L^2-function, then

$$\lambda_1 = \inf \left\{ \frac{\|\nabla w\|^2}{\|w\|^2} : w \in \mathcal{C}^2, \ w \neq 0 \right\}. \tag{2.11}$$

In a similar fashion we can derive a variational expression for any λ_n. Thought we do not know yet that (2.10) is true. To prove (2.10) we first verify (2.11) and its generalization for any other eigenvalues. We then use these formulas to verify the validity of (2.9).

Proposition 2.3 *Assume either Dirichlet, or Neumann homogeneous boundary condition. Then the formula* (2.10) *holds true. Moreover, for each* $n \in \mathbb{N}$, $n > 1$,

$$\lambda_n = \inf\left\{ \frac{\|\nabla w\|^2}{\|w\|^2} : \ w \in \mathcal{C}^2, \ w \neq 0, \ w \perp w_1, \dots, w_{n-1} \right\} \tag{2.12}$$
$$= \inf\left\{ \|\nabla w\|^2 : \ w \in \mathcal{C}^2, \ \|w\| = 1, \ w \perp w_1, \dots, w_{n-1} \right\}.$$

Proof We give a partial proof by assuming that a classical minimizer exists. The proof of the existence uses a classical result of Rellich, namely any sequence h_n with $\|\nabla h_n\|$ uniformely bounded, has a subsequence that converges strongly in $L^2(\Omega)$. For our variational problem (**??**), we may assume $\|h_n\| = 1$, so that any limit point $\bar{w}$ of $\|h_n\}_{n\in\mathbb{N}}$ satisfies $\|\bar{w}\| = 1$ (and hence nonzero).

We present the proof when $n > 1$ because the proof of $n = 1$ is similar. Assume that there exists a function $\bar{w}$ such that the infimum is achieved at $\bar{w} \in \mathcal{C}^2$. This means that $\bar{w} \perp w_1, \dots, w_n$, and for any $v \in \mathcal{C}^2$, $v \perp w_1, \dots, w_n$, we have

$$\varphi(t) := \frac{\|\nabla(w + tv)\|^2}{\|w + tv\|^2} \leq \varphi(0),$$

for every $t \in \mathbb{R}$. As a result

$$0 = \dot{\varphi}(0) = 2\frac{\langle \nabla\bar{w}, \nabla v\rangle}{\|\bar{w}\|^2} - 2\frac{\|\nabla\bar{w}\|^2}{\|\bar{w}\|^2}\frac{\langle \bar{w}, v\rangle}{\|\bar{w}\|^2} = -2\frac{\langle \Delta\bar{w}, v\rangle}{\|\bar{w}\|^2} - 2\frac{\|\nabla\bar{w}\|^2}{\|\bar{w}\|^2}\frac{\langle \bar{w}, v\rangle}{\|\bar{w}\|^2} = -2\frac{\langle \Delta\bar{w} - \bar{\lambda}\bar{w}, v\rangle}{\|\bar{w}\|^2},$$

where $\bar{\lambda}$ denotes the right-hand side of (2.12) (the minimum value). As a result,

$$v \in \mathcal{C}^2, \ v \perp w_1, \dots, w_{n-1} \quad \Longrightarrow \quad \langle \Delta\bar{w} + \bar{\lambda}\bar{w}, v\rangle = 0.$$

Since $\bar{w} \perp w_1, \dots, w_{n-1}$, we also have

$$\langle \Delta\bar{w} + \bar{\lambda}\bar{w}, w_j\rangle = \langle \Delta\bar{w}, w_j\rangle = \langle \bar{w}, \Delta w_j\rangle = -\lambda_j\langle \bar{w}, w_j\rangle = 0,$$

for $j = 1, \dots, n-1$. As a result $\Delta\bar{w} + \bar{\lambda}w = 0$. In other words, $\bar{w}$ is an eigenfunction and the corresponding eigenvalue is $\bar{\lambda}$. This in turn implies that $\bar{\lambda} \geq \lambda_n$. On the other hand

$$\bar{\lambda} \leq \frac{\|\nabla w_n\|^2}{\|w_n\|^2} = \lambda_n.$$

This completes the proof. □

We are now ready to establish (2.9).

Theorem 2.1 *Assume either Dirichlet, or Neumann homogeneous boundary condition. Then the formula* (2.9) *holds true for every* $g \in \mathcal{C}^1$.

Proof Let us write
$$R_n = g - \sum_{m=1}^{n-1} c_m w_m.$$
We wish to show $\|R_n\| \to 0$ in large n limit. Since $R_n \perp w_1, \ldots, w_{n-1}$, we use (2.12) to assert
$$\|R_n\|^2 \le \lambda_n^{-1} \|\nabla R_n\|^2$$
which would go to 0 if we can show that $\sup_n \|\nabla R_n\| < \infty$, and $\lambda_n \to \infty$ as $n \to \infty$. The latter will be established later in this chapter after we learn how to compare the eigenvalues of the domain of Ω with a rectangular domain Ω' that contains Ω.

It remains to find a uniform bound on $\|\nabla R_n\|$. Evidently
$$\nabla R_n = \nabla g - \sum_{m=1}^{n-1} c_m \nabla w_m.$$
Observe that the set $\{\nabla w_n : \ n \in \mathbb{N}\}$ is an orthogonal set. Indeed,
$$\langle \nabla w_j, \nabla w_k \rangle = -\langle w_j, \Delta w_k \rangle = \lambda_k \langle w_j, w_k \rangle = \lambda_k \delta_{jk}.$$
As a result,
$$\|\nabla R_n\|^2 = \left\| \nabla g - \sum_{m=1}^{n-1} c_m \nabla w_m \right\|^2 = \|\nabla g\|^2 - 2 \left\langle \nabla g, \sum_{m=1}^{n-1} c_m \nabla w_m \right\rangle + \sum_{m=1}^{n-1} c_m^2 \lambda_m \le \|\nabla g\|^2,$$
because
$$\left\langle \nabla g, \sum_{m=1}^{n-1} c_m \nabla w_m \right\rangle = -\left\langle g, \sum_{m=1}^{n-1} c_m \Delta w_m \right\rangle = \sum_{m=1}^{n-1} c_m \lambda_m \langle g, w_m \rangle = \sum_{m=1}^{n-1} c_m^2 \lambda_m.$$
This completes the proof. □

We now turn our attention to the proof of $\lambda_n \to \infty$ in large n limit. First let us comment that a variational expression for an eigenvalue is desirable because in general no explicit formula can be found for λ_n. Our formula (2.12) does not serve our purposes because the eigenfunctions are not known in general. The following *maximin principle* of *Courant and Hilbert* provides us with a better alternative.

Proposition 2.4 *Assume either Dirichlet, or Neumann homogeneous boundary condition. Then for $n > 1$,*

$$\lambda_n = \max_{v_1, \ldots, v_{n-1}} \lambda_n(v_1, \ldots, v_{n-1}), \tag{2.13}$$

where

$$\lambda_n(v_1,\ldots,v_{n-1}) := \inf\left\{\frac{\|\nabla w\|^2}{\|w\|^2} :\ w\in\mathcal{C}^2,\ w\perp v_1,\ldots,v_{n-1}\right\}. \tag{2.14}$$

(Here the maximum is over continuous or even square integrable functions and we do not assume any boundary conditions.)

Proof Let us write $\bar\lambda$ for the right-hand side of (2.13). We certainly have $\lambda_n \le \bar\lambda$ by Proposition 2.3. On the other hand, given $v = (v_1,\ldots,v_{n-1}) \in \mathcal{C}^2$, choose $\alpha = (\alpha_1,\ldots,\alpha_n) \neq 0$ so that

$$w := \sum_{j=1}^n \alpha_j w_j \perp v_1,\ldots,v_{n-1}.$$

Such a nonzero α exists because α satisfies a system of $n-1$ linear equations. We have

$$\lambda_n(v_1,\ldots,v_n) \le \frac{\|\nabla w\|^2}{\|w\|^2} = \frac{\langle -\Delta w, w\rangle}{\|w\|^2} = \frac{\sum_{j=1}^n \lambda_j\alpha_j^2}{\sum_{j=1}^n \alpha_j^2} \le \lambda_n.$$

This being true for every such v implies that $\bar\lambda \le \lambda_n$, completing the proof of (2.13). $\square$

It is straightforward to show

$$\lambda_n = \max\left\{\frac{\|\nabla w\|^2}{\|w\|^2} :\ w\in span\{w_1,\ldots w_n\},\ w\neq 0\right\}. \tag{2.15}$$

We can use this to find a *minimax principle* for the eigenvalues:

Proposition 2.5 *Assume either Dirichlet, or Neumann homogeneous boundary condition. Then for $n>1$,*

$$\lambda_n = \min_{v_1,\ldots,v_n\in\mathcal{C}} \hat\lambda_n(v_1,\ldots,v_{n-1}), \tag{2.16}$$

where

$$\hat\lambda_n(v_1,\ldots,v_n) := \sup\left\{\frac{\|\nabla w\|^2}{\|w\|^2} :\ w\in span\{v_1,\ldots,v_n\},\ w\neq 0\right\}.$$

(Here the minimum is over continuous functions satisfying the corresponding boundary conditions.)

Proof Let us write $\bar{\lambda}$ for the right-hand side of (2.16). We certainly have $\lambda_n \geq \bar{\lambda}$ by (2.15). On the other hand, given $v = (v_1, \ldots, v_{n-1}) \in \mathcal{C}$, choose $\alpha = (\alpha_1, \ldots, \alpha_n) \neq 0$ so that

$$\bar{w} := \sum_{j=1}^{n} \alpha_j v_j \perp w_1, \ldots, w_{n-1}.$$

Such a nonzero α exists because α satisfies a system of $n-1$ linear equations. We have

$$\hat{\lambda}_n(v_1, \ldots, v_n) \geq \frac{\|\nabla \bar{w}\|^2}{\|\bar{w}\|^2} \geq \inf \left\{ \frac{\|\nabla w\|^2}{\|w\|^2} : \ w \perp w_1, \ldots, w_{n-1}, \ w \neq 0 \right\} = \lambda_n.$$

Since this is true for every choices of $v_1, \ldots, v_{n-1} \in \mathcal{C}$, we deduce that $\bar{\lambda} \geq \lambda_n$. □

To display the dependence on the domain, let us write $\lambda_n(\Omega)$ for the n-th eigenvalue. To emphasis on the type of boundary conditions we have, we may write $\lambda_n^D(\Omega)$ and $\lambda_n^N(\Omega)$ for the eigenvalues with the Dirichlet and Neumann homogeneous boundary conditions respectively. As we know from experience, a longer string (or a larger drum-head) plays lower notes. The next result is a mathematical justification of this fact.

Proposition 2.6 *If $\Omega \subset \Omega'$, then $\lambda_n^D(\Omega) \geq \lambda_n^D(\Omega')$.*

Proof Given a function $w \in \mathcal{C}_D^2(\Omega)$, define $\hat{w} : \Omega' \to \mathbb{R}$ by

$$w'(x) = w(x)\ \mathbb{1}(x \in \Omega), \tag{2.17}$$

so that $w' = 0$ on $O' \setminus \Omega$. This function is not necessarily twice differentiable on ∂O, but it is always continuous (in fact w' is weakly differentiable with $\nabla w \in L^2(O')$). Since such functions can be approximated by smooth functions in the norm $\|w\| + \|\nabla w\|$, we may use them in our variational representation of eigenvalues. We write $\hat{\mathcal{C}}(\Omega, \Omega')$ for the set of function w' as in (2.17). We can now use (2.13) to assert

$$\begin{aligned}
\lambda_n(\Omega') &= \sup_{v_1', \ldots, v_{n-1}'} \inf \left\{ \frac{\|\nabla w'\|^2}{\|w'\|^2} : \ w' \in \mathcal{C}_D^2(\Omega), \ w' \neq 0, \ w' \perp v_1', \ldots, v_{n-1}' \right\} \\
&\leq \sup_{v_1', \ldots, v_{n-1}'} \inf \left\{ \frac{\|\nabla w'\|^2}{\|w'\|^2} : \ w' \in \mathcal{C}(\Omega, \Omega'), \ w' \neq 0, \ w' \perp v_1', \ldots, v_{n-1}' \right\} \qquad (2.18)
\end{aligned}$$

Let us write $v_1, \ldots, v_{n-1}$ and w for the restrictions of $v_1', \ldots, v_{n-1}'$ and w' to the set Ω. Since

$$w' \in \mathcal{C}(\Omega, \Omega'), \ w' \perp v_1', \ldots, v_{n-1}' \quad \Longrightarrow \quad w' \perp v_1', \ldots, v_{n-1}', \ \|w\| = \|w'\|, \ \|\nabla w\| = \|\nabla w'\|,$$

we deduce that the right-hand side of (2.18) is simply $\lambda_n(\Omega)$, as desired. □

Remark 1.1(i) As we discussed in the proof of Proposition 2.4, we can allow the trial function to be weakly differentiable with a square integrable derivative. The set of such functions is denoted by $H^1(\Omega)$ and this is in some sense the largest set of functions w for which $\|w\|$ and $\|\nabla w\|$ are well-defined. To satisfy the homogeneous Dirichlet condition, we need to assume that the *trace* of w on $\partial\Omega$ is zero. The set of such functions is denoted by $H_0^1(\Omega)$. Alternatively, $w \in H_0^1(\Omega)$ if w can be approximated (with respect to the norm $\|w\| + \|\nabla w\|$) by smooth functions that vanish near the boundary. In summary we can write

$$\lambda_n^D(v_1, \dots, v_{n-1}) := \inf \left\{ \frac{\|\nabla w\|^2}{\|w\|^2} : \ w \in H_0^1(\Omega), \ w \neq 0, \ w \perp v_1, \dots, v_{n-1} \right\}. \tag{2.19}$$

As for the Neumann boundary condition, we can drop the assumption $\partial u/\partial n = 0$ and write

$$\lambda_n^N(\Omega) = \inf \left\{ \frac{\|\nabla w\|^2}{\|w\|^2} : \ w \in H^1(\Omega), \ w \neq 0, \ w \perp w_1, \dots, w_{n-1} \right\}, \tag{2.20}$$

$$= \max_{v_1, \dots, v_{n-1}} \inf \left\{ \frac{\|\nabla w\|^2}{\|w\|^2} : \ w \in H^1(\Omega), \ w \neq 0, \ w \perp v_1, \dots, v_{n-1} \right\}. \tag{2.21}$$

The proof of these formulas are left as an exercise. From comparing (2.21) with (2.13) we learn

$$\lambda_n^N(\Omega) \leq \lambda_n^D(\Omega). \tag{2.22}$$

□

As an immediate consequence of Proposition 2.4, we learn that $\lambda_n^D(\Omega) \to \infty$ in large n limit because we can choose two rectangular domains D^-, and D^+ such that $D^- \subset \Omega \subset D^+$, and $\lambda_n^D(D^-) \geq \lambda_n^D(\Omega) \geq \lambda_n^D(D^+)$. We wish to find the asymptotic behavior of λ_n. For this, let us define

$$\mathcal{N}^{D(N)}(\lambda) = \sharp\{n : \ \lambda_n^{D(N)} \leq \lambda\}.$$

Let us take a closer look at the eigenvalues of rectangular domains.

Example 2.2 Let Ω be as in Example 2.1. From (2.4) we learn

$$\mathcal{N}^D(\lambda) = \sharp E^D(\lambda) := \sharp \left\{ k = (k_1, \dots, k_d) \in \mathbb{N}^d : \sum_{j=1}^d \left(\frac{k_j}{\ell_j} \right)^2 \leq \frac{\lambda}{\pi^2} \right\}.$$

In other words, $k \in E^D(\lambda)$ iff k is an integer lies in Q, the first quadrant of an ellipsoid with radii $\pi^{-1}\ell_j\sqrt{\lambda}$. Such an integer k is a corner of the cube $\prod_j [k_j - 1, k_j]$ that fully lies in Q. Hence

$$\mathcal{N}^D(\lambda) \leq Vol(Q) = 2^{-d}\omega_d \prod_{j=1}^d \frac{\ell_j\sqrt{\lambda}}{\pi} = (2\pi)^{-d} \ \omega_d \ \lambda^{d/2} \ Vol(\Omega), \tag{2.23}$$

where ω_d is the volume of the unit ball in dimension d. On the other hand, if

$$Q^- = \left\{ x = (x_1, \dots, x_d) \in (0,\infty)^d : \sum_{j=1}^d \left(\frac{x_j + 1}{\ell_j} \right)^2 \le \frac{\lambda}{\pi^2} \right\},$$

then

$$Vol(Q^-) \le \mathcal{N}^D(\lambda). \tag{2.24}$$

From this and (2.23) we can readily deduce

$$\lim_{\lambda\to\infty} \lambda^{-d/2} \mathcal{N}^D(\lambda) = (2\pi)^{-d}\ \omega_d\ Vol(\Omega) =: c_d(\Omega). \tag{2.25}$$

□

Hermann Weyl in 1911 discovered that (2.25) is true for every bounded domain. He also conjectured the following asymptotic expansions:

$$\mathcal{N}^D(\lambda) = (2\pi)^{-d}\ \omega_d\ Vol_d(\Omega)\lambda^{d/2} - 4^{-1}(2\pi)^{-d+1}\ \omega_{d-1}\ \lambda^{(d-1)/2}\ Vol_{d-1}(\partial\Omega) + o\big(\lambda^{(d-1)/2}\big),$$
$$\mathcal{N}^N(\lambda) = (2\pi)^{-d}\ \omega_d\ Vol_d(\Omega)\lambda^{d/2} + 4^{-1}(2\pi)^{-d+1}\ \omega_{d-1}\ \lambda^{(d-1)/2}\ Vol_{d-1}(\partial\Omega) + o\big(\lambda^{(d-1)/2}\big).$$

Theorem 2.2 *Let Ω be a bounded domain with C^1 boundary. Then* (2.25) *holds.*

Proof *(Step 1)* Assume that $\Omega = \Omega_1 \cup \dots \cup \Omega_k$ is a partition of Ω into k many subdomains. We assume that each Ω_j has a C^1 boundary. Let us we write $\lambda_{j,n}^D$ for the n-th Dirichlet eigenvalue of the subdomain Ω_j, and arrange all $\lambda_{j,n}^D$ in a non-decreasing order $\mu_1^D \le \mu_2^D \le \dots$. We also write $\hat{w}_1^D, \hat{w}_2^D, \dots$ for the corresponding eigenfunctions. We then define $\widehat{\mathcal{C}}$ to be the set of functions $u \in H_0^1(\Omega)$ such that $u_j = u 1\!\!1_{\Omega_j} \in H_j^1(\Omega_j)$, for every $j \in \{1, \dots, k\}$. In other words, $u \in H^1(\Omega)$, and vanishes on the boundaries of all the subdomains. As before we can show

$$\mu_n^D = \inf\left\{ \frac{\|\nabla w\|^2}{\|w\|^2} :\ w \in \widehat{\mathcal{C}},\ w \ne 0,\ w \perp \hat{w}_1^D, \dots, \hat{w}_{n-1}^D \right\}. \tag{2.26}$$

Here

$$\|\nabla w\|^2 = \sum_{j=1}^k \int_{\Omega_j} |\nabla w\|^2\ dx. \tag{2.27}$$

The formula (2.26) can be established is just the same way we proved (2.12). Indeed if $\bar{w}$ is a minimizer of (2.26), and we consider $\varphi(t) = \|\nabla(\bar{w} + tv)\|^2 / \|\bar{w} + tv\|^2$, for a function $v \in \widehat{\mathcal{C}}$, then $\varphi'(0) = 0$ yields $\langle(\Delta\bar{w} + \bar{\lambda}\bar{w}), v\rangle = 0$ because as we perform an integration by parts in each subdomain, there would be no boundary contribution. Here $\bar{\lambda}$ denotes the right-hand side of (2.26). Without loss of generality, we may assume that $\|\bar{w}\| = 1$. Observe that if $\bar{w}_j = \bar{w}\mathbb{1}_{\Omega_j}$, then using the elementary inequality

$$\min_j \frac{a_j}{b_j} \leq \frac{\sum_j a_j}{\sum_j b_j}, \quad a_j, b_j > 0,$$

we have

$$\frac{\|\nabla\bar{w}\|^2}{\|\bar{w}\|^2} = \frac{\sum_j \|\nabla\bar{w}_j\|^2}{\sum_j \|w_j\|^2} \geq \min\left\{\frac{\|\nabla\bar{w}_j\|^2}{\|\bar{w}_j\|^2} : \ \bar{w}_j \neq 0\right\}.$$

This means that if the minimum on the left-hand side is achieved at $\bar{j} \in \{1, \dots, n-1\}$, then $\bar{w}_{\bar{j}}$ is also a minimizer (and that the inequality must be an equality). Because of this we may assume that the minimizer $\bar{w}$ satisfies $\bar{w} = \bar{w}\mathbb{1}_{\Omega_{\bar{j}}}$ for some $\bar{j}$. From $\bar{w} \perp \hat{w}_1^D, \dots, \hat{w}_{n-1}^D$, we can readily deduce that $\bar{\lambda} \geq \mu_n$. The proof of $\bar{\lambda} \leq \mu_n$ follows from choosing $w = \hat{w}_n^D$ for our trial function. This completes the proof of (2.26).

A repetition of the proof of Proposition 2.4 yields

$$\mu_n^D = \max_{v_1,\dots,v_{n-1}} \inf\left\{\frac{\|\nabla w\|^2}{\|w\|^2} : \ w \in \widehat{\mathcal{C}}, \ w \neq 0, \ w \perp v_1, \dots, v_{n-1}\right\}. \tag{2.28}$$

(Step 2) Similarly, let us define $\widehat{\mathcal{C}}'$ to be the set of functions u such that $u_j = u\mathbb{1}_{\Omega_j} \in H^1(\Omega_j)$ for every $j \in \{1, \dots, k\}$. In other words, u is in H^1 in each subdomain, but is allowed to be discontinuous across the boundary of subdomains. Let us we write $\lambda_{j,n}^N$ for the n-th Neumann eigenvalue of the subdomain Ω_j, and arrange all $\lambda_{j,n}^N$ in a non-decreasing order $\mu_1^N \leq \mu_2^N \leq \dots$. We also write $\hat{w}_1^N, \hat{w}_2^N, \dots$ for the corresponding eigenfunctions. We claim

$$\mu_n^N = \inf\left\{\frac{\|\nabla w\|^2}{\|w\|^2} : \ w \in \widehat{\mathcal{C}}', \ w \neq 0, \ w \perp \hat{w}_1^N, \dots, \hat{w}_{n-1}^N\right\}. \tag{2.29}$$

Again $\|\nabla w\|^2$ is defined by (2.27). Let us write $\bar{w}$ for a minimizer in (2.29), and $\bar{\lambda}$ for the right-hand side of (2.29). A repetition of the proof of (2.20) yields $\Delta\bar{w} + \bar{\lambda}\bar{w} = 0$ strictly inside each subdomain, and that $\partial\bar{w}/\partial n = 0$ on the boundary of each subdomain. As in Step 1, we can argue that there exists k such that $\bar{w}\mathbb{1}_{\Omega_k}$ is also a minimizer. We can now repeat our reasoning in Step 1 to complete the proof of (2.29). Similarly, we can show

$$\mu_n^N = \max_{v_1,\dots,v_{n-1}} \inf\left\{\frac{\|\nabla w\|^2}{\|w\|^2} : \ w \in \tilde{\mathcal{C}}, \ w \perp v_1, \dots, v_{n-1}\right\}. \tag{2.30}$$

From (2.30), (2.28), and (2.22) we deduce

$$\mu_n^N \leq \lambda_n^N \leq \lambda_n^D \leq \mu_n^D. \tag{2.31}$$

(Final Step) Define

$$\widehat{\mathcal{N}}^D(\lambda) = \sharp\{n: \ \mu_n^D \le \lambda\}, \quad \widehat{\mathcal{N}}^N(\lambda) = \sharp\{n: \ \mu_n^N \le \lambda\}.$$

From (2.31) we learn

$$\widehat{\mathcal{N}}^D(\lambda) \le \mathcal{N}^D(\lambda) \le \mathcal{N}^N(\lambda) \le \widehat{\mathcal{N}}^N(\lambda).$$

On the other hand if we write $\mathcal{N}_i^{D(N)}(\lambda)$ for the eigenvalue counting number of the domain Ω_i, then it is not hard to see

$$\widehat{\mathcal{N}}^{D(N)}(\lambda) = \sum_{j=1}^{k} \mathcal{N}_j^{D(N)}(\lambda),$$

which in turn implies

$$\lim_{\lambda\to\infty} \lambda^{-d/2}\widehat{\mathcal{N}}^{D(N)}(\lambda) = \lim_{\lambda\to\infty} \sum_{j=1}^{k} \lambda^{-d/2}\mathcal{N}_j^{D(N)}(\lambda). \tag{2.32}$$

From this we can readily derive (2.25) when Ω is a finite union of rectangular domains. Since we can find a sequence of domains $\Omega_n^{\pm}$ such that each $\Omega_n^{\pm}$ is a union of rectangular domains, and

$$\Omega_n^- \subset \Omega \subset \Omega_n^+, \quad \lim_{n\to\infty} Vol\big(\Omega_n^+ \setminus \Omega_n^-\big),$$

we are done. □

Corollary 2.1 *Let Ω be as in Theorem 2.2. Then*

$$\lim_{n\to\infty} n^{-2/d}\lambda_n(\Omega) = c_d(\Omega)^{-2/d}.$$

Proof The function $\mathcal{N}(\lambda)$ is a piecewise constant function with jumps at $\mu_1 < \mu_2 < \dots < \mu_n < \dots$, where μ_j is the j-th distinct eigenvalue, and $\mathcal{N}(\mu_j+) - \mathcal{N}(\mu_j-)$ is the multiplicity of μ_j. Given $c_\pm$ with $c_- < c_d(\Omega) < c_+$, we have

$$c_-\lambda^{d/2} \le \mathcal{N}(\lambda) \le c_+\lambda^{d/2},$$

for sufficiently large λ. This implies

$$(n/c_+)^{-d/2} \le \mathcal{N}^{-1}(n) \le (n/c_-)^{-d/2},$$

for sufficiently large n. This completes the proof, because $\mathcal{N}^{-1} = n = \lambda_n$ for $n \in \mathbb{N}$, and we can send $c_\pm$ to $c_d(\Omega)$. □

Remark 2.1(i) In 1966, Marc Kac raised the following question: Is the domain Ω determined up to isometries from the its Dirichlet or Neumann eigenvalues $\lambda_n(\Omega)$? It turns out that the answer is no in general. However the eigenvalues do provide many goemetric information about Ω. It is conjectured that under some additional assumptions on Ω, we should be able to determine Ω fully from its spectrum. Let us discuss some reformulation of Kac's question. Observe that the Laplace transform of the counting function $\mathcal{N}$ is simply

$$\begin{aligned}\int_0^\infty e^{-t\lambda}\mathcal{N}(\lambda)\ d\lambda &= \int_0^\infty e^{-t\lambda}\sum_{n=1}^\infty \mathbb{1}(\lambda_n \le \lambda)\ d\lambda = \sum_{n=1}^\infty \int_{\lambda_n}^\infty e^{-t\lambda}\ d\lambda \\ &= t^{-1}\sum_{n=1}^\infty e^{-t\lambda_n} = t^{-1}Tr\left(e^{t\Delta}\right).\end{aligned}$$

On the other hand

$$\begin{aligned}\int \lambda^{d/2}\ e^{-t\lambda}\ d\lambda &= t^{-1-\frac{d}{2}}\Gamma\left(\frac{d}{2}+1\right), \\ \int \lambda^{(d-1)/2}\ e^{-t\lambda}\ d\lambda &= t^{-1-\frac{d-1}{2}}\Gamma\left(\frac{d-1}{2}+1\right),\end{aligned}$$

where for example

$$\Gamma\left(\frac{d}{2}+1\right) = \begin{cases} k! & \text{if } d = 2k, \\ \frac{(2k+2)!}{4^k(k+1)!}\sqrt{\pi} & \text{if } d = 2k+1. \end{cases}$$

This suggests an expansion

$$Tr\left(e^{t\Delta}\right) = t^{-\frac{d}{2}}\sum_{k=0}^\infty a_k t^{k/2}, \tag{2.33}$$

for small $t > 0$.

(ii) The variational techniques we have developed work also when we add a potential to $-\Delta$. For example, if $V : \Omega \to \mathbb{R}$ is a continuous function, and $\mathcal{L}$ is the operator

$$\mathcal{L}w = -\alpha\Delta w + Vw,$$

then under either Dirichlet or Neumann boundary condition, we have

$$\langle \mathcal{L}w, w\rangle = \|\nabla w\|^2 + \langle Vw, w\rangle.$$

Again we write $\lambda_1 \le dots \le \lambda_n \le \dots$ for the eigenvalues and $w_1, w_2, \dots, w_n, \dots$ and eigenfunctions:

$$\mathcal{L}w_n = \lambda_n w_n, \quad \|w_n\| = 1.$$

With a verbatim argument we can show

$$\lambda_n = \inf \left\{ \frac{\|\nabla w\|^2 + \langle Vw, w\rangle}{\|w\|^2} \ : \ w \in \mathcal{C}^2,\ w \perp w_1, \ldots, w_{n-1} \right\}.$$

Note that the operator $\mathcal{L}$ is symmetric, but not necessarily positive unless $V \geq 0$. $\square$

2.1 Fundamental solution

The diffusion (1.1) in the domain Ω has a solution of the form

$$u(x,t) = \sum_{n=1}^{\infty} e^{-\alpha\lambda_n t} \langle g, w_n\rangle w_n(x),$$

where $g(x) = u(x,0)$ is the initial condition. This can be rewritten as

$$u(x,t) = \int_\Omega S(x,y,t)g(y)\ dy, \quad \text{where} \quad S(x,y,t) = \sum_{n=1}^{\infty} e^{-\alpha\lambda_n t} w_n(x) w_n(y). \tag{2.34}$$

We refer to S as the *fundamental solution.* In fact S solves the diffusion equation in x for each y (or the other way around) so long as $t > 0$:

$$S_t = \alpha \Delta_x S. \tag{2.35}$$

Since $u(x,t) \to g(x)$ as $t \to \infty$, we interpret this as

$$\lim_{t\to 0} S(x,y,t) = \delta_y(x), \qquad \text{or} \qquad S(x,y,0) = \delta_y(x).$$

With the aid of S we can solve (1.1) with an external force:

$$u_t = \alpha\Delta u + f, \qquad u(x,0) = g, \tag{2.36}$$

By Duhamel's formula

$$u(x,t) = \int_\Omega S(x,y,t)g(y)\ dy + \int_0^t \int_\Omega S(x,y,t-s) f(y,s)\ dyds. \tag{2.37}$$

We now ready to treat inhomogeneous boundary conditions. For example if we require

$$u(x,t) = h(x,t), \qquad t \geq 0,\ x \in \partial\Omega,$$

then we search for a C^2 function $H : \Omega \times [0,\infty) \to \mathbb{R}$ such that the restriction of H to the boundary coincides with h. Then the function $w = u - H$ satisfies a homogeneous Dirichlet boundary condition, and solves

$$w_t = \alpha\Delta w + \hat{f}, \qquad w(x,0) = \hat{g},$$

where $\hat{f} = f - (H_t - \alpha\Delta H)$, and $\hat{g}(x) = g(x) - H(x,0)$.

2.2 Brownian motion

When the domain Ω is $\mathbb{R}^d$, we can explicitly determine the fundamental solution. To find S, observe that if u satisfies (1.1) in $\mathbb{R}^d$, and $c > 0$ is a scalar, then $w(x,t) = u(cx, c^2t)$ is also a solution. This suggests looking for a scaling invariant solution of the form $u(x,t) = \varphi\big(x/\sqrt{t}\big)$. Let us first assume that $d = 1$. Substituting such a function u in (1.1) yields

$$-\frac{x}{2t^{3/2}}\varphi'\left(\frac{x}{t^{1/2}}\right) = \frac{\alpha}{t}\varphi''\left(\frac{x}{t^{1/2}}\right), \qquad \text{or} \qquad -r\varphi'(r) = 2\alpha\varphi''(r).$$

This leads to a solution of the form

$$w(x,t) = \int_0^{x/\sqrt{t}} e^{-\frac{r^2}{4\alpha}}\ dr.$$

Observe

$$w(x,0) = \begin{cases} \sqrt{\alpha\pi}, & x > 0, \\ -\sqrt{\alpha\pi}, & x < 0. \end{cases}$$

We wish to find a solution with δ_0 for initial data. Since a constant multiple of w_x is also a solution, we arrive at

$$\bar{S}(x,0,t) = \frac{1}{2\sqrt{\alpha\pi}} w_x(x,t) = \frac{1}{2\sqrt{\alpha\pi t}} e^{-\frac{x^2}{4\alpha t}},$$

for the fundamental solution. We can extend this to higher dimensions, and by translation to any y:

$$\bar{S}(x,y,t) = (4\pi t\alpha)^{-d/2}\ e^{-\frac{|x-y|^2}{4\alpha t}}. \tag{2.38}$$

We note that $x \mapsto \bar{S}(x,y,t)$ can serve as a probability density because

$$\int \bar{S}(x,y,t)\ dy = 1.$$

Indeed we may regard $x \mapsto \bar{S}(x,y,t)$ as the probability density of the location of a particle that is suspended in a motionless fluid. The particle is initially located at x and reaches y at time t. Its motion comes from kicks it receives from the fluid particles. A simple mathematical model for its motion was proposed by Einstein in 1905 and is known as Brownian motion. (It was also developed by Bachelier in his 1900 thesis to model the stock market fluctuations.) The first rigorous construction of a Brownian motion was carried out by Wiener in 1920's. By a Brownian motion or Wiener process $B(t)$, we mean a probability measure $\mathbb{P}$ on the set of continuous path $B : [0,\infty) \to \mathbb{R}^d$ with the following properties:

- $B(0) = 0$ and $\mathbb{P}(B(t) \in A) = \int_A \bar{S}(0, y, t)\ dy$ for $\alpha = 1/2$.
- The process $\hat{B}(t) = B(t+s) - B(s),\ t \geq 0$ is again a Brownian motion that is independent of $\big(B(\theta):\ \theta \in [0, s]\big)$.

Given a Brownian motion, we may write

$$u(x, t) = \mathbb{E}\ g\big(x + \sqrt{2\alpha}\ B(t)\big),$$

where $\mathbb{E}$ denotes the expectation with respect to $\mathbb{P}$. Moreover, we can readily calculate the finite dimensional density of $\big(B(t_1), \dots, B(t_k)\big)$ for $0 = t_0 < t_1 < \cdots < t_k = T$. Indeed if

$$\big(B(t_1), B(t_2), \dots, B(t_k)\big) = (x_1, x_2, \dots, x_k),$$

then

$$\big(B(t_1), B(t_2) - B(t_1), \dots, B(t_k) - B(t_{k-1})\big) = (x_1, x_2 - x_1, \dots, x_k - x_{k-1}),$$

and by the aforementioned properties of Brownian motion,

$$\mathbb{E} f\big(B(t_1), \dots, B(t_k)\big) = \int f(x_1, \dots, x_k)\ Z(t_1, \dots, t_k)^{-1} \exp\left[-\frac{1}{2} \sum_{j=1}^{k} \frac{|x_j - x_{j-1}|^2}{t_j - t_{j-1}}\right] \prod_{j=1}^{k} dx_j,$$

where

$$Z(t_1, \dots, t_k) = \prod_{j=1}^{k} \big(2\pi(t_j - t_{j-1})\big)^{1/2}.$$

If we write $\big(y(t):\ t \in [0, T]\big)$ for the (polygonal) path that interpolates linearly between points

$$(0, B(0)),\ (t_1, B(t_1)), \dots, (t_k, B(t_k)),$$

then the exponent can be written as

$$-\frac{1}{2} \int_0^T |\dot{y}(s)|^2\ ds.$$

We are tempted to choose finer and finer grid for $[0, T]$, and hope to have a limit for our formula as $\max_j (t_j - t_{j-1})$ tends to 0. If we succeed, we would have a representation of the Wiener measure in the interval $[0, T]$ in the form

$$Z([0, T])^{-1} \exp\left[-\frac{1}{2} \int_0^T |\dot{B}(s)|^2\ ds\right] \prod_{s \in [0, T]} dB(s). \tag{2.39}$$

Unfortunately such a limit does not exist, and various terms that appear in (2.39) are not mathematically well-defined. Nonetheless, if we think of the diffusion equation

$$u_t(x,t) = \frac{1}{2}\Delta u(x,t) + V(x)u(x,t), \qquad u(x,0) = g(x), \tag{2.40}$$

as the Euclidean analog of the Schrodinger equation, then a possible candidate for the solution would be

$$u(x,t) = \int g(x+B(t))\ Z([0,t])^{-1} \exp\left[-\int_0^t \left(\frac{1}{2}|\dot{B}(s)|^2 - V(x+B(s))\right)\ ds\right] \prod_{s\in[0,T]} dB(s).$$

Motivated by this we have the following representation of solution that is known as *Feynmann-Kac Formula.*

Theorem 2.3 *Assume that V and g are bounded continuous functions.Then the solution of* (2.40) *can be represented as*

$$u(x,t) = \mathbb{E}\ g(x+B(t))\ e^{\int_0^t V(x+B(s))\ ds}. \tag{2.41}$$

Proof *(Step 1)* We wish to show that u given by (**??**) satisfies (2.40). Let us first assume that $g, V \in C^2$ with bounded second derivative. This would guarentee that $u \in C^2$ because we can differentiate inside the expectation.

Give $h > 0$, set $\hat{B}(t) = B(t+h) - B(h)$. Observe

$$\begin{aligned}
u(x,t+h) =& \mathbb{E}\ g\big(x+B(t+h)\big)\ e^{\int_0^{t+h} V(x+B(s))\ ds} \\
=& \mathbb{E}\ g\big(x+B(h)+\hat{B}(t)\big)\ e^{\int_0^t V(x+B(h)+\hat{B}(s))\ ds}\ e^{\int_0^h V(x+B(s))\ ds} \\
=& \mathbb{E}\ u\big(x+B(h),t\big)\ e^{\int_0^h V(x+B(s))\ ds} \\
=& \mathbb{E}\ u\big(x+B(h),t\big)\ \left(1+\int_0^h V\big(x+B(s)\big)\ ds\right) + O(h^2) \\
=& \mathbb{E}\ u\big(x+B(h),t\big) + \ (1+hV(x)) + o(h) \\
=& \mathbb{E}\ u\big(x+B(h),t\big) + hV(x)u(x,t) + o(h) \\
=& u(x,t) + 2^{-1}h\Delta u(x,t) + hV(x)u(x,t) + o(h).
\end{aligned}$$

Hence u given by (2.41) satisfies (2.40).

(Step 2) We now replace the differentiability assumption on (g,V). Choose a sequence $(g^n, V^n) \in C^2$ with bounded derivatives such that $(g^n, V^n) \to (g,V)$ locally uniformly. We write u^n for the corresponding u as we replace g and V in (2.41) with g^n and V^n. Evidently $u^n \to u$ pointwise. By Step 1

$$u^n_t = \frac{1}{2}\Delta u^n + V^n u^n, \qquad u^n(x,0) = g^n(x).$$

We may use Duhamel's formula to write

$$u^n(x,t) = \int \bar{S}(x,y,t)g^n(y)\ dy + \int_0^t \int \bar{S}(x,y,t-s)(V^n u^n)(y,s)\ dy,$$

where S is given in (2.38). We can pass to the limit to deduce

$$u(x,t) = \int \bar{S}(x,y,t)g(y)\ dy + \int_0^t \int \bar{S}(x,y,t-s)(Vu)(y,s)\ dy.$$

This in turn implies that u satisfies (2.40). (We only calculated the right derivative, but this is good enough to show that u is weakly differentiable, and since its weak derivative is continuous, u is classically differentiable.) $\square$

2.3 Green's function

Given a domain Ω, the kernel G of the operator Δ^{-1} is known as the Green's function. We can use our eigenvalues and eigenfunctions to find an explicit expression for G:

$$-\Delta^{-1}(x,y) = G^D(x,y) = \sum_{n=1}^{\infty} (\lambda_n^D)^{-1} w_n^D(x) w_n^D(y). \tag{2.42}$$

This is an immediate consequence of $-\Delta^{-1} w_n = \lambda_n^{-1} w_n$. The question of convergence of the series in (2.42) is subtle we do not address it here. Note that by (2.25) we know that λ_n^{-1} behaves like a constant multiple of $n^{-2/d}$, which converges rather slowly to zero when d is large. Assuming Dirichlet boundary condition, the Green's function $G = G^D$ can be specified by

$$\begin{cases} -\Delta_y G^D(x,y) = \delta_x(y), & y \in \Omega, \\ G^D(x,y) = 0, & y \in \partial\Omega. \end{cases} \tag{2.43}$$

We now apply (2.7) to assert that for any C^2 function u,

$$u(x) = -\int_\Omega G^D(x,y)\ \Delta u(y)\ dy - \int_{\partial\Omega} \frac{\partial G^D}{\partial n}(x,y) u(y)\ dS(y). \tag{2.44}$$

The kernel $-\partial G^D/\partial n$ is known as *Poisson kernel.* With the aid of (2.44) we can solve the problem

$$\begin{cases} -\Delta u = f, & \text{in } \Omega, \\ u = h, & \text{in } \partial\Omega. \end{cases} \tag{2.45}$$

Assuming Neumann boundary condition, the Green's function $G = G^N$ is defind by

$$G^N(x,y) = \sum_{n=2}^{\infty} (\lambda_n^N)^{-1} w_n^N(x) w_n^N(y). \tag{2.46}$$

Note that the sum avoids the first eigenvalue $\lambda_1^N = 0$. Observe

$$-\Delta_y G^N(x,y) = \sum_{n=2}^{\infty} w_n^N(x) w_n^N(y) = \delta_x(y) - 1.$$

Hence G^N can be specified by

$$\begin{cases} -\Delta_y G^N(x,y) = \delta_x(y) - 1, & y \in \Omega, \\ \frac{\partial G^N}{\partial n}(x,y) = 0, & y \in \partial\Omega. \end{cases} \tag{2.47}$$

Applying (2.7) again yields,

$$u(x) = -\int_\Omega G^N(x,y)\ \Delta u(y)\ dy + \int_\Omega u(y)\ dy + \int_{\partial\Omega} G^N(x,y) \frac{\partial u}{\partial n}(y)\ dS(y). \tag{2.48}$$

With the aid of (2.48) we can solve the problem

$$\begin{cases} -\Delta u = f, & \text{in } \Omega, \\ \frac{\partial u}{\partial n} = h, & \text{in } \partial\Omega. \end{cases} \tag{2.49}$$

For this problem to have a solution, we need

$$\int_\Omega f\ dx + \int_{\partial\Omega} h\ dS = 0. \tag{2.50}$$

Also note that if u is a solution to (2.51), then $u + c$ is also a solution for any constant c. To have a unique solution, we may require that $\int_\Omega u(y)\ dy = 0$.

When $\Omega = \mathbb{R}^d$, by translation invariance of the domain and Δ, the corresponding Green's function $\bar{G}$ satisfies $\bar{G}(x,y) = \bar{G}(0, y-x)$. When $d \geq 3$, we may find the Green's function by integrating the fundamental solution (2.38) in t:

$$\begin{aligned} \bar{G}(x) :=& \bar{G}(0,x) = -\Delta^{-1}(0,x) = \int_0^\infty \bar{S}(0,x,t)dt = \int_0^\infty (4\pi t)^{-d/2} e^{-\frac{|x|^2}{4t}}\ dt \\ =& \frac{1}{4\pi^{d/2}} \int_0^\infty \theta^{\frac{d}{2}-2}\ e^{-\theta|x|^2}\ d\theta = \frac{1}{4\pi^{d/2}} \int_0^\infty \theta^{\frac{d}{2}-2}\ e^{-\theta}\ d\theta\ |x|^{2-d} \\ =& \frac{\Gamma(d/2-1)}{4\pi^{d/2}}\ |x|^{2-d} = \frac{\Gamma(d/2)}{2(d-2)\pi^{d/2}}\ |x|^{2-d} = \frac{1}{d(d-2)\omega_d}\ |x|^{2-d} =: c_d|x|^{2-d}. \end{aligned}$$

We can verify this directly. It is straightforward to check that $\Delta\bar{G} = 0$ off of the origin. On the other hand, we can use the integrability of $\bar{G}$ near the origin to assert that for every smooth φ of compact support,

$$\int \bar{G}\Delta\varphi\; dx = \lim_{\delta\to 0}\int_{|x|>\delta} \bar{G}\Delta\varphi\; dx = \lim_{\delta\to 0}\left[\int_{|x|>\delta} \varphi\Delta\bar{G}\; dx + \int_{|x|=\delta}\left(\frac{\partial\varphi}{\partial n}\,\bar{G} - \frac{\partial\bar{G}}{\partial n}\,\varphi\right)\, dS\right]$$
$$= -\lim_{\delta\to 0}\int_{|x|=\delta} \frac{\partial\bar{G}}{\partial n}\,\varphi\; dS = -\varphi(0)\;\lim_{\delta\to 0}\int_{|x|=\delta} \frac{\partial\bar{G}}{\partial n}\; dS.$$

From

$$\nabla\bar{G}(x) = -(d-2)c_d|x|^{-d}x, \qquad \frac{\partial\bar{G}}{\partial n}(x) = (d-2)c_d|x|^{1-d},$$

we deduce

$$\int_{|x|=\delta} \frac{\partial\bar{G}}{\partial n}\; dS = 1, \tag{2.51}$$

because $d\omega_d$ is the surface area of a sphere of radius 1. When $d = 2$,

$$\bar{G}(x) = -\frac{1}{2\pi}\log|x|, \tag{2.52}$$

because $\bar{G}$ satisfies $\Delta\bar{G} = 0$ off of the origin, and (2.51) holds. In summary,

$$\int (-\Delta\varphi)\bar{G}\; dy = \varphi(0),$$

for any smooth φ of compact support. This is exactly (2.48) for $u = \varphi$, and can be interpreted as saying that $-\Delta\bar{G} = \delta_0$ *weakly*.

Remark 2.2 According Coulomb's law the (potential) energy associated with a charge density $\rho(x)$ (in dimension 3) is given by

$$V(x) = \frac{1}{4\varepsilon_0\pi}\int \frac{\rho(y)}{|x-y|}\; dy = \frac{1}{\varepsilon_0}\int \bar{G}(x,y)\rho(y)\; dy,$$

where ε_0 is the *electric constant*. Hence the electric field E is given by

$$E(x) = -\nabla V(x) = -\frac{1}{4\varepsilon_0\pi}\int \rho(y)\frac{x-y}{|x-y|^3}\; dy.$$

As a consequence we have the Gauss' law $\nabla\cdot E = -\Delta V = \varepsilon_0^{-1}\rho$. □

On account of (2.44) and (2.48), we can solve the problems (2.45) and (2.51), provided that the corresponding Green's functions are known. In practice, no explicit formula for the Green's function is available. Since $\Delta(G-\bar{G})=0$, $G-\bar{G}$ is a harmonic motion and is smooth. This implies that the type of singularity G has near the diagonal is the same as $\bar{G}$. Note also that by (2.7)

$$u(x) = -\int_{\Omega} \bar{G}(x,y)\ \Delta u(y)\ dy - \int_{\partial\Omega} \frac{\partial \bar{G}}{\partial n}(x,y) u(y)\ dS(y) + \int_{\partial\Omega} \bar{G}(x,y)\frac{\partial u}{\partial n}(y)\ dS(y). \tag{2.53}$$

Motivated by this, let us set

$$w(x) = \Gamma v(x) =: -\int_{\partial\Omega} \frac{\partial \bar{G}}{\partial n}(x,y) v(y)\ dS(y),$$

for a given function v. This is the analog of Cauchy's integral in complex analysis and $\Delta w = 0$ off of $\partial\Omega$. We way wonder whether the operator Γ can be used to solve (2.51) for $f=0$. For this we need to examine the behavior of $w(x)$ as x approaches a point $a \in \partial\Omega$ within Ω. We note that the function w may not be continuous on $\partial\Omega$. For the limiting behavior of w at a, we need to the evaluate the total integral of the kernel that appears on the right-hand side of (2.53).

Lemma 2.1 *(Gauss Lemma)*

$$-\int_{\partial\Omega} \frac{\partial \bar{G}}{\partial n}(x,y)\ dS(y) = \frac{1}{2}\mathbb{1}\big(x \in \partial\Omega\big) + \mathbb{1}\big(x \in \Omega\big). \tag{2.54}$$

Proof Note that by Gauss divergence formula

$$\int_{\partial\Omega} \frac{\partial \bar{G}}{\partial n}(x,y)\ dS(y) = \int_{\partial B_\delta(x)\cap\Omega} \frac{\partial \bar{G}}{\partial n}(x,y)\ dS(y),$$

because $\Delta_y \bar{G}(x,y) = 0$ in $\Omega \setminus B_\delta(x)$. This implies (2.54) when $x \in \Omega$ by (**??**). In the case of $x \in \partial\Omega$, we can show

$$\lim_{\delta\to 0}\int_{\partial B_\delta(x)\cap\Omega} \frac{\partial \bar{G}}{\partial n}(x,y)\ dS(y) = \frac{1}{2},$$

because for δ small, the domain of integration is almost half of $\partial B_\delta(x)$. □

Theorem 2.4 *Let v be a continuous function. Then*

$$\lim_{x\in\Omega\to a} (\Gamma v)(x) = \frac{1}{2}v(a) + (\Gamma v)(a), \tag{2.55}$$

for every $a \in \partial\Omega$.

Proof For $x \in \Omega$, we use (2.54) to write,

$$(\Gamma v)(x) - \frac{1}{2}v(a) - (\Gamma v)(a) = -\int_{\partial\Omega} \left[\frac{\partial \bar{G}}{\partial n}(x,y) - \frac{\partial \bar{G}}{\partial n}(a,y)\right] \big(v(y) - v(a)\big)\ dS(y)$$
$$=: \int A(x,y)\ dS(y).$$

We write this integral as $I(\delta) + II(\delta)$, with I representing the integral of A over $\partial\Omega \cap B_\delta(a)$. We use the continuity of v to show that $I(\delta)$ is small δ. For $II(\delta)$, we are δ-away from the singularity of G and use the continuity of Γ to show that $II(\delta)$ is small whenever $|x-a|$ is small. □

The formula (2.55) offers a strategy for solving (2.45) when $f = 0$. The solution can be expressed as $u = \Gamma v$ for

$$v = \left(\frac{1}{2}id + \Gamma\right)^{-1} h.$$

This strategy can be carried out to prove the existence of a solution by taking advantage of the compactness of the operator Γ.

2.4 Exercise

(i) Determine the radial part of the operator Δ in dimension d. In other words, find Δf, where $f(x) = \varphi(|x|)$.

(ii) When $d = 2$, determine the Laplace operator in polar coordinates.

(iii) When $d = 2$, and Ω is the disc $\{x : \ |x| \le a\}$, find eigenvalues and eigenfunctions of Δ for the homogeneous Dirichlet boundary conditions. (Hint: The eigenfunctions are not explicit and satisfy ODEs known as Bessel's differential equations.)

(iv) Assume Robin homogeneous boundary condition with $a \ge 0$. Then for each $n \in \mathbb{N}$, $n > 1$,

$$\lambda_n = \inf\left\{\frac{\|\nabla w\|^2 + \mathcal{M}(w)}{\|w\|^2} :\ w \in \mathcal{C}^2,\ w \perp w_1, \dots, w_{n-1}\right\},$$

where

$$\mathcal{M}(w) = \int_{\partial\Omega} aw^2\ dS.$$

(Remark: As in the proof of (2.11)*, assume that a minimizer exists. The condition* $a \ge 0$ *may be used to guarantee the existence of a minimizer.)*

(v) Verify (2.20). *(Hint: Repeat the proof of Proposition 2.3 for* $v \in C^2$ *and* $v \perp w_1, \dots, w_{n-1}$*. If we additionally assume that* v *vanishes on* $\partial\Omega$*, then we deduce* $\Delta\bar{w} + \bar{\lambda}w = 0$ *inside* Ω*. Then choose* v *that does not vanish on boundary to deduce that* $\partial\bar{w}/\partial n = 0$ *on* $\partial\Omega$*.)*

(vi) Verify (2.24).

(vii) Show that (2.25) holds when $\lambda^D(\Omega)$ is replaced with $\lambda^N(\Omega)$, and Ω is a rectangular domain.

(viii) Show

$$\left|\mathcal{N}^D(\lambda) - (2\pi)^{-d}\ \omega_d\ Vol_d(\Omega)\lambda^{d/2}\right| \le 2^{-1}(2\pi)^{-d+1}\ \omega_{d-1}\ \lambda^{(d-1)/2}\ Vol_{d-1}(\partial\Omega),$$

for a rectangular Ω as in Example 2.2. *(Hint: Bound $Vol(Q) - Vol(Q^-)$).*

(ix) Show that $\int w_n^N\ dx = 0$ for $n > 1$. Use this to verify

$$\int_\Omega S^N(x, y, t)\ dy = 1,$$

where S^N denotes the fundamental solution of the diffusion equation when we have Neumann condition.

(x) Check directly that u given by (2.37) satisfies (2.36).

(xi) Assume that $u : \mathbb{R}^d \to \mathbb{R}$ is a uniformly positive twice continuously differentiable function such that Δu is bounded. Show

$$u(x) = \mathbb{E}\ u(x + B(t))\ e^{-\int_0^t \frac{\Delta u}{2u}(x+B(s))\ ds},$$

for every $t \ge 0$. (The assumptions on u guarantee that the right-hand side is well-defined.)

(xii) For G given by (2.42), show

$$\int_{\Omega\times\Omega} G(x, y)^2\ dxdy = \sum_{n=1}^\infty \lambda_n^{-2}.$$

When this is finite? *(Hint: Use Theorem 2.2.)*

(xiii) When

$$\int_{|x|\le 1} \bar{G}(x)^2\ dx < \infty?$$

Explain why your answer coincides with your answer in **(xii)**.

(xiv) In the case of the upper half space

$$\Omega = \left\{(x_1, \dots, x_d) \in \mathbb{R}^d :\ x_d > 0\right\},$$

show

$$G^D(x, y) = \bar{G}(x - y) - \bar{G}(x - \bar{y}),$$

where $y = (y_1, \ldots, y_{d-1}, y_d)$, $\bar{y} = (y_1, \ldots, y_{d-1}, -y_d)$.

(xv) Assume that $u : \Omega \times [0, \infty) \to \mathbb{R}$ solves the wave equation

$$u_{tt} = c^2 u_{xx}, \qquad x \in \Omega, t > 0,$$

subject to the initial conditions

$$u(x, 0) = f(x), \quad u_t(x, 0) = g(x), \quad x \in \Omega,$$

and the Dirichlet boundary condition $u(x,t) = 0$, for $x \in \partial\Omega$. Use the eigenvalues and eigenfunctions of $-\Delta$ in the domain Ω to represent the solution in terms of its initial data. (*Hint*: First ignore initial conditions and separate variables to find solutions of the form $u(x,t) = T(t)X(x)$.)

(xvi) Consider the wave equation in $\mathbb{R}$:

$$u_{tt}(x,t) = c^2 u_{xx}(x,t) + h(x,t), \qquad x \in \mathbb{R},\ t > 0,$$

with the initial conditions $u(x, 0) = f(x)$, $u_(t(x, 0) = g(x)$. Directly show that u given by

$$u(x,t) = \frac{1}{2}\big(f(x+ct) + f(x-ct)\big) + \frac{1}{2c}\int_{x-ct}^{x+ct} g(y)\ dy + \frac{1}{2c}\int_0^t \int_{x-c(t-s)}^{x+c(t-s)} h(y,s)\ dyds,$$

is a solution.

3 Schrodinger Operator

For our purposes, we wish to analyze the spectrum of $\mathcal{L} = -\Delta + V$. As we will see later, if V vanishes sufficiently fast at ∞, then we always have $\sigma_{ess}(\mathcal{L}) = [0, \infty)$, and that $\sigma_d(\mathcal{L}) \subset (-\infty, 0)$ is a finite set (possibly empty). Let us first discuss some examples.

Example 3.1(i) Let $\mathcal{X} = L^2(\mathbb{R}^d)$, and $\mathcal{L} = -\Delta$, with $Dom(\mathcal{L}) = H^2(\mathbb{R}^d)$. We claim that $\sigma(\mathcal{L}) = \sigma_{ess}(\mathcal{L}) = [0, \infty)$. Note that for every $k \in \mathbb{R}^d$, we have $\mathcal{L}(w_k) = 4\pi^2|k|^2 w_k$, where $w_k(x) = e^{2\pi i k\cdot x}$. But $w_k \notin L^2(\mathbb{R}^d)$. Nonetheless the presence of such w_k prevents the operator $\Delta + |k|^2$ to be invertible. To explain this, let us use the Fourier Transform

$$\hat{f}(\xi) = \mathcal{F}(f)(\xi) = \int e^{-2\pi i x\cdot\xi} f(\xi)\ d\xi, \quad \check{g}(x) = \mathcal{F}^{-1}(f)(x) = \int e^{2\pi i x\cdot\xi} g(x)\ dx.$$

Define $f_n = \check{g}_n$, where

$$g_n(\xi) = (2\pi n)^{d/2} e^{-n^2|\xi - k|^2}.$$

We claim

$$\|f_n\| = 1, \quad \lim_{n\to\infty} \|(\Delta + 4\pi^2|k|^2) f_n\| = 0, \quad f_n \rightharpoonup 0.$$

Indeed $\|f_n\|^2 = \|g_n\|^2 = 1$, and

$$\begin{aligned}\|(\Delta + 4\pi^2|k|^2) f_n\|^2 &= 16\pi^4 (2\pi n)^{d/2} \int (|\xi|^2 - |k|^2)^2 e^{-n^2|\xi-k|^2}\ d\xi \\ &= 16\pi^4 (2\pi)^{d/2} n^{-d/2} \int (|k + n^{-1}\xi|^2 - |k|^2)^2 e^{-|\xi|^2}\ d\xi \to 0,\end{aligned}$$

in large n limit.

Also if $-(\Delta + \lambda)u = w$, then

$$\hat{w}(\xi) = (4\pi^2|\xi|^2 - \lambda)\hat{u}(\xi),$$

which leads to

$$-(\Delta + \lambda)^{-1} w = K * w, \quad \text{where} \quad \hat{K}(\xi) = (4\pi^2|\xi|^2 - \lambda)^{-1} =: L(\xi).$$

Note that $\hat{K}$ is well-defined and analytic if $\lambda \notin [0, \infty)$. Moreover,

$$\begin{aligned}K(x) =& \check{L}(x) = \int (4\pi^2|\xi|^2 - \lambda)^{-1} e^{2\pi i x\cdot\xi}\ d\xi = \int_0^\infty \int e^{2\pi i x\cdot\xi - t(4\pi^2|\xi|^2 - \lambda)}\ d\xi\ dt \\ =& \int_0^\infty e^{t\lambda - \frac{|x|^2}{4t}} \int e^{2\pi i x\cdot\xi - 4\pi^2|\xi|^2 t + \frac{|x|^2}{4t}}\ d\xi\ dt = \int_0^\infty e^{t\lambda - \frac{|x|^2}{4t}} \int e^{t|2\pi i\xi + \frac{x}{2t}|^2}\ d\xi\ dt \\ =& \int_0^\infty e^{t\lambda - \frac{|x|^2}{4t}} \int e^{t|2\pi i \xi|^2}\ d\xi\ dt = \int_0^\infty e^{t\lambda - \frac{|x|^2}{4t}} \int e^{-|2\pi\sqrt{t}\ \xi|^2}\ d\xi\ dt \\ =& \pi^{d/2} \int_0^\infty e^{t\lambda - \frac{|x|^2}{4t}}\ (2\pi\sqrt{t})^{-d}\ dt = (4\pi)^{-d/2} \int_0^\infty e^{t\lambda - \frac{|x|^2}{4t}}\ t^{-d/2}\ dt\end{aligned}$$

(iii) Consider $\mathcal{L} = -\frac{d^2}{dx^2} - V_0 1\!\!1(|x| \le 1)$. As we mentioned before, if λ is an eigenvalue, then $\lambda \in (-\infty, 0)$. We write $\lambda = -\ell^2$. Since outside $[-1,1]$, the eigenfunction must satisfy $\psi'' = \ell^2\psi$, we learn that $\psi(x) = c_0 e^{-\pm x}$. Since we require $\psi \in L^2(\mathbb{R})$, we must have $\psi(x) = c_0 e^{-\ell x}$, for $x > \ell$, and $\psi(x) = c_0' e^{\ell x}$, for $x < -\ell$. For simplicity, we assume that $c_0 = c_0'$. In summary, We first concentrate on its eigenvalues. We search for ψ such that $\psi(x) = c_0 e^{-\ell|x|}$ outside the interval $[-1,1]$. Inside the interval $[-1,1]$, we wish to solve

$$\mathcal{L}\psi = -\psi'' - V_0\psi = -\ell^2\psi, \quad \text{or} \quad \psi'' = (\ell^2 - V_0)\psi.$$

We now argue that $\ell^2 - V_0 < 0$. If to the contrary $\ell^2 - V_0 = \eta^2$ for some $\eta \ge 0$, then $\psi(x) = c_1 e^{\eta x} + c_2 e^{-\eta x}$, and the condition $\psi(1) = \psi(-1) = c_0 e^{-\ell}$ implies that $c_1 = c_2$, $c_1(e^{-\eta} + e^{\eta}) = c_0 e^{-\ell}$. On the other hand the conditions $\psi'(1) = -c_0\ell e^{-\ell}$, $\psi'(-1) = c_0\ell e^{-\ell}$, lead to $c_1\eta(e^{\eta} - e^{-\eta}) = -c_0\ell e^{-\ell}$. Note that since $\ell > 0$, we must have $\eta > 0$. In summary

$$c_1(e^{-\eta} + e^{\eta}) = c_0 e^{-\ell}, \qquad c_1\eta(e^{\eta} - e^{-\eta}) = -c_0\ell e^{-\ell},$$

which in particular implies

$$\eta\frac{e^{\eta} - e^{-\eta}}{e^{\eta} + e^{-\eta}} = -\ell.$$

This is impossible because the left-hand side is positive. In summary, we must have $V_0 - \ell^2 = \mu^2 > 0$. As a result, we have $\psi(x) = c_1\cos(\mu x) + c_2\sin(\mu x)$, inside $[-1,1]$. The boundary conditions $\psi(1) = \psi(-1) = c_0 e^{-\ell}$ imply that either $c_2 = 0$, or $\sin\mu = 0$. Additionally we require

$$\psi'(1) = -c_0\ell e^{-\ell}, \qquad \psi'(-1) = c_0\ell e^{-\ell}.$$

This means,

$$-c_1\mu\sin\mu + c_2\mu\cos(\mu) = -c_0\ell e^{-\ell}, \qquad c_1\mu\sin\mu + c_2\mu\cos(\mu) = c_0\ell e^{-\ell}.$$

These equations rule out the possibility of $\sin\mu = 0$, because we are assuming that $c_0 \ne 0$ and $\ell > 0$. Hence $c_2 = 0$, and

$$c_1\cos\mu = c_0 e^{-\ell}, \qquad c_1\mu\sin\mu = c_0\ell e^{-\ell}.$$

As a result, we must have $\mu\tan\mu = \ell = \sqrt{V_0 - \mu^2}$. Hence $\mu^2\tan^2\mu = V_0 - \mu^2$. In summary,

$$\sigma_d(\mathcal{L}) = \left\{V_0 - \mu^2 : \ \mu \in (0, \sqrt{V_0}), \ \mu|\cos\mu|^{-1} = \sqrt{V_0}\right\}.$$

Clearly this set is nonempty and finite. Indeed if we write $\zeta(\mu) = \mu|\cos\mu|^{-1}$, then ζ is monotone restricted to an interval $\big(j\pi/2, (j+1)\pi/2\big)$, $j \in \mathbb{N} \cup \{0\}$ with $\zeta\big(j\pi/2, (j+1)\pi/2\big) = \big(j\pi/2, \infty\big)$, for j even, and $\zeta\big(j\pi/2, (j+1)\pi/2\big) = \big(((j+1)\pi/2, \infty\big)$, for j odd.

We next turn our attention to the essential spectrum. Given $\lambda = k^2 \in \sigma_{ess}(\mathcal{L}) = [0, \infty)$, we wish to find ψ such that $\mathcal{L}\psi = \lambda\psi$. Note that now ψ is not in $\mathcal{L}^2(\mathbb{R})$. Since $\psi'' = -k^2\psi$

outside $[-1,1]$, we must be able to express ψ as a linear combination of e^{ikx} and e^{-ikx}. For the sake of simplicity, let us assume that $\psi(x) = c_1 e^{-ikx}$ for $x < -1$, and $\psi(x) = c_2 e^{ikx} + c_3 e^{-ikx}$ for $x > 1$. Inside $[-1,1]$, we have $\psi'' = -r^2\psi$, where $r^2 = V_0 + k^2$. Hence $\psi(x) = c_4 e^{irx} + c_5 e^{-irx}$ inside $[-1,1]$. Matching these functions and their first derivatives at ± 1 yield

$$
\begin{aligned}
&c_4 e^{-ir} + c_5 e^{ir} = c_1 e^{ik}, && c_4 r e^{-ir} - c_5 r e^{ir} = -c_1 k e^{ik},\\
&c_4 e^{ir} + c_5 e^{-ir} = c_2 e^{ik} + c_3 e^{-ik}, && c_4 r e^{ir} - c_5 r e^{-ir} = c_2 k e^{ik} - c_3 k e^{-ik}.
\end{aligned}
$$

As a result,

$$
\begin{aligned}
&2c_4 = c_1\left(1 - \frac{k}{r}\right)e^{i(k+r)}, \qquad 2c_5 = c_1\left(1 + \frac{k}{r}\right)e^{i(k-r)},\\
&2c_4 = c_2\left(1 + \frac{k}{r}\right)e^{i(k-r)} + c_3\left(1 - \frac{k}{r}\right)e^{-i(k+r)},\\
&2c_5 = c_2\left(1 - \frac{k}{r}\right)e^{i(k+r)} + c_3\left(1 + \frac{k}{r}\right)e^{-i(k-r)}.
\end{aligned}
$$

These equations allow us to determine the coefficients $c_2, \dots, c_5$ in terms of c_1. □

We now consider the operator

$$
\mathcal{L} : H^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d), \quad \mathcal{L} = -\Delta + V, \tag{3.1}
$$

for a potential $V : \mathbb{R}^d \to \mathbb{R}$.

Definition 3.1 We say V is a *Kato potential*, if for every $\varepsilon > 0$, there exists a decomposition $V = V_1 + V_2$ such that $V_1 \in L^2(\mathbb{R}^d)$, and $\sup_x |V_2(x)| \le \varepsilon$. In particular, if $V \in L^2(\mathbb{R}^d)$, then V is a Kato potential. □

Example 3.2 If $V(x) = c|x|^{-\alpha}$, for some $\alpha > 0$, then we can write $V = V_1 + V_2$, where $V_1(x) = V(x)\mathbb{1}(|x| \le \ell)$. Clearly V_2 is small for ℓ large. On the other hand, $V_1 \in L^2$ iff $2\alpha < d$. In particular, the Coulomb potential ($\alpha = 1$, $d = 3$) is a Kato potential. □

Theorem 3.1 *Let $\mathcal{L}$ be as in* (3.1)*.*
(i) *If $V \ge 0$, and $V(x) \to \infty$ as $|x| \to \infty$, then $\sigma(\mathcal{L}) = \sigma_d(\mathcal{L})$.*

(ii) *If V is a Kato potential, then $\sigma_{ess}(\mathcal{L}) = \sigma_{ess}(-\Delta) = [0, \infty)$.*

Remark 3.1 Give a bounded set Ω, consider the potential $V(x) = \infty\mathbb{1}(x \notin \Omega)$. We interpret $-\Delta + V$ as the restriction of $-\Delta$ to Ω, which has a discrete spectrum. □

We now focus on the case of $\mathcal{L}$ as in (A.1) when $d = 1$, and V satisfies

$$\int (1 + |x|)|V(x)|\ dx < \infty. \tag{3.2}$$

Definition 3.2(i) Let $\lambda = -\ell^2 \in \sigma_d(\mathcal{L}^W),\ \ell > 0$. Then there exists a unique C^2 function $\psi^\ell : \mathbb{R} \to \mathbb{R}$ such that

$$\int (\psi^\ell(x))^2\ dx = 1, \qquad (\mathcal{L}^W + \ell^2)\psi^\ell = 0,$$

and $\psi^\ell \cong a_\pm(\ell)e^{-\ell|x|}$ as $x \to \pm\infty$, for constants $a_\pm(\ell) = a^W_\pm(\ell) \in \mathbb{R}$.

(ii) Let $\lambda = k^2 \in \sigma_{ess}(\mathcal{L}^W) = [0, \infty)$. Then there exists a unique C^2 function φ^k such that $(\mathcal{L}^W - k^2)\varphi^k = 0$, and $\varphi \cong b(k)e^{-ikx}$ as $x \to -\infty$, and $\varphi \cong e^{-ikx} + A(k)e^{ikx}$ as $x \to \infty$, for constants $b(k) = b^W(k), A(k) = A^W(k) \in \mathbb{R}$.

(ii) Define $X(W) : P(W) \to \mathbb{R}$ by $X(W)(-\ell^2) = a_+(\ell),\ X(W)(k^2) = A(k)$.

Proposition 3.1 *Given two C^2 functions $\psi : \mathbb{R} \to \mathbb{C}$ and $\varphi : \mathbb{R} \to \mathbb{C}$, recall that its Wronskian is defined by*

$$\mathcal{W}(\psi, \varphi) = \det \begin{bmatrix} \psi & \varphi \\ \psi' & \varphi' \end{bmatrix}.$$

If ψ and φ satisfy

$$(\mathcal{L}^W + \lambda)\varphi = (\mathcal{L}^W + \lambda)\psi = 0,$$

then $\mathcal{W}(\psi, \varphi)$ is constant (independent of x).

Proof We certainly have

$$\frac{d}{dx}\mathcal{W}(\psi, \varphi) = \det \begin{bmatrix} \psi' & \varphi' \\ \psi' & \varphi' \end{bmatrix} + \det \begin{bmatrix} \psi & \varphi \\ \psi'' & \varphi'' \end{bmatrix} = \det \begin{bmatrix} \psi & \varphi \\ (W - \lambda)\psi & (W - \lambda)\varphi \end{bmatrix} = 0.$$

□

Definition 3.2 In what follows, we write $f \cong g$ at ∞ for

$$\lim_{x\to\infty} \frac{f(x)}{g(x)} = 1, \qquad \lim_{x\to\infty} \frac{f'(x)}{g'(x)} = 1.$$

In the same fashion, by $f \cong g$ at $-\infty$ we mean that the above limits hold as $x \to -\infty$.

□

Proposition 3.2 *Assume that a C^2 function $\psi : \mathbb{R} \to \mathbb{C}$ satisfies the following conditions: $\mathcal{L}\varphi = k^2\varphi$, for $k \in \mathbb{R}$, and*

$$\varphi(x) \cong c_1 e^{-ikx} \quad as \quad x \to -\infty, \qquad \varphi(x) \cong c_2 e^{-ikx} + c_3 e^{ikx} \quad as \quad x \to \infty. \tag{3.3}$$

Then we have

$$c_2^2 = c_1^2 + c_3^2. \tag{3.4}$$

Proof Note that since V and k are real, we have $\mathcal{L}\bar{\varphi} = \lambda\bar{\varphi}$. We then use Proposition 3.1 to assert that $\mathcal{W}(\varphi, \bar{\varphi}) = c$ is constant. On the other hand

$$\mathcal{W}(\varphi, \bar{\varphi})(-\infty) = \det \begin{bmatrix} c_1 e^{-ikx} & \bar{c}_1 e^{ikx} \\ -ikc_1 e^{-ikx} & ik\bar{c}_1 e^{ikx} \end{bmatrix} = 2ik|c_1|^2,$$

$$\mathcal{W}(\varphi, \bar{\varphi})(+\infty) = \det \begin{bmatrix} c_2 e^{-ikx} + c_3 e^{ikx} & \bar{c}_2 e^{ikx} + \bar{c}_3 e^{-ikx} \\ -ikc_2 e^{-ikx} + ikc_3 e^{ikx} & ik\bar{c}_2 e^{ikx} - ik\bar{c}_3 e^{-ikx} \end{bmatrix} = 2ik(|c_2|^2 - |c_3|^2).$$

From this and $\mathcal{W}(\varphi, \bar{\varphi})(-\infty) = \mathcal{W}(\varphi, \bar{\varphi})(\infty)$ we deduce (3.4). □

Remark 3.2 The intuition behind (3.4) is as follows. We send a wave $\varphi(x) = c_2 e^{-ikx}$ from ∞ to the left. Its kinetic energy is associated with $|\varphi'(x)|^2 = k^2|c_2|^2$. A part of this wave is transmitted as $c_1 e^{-ikx}$, and a part of it is reflected back as $c_3 e^{ikx}$. With this interpretation, (**??**) is the conservation of energy. □

3.1 Inverse Scattering Transform

We wish to recover the potential W from its spectral/scattering data $\big(\sigma(\mathcal{L}^W), a^W(\ell), A^W(k)\big)$. In this subsection we derive a celebrated formula of *Gelfand-Levitan-Marchenko (GLM)* equation is the key identity for building the potential W from its the spectral/scattering data.

Theorem 3.2 *Given a potential W, define $B^W = B = B_d + B_c$, where*

$$B_d(x) = \sum_{-\ell^2 \in \sigma_d(\mathcal{L}^W)} a^W(\ell)^2 e^{-\ell x}, \qquad B_c(x) = \frac{1}{2\pi} \int A(k) e^{ikx}\, dk. \tag{3.5}$$

Find $E(x, \xi)$ from the linear integral equation

$$E(x, \xi) + B(\xi + x) + \int_x^\infty B(\xi + \zeta) E(x, \zeta)\, d\zeta = 0. \tag{3.6}$$

Then

$$W(x) = -2 \frac{d}{dx} E(x, x). \tag{3.7}$$

In our setting, we have a wave function $\varphi(x,k)$ such that

$$\varphi_{xx} + k^2\varphi = W\varphi, \tag{3.8}$$

We may use Duhammel principle to solve (3.8). The space of all solutions is 2-dimensional, and we produce a basis $\{f^-, f^+\}$ for this space by requiring $f^\pm \cong e^{\pm ikx}$ as $x \to \pm\infty$. More precisely, we require $f^\pm(x,k)$ to satisfy

$$\begin{aligned} f^+(x,k) =& e^{ikx} - k^{-1}\int_x^\infty \sin(k(x-y))W(y)f^+(y,k)\ dy, \\ f^-(x,k) =& e^{-ikx} + k^{-1}\int_{-\infty}^x \sin(k(x-y))W(y)f^-(y,k)\ dy. \end{aligned} \tag{3.9}$$

The functions $f^\pm$ are called the *Jost functions/solutions.* Note that if

$$G^\pm(x,k) = \mp k^{-1}\sin(kx)\mathbb{1}\big(\mp x \geq 0\big),$$

then

$$G^\pm_{xx} + k^2 G^\pm = \delta_0, \qquad G^\pm(\pm\infty,k) = G^\pm_x(\pm\infty,k) = 0. \tag{3.10}$$

As a result, $f^\pm$ satisfy (3.8)

$$f^\pm_{xx} + k^2 f^\pm = W f^\pm, \tag{3.11}$$

with $f^\pm \cong e^{\pm ikx}$, as $x \to \pm\infty$. Note that if we write $g(x,k) = b(k)f^-(x,k)$, then $g \cong b(k)e^{-ikx}$, as $x \to -\infty$. As a result, $\mathcal{W}(\varphi, g)(-\infty) = 0$. This and Proposition 4.5 imply that $\mathcal{W}(\varphi, g) = 0$, which in turn imply that φ is a constant multiple of g. Since $\varphi, g \cong b(k)e^{-ikx}$, as $x \to -\infty$, we deduce that $\varphi = g$. In the same fashion, we can use f^+ to represent φ. In summary,

$$\varphi^W(x,k) = \varphi(x,k) = b(k)f^-(x,k) = f^+(x,-k) + A(k)f^+(x,k). \tag{3.12}$$

As an immediate consequence of this, we have the following formula for f^- in terms of f^+:

$$f^-(x,k) = \beta(k)f^+(x,-k) + \alpha(k)f^+(x,k), \tag{3.13}$$

where $\beta(k) = b(k)^{-1}$, and $\alpha(k) = A(k)b(k)^{-1}$.

Proposition 3.3 **(i)** *Functions $f^\pm$ have extensions from $\mathbb{R} \times [0,\infty)$ to*

$$\mathbb{R} \times \big\{(x,k) :\ x \in \mathbb{R},\ k \in \mathbb{C},\ k \neq 0,\ Im(k) \geq 0\big\}.$$

This extension (still denoted by $f^\pm$) is continuous, and analytic when restricted to the upper-half plane $Im(k) > 0$.

(ii) *The functions α, β and A are analytic in the upper-half plane.*

Proof(i) We only provide a proof for f^+, as the case of f^- can be established by a verbatim argument. We define a sequence f_n inductively by starting from $f_0(x,k) = e^{ikx}$, and

$$f_{n+1}(x,k) = e^{ikx} - \int_x^\infty \sin(k(x-y))W(y)f_n(y,k)\ dy.$$

Evidently each f_n is analytic in k away from $k=0$. If we can show that f_n converges locally uniformly when $Imk > 0$, we deduce the analytic property of f^+. Observe that if $g_n = f_n - f_{n-1}$, with $f_{-1} = 0$, then $g_0 = e^{ikx}$, and

$$g_{n+1}(x,k) = -\int_x^\infty \sin(k(x-y))W(y)g_n(y,k)\ dy.$$

On the other hand, if $h_n(x,k) = g_n(x,k)e^{-ikx}$, then $h_0 = 1$, and

$$\begin{aligned} h_{n+1}(x,k) &= -\int_x^\infty \sin(k(x-y))e^{ik(y-x)}W(y)h_n(y,k)\ dy \\ &= \int_x^\infty \frac{1}{2ik}\big(e^{2ik(y-x)} - 1\big)W(y)h_n(y,k)\ dy. \end{aligned}$$

Since

$$\left|e^{2ik(y-x)} - 1\right| \le \left(e^{-2(y-x)Im(k)} + 1\right) \le 2,$$

by $y - x \ge 0, Im(k) \ge 0$, we deduce

$$|h_{n+1}(x,k)| \le |k|^{-1}\int_x^\infty |W(y)|\ |h_n(y,k)|\ dy.$$

From this we can readily deduce

$$|h_n(x,k)| \le \frac{C_0(x)^n}{|k|^n n!}, \tag{3.14}$$

where $C_0(x) = \int_x^\infty |W(y)|\ dy$. To see this, assume (3.14) is true. Then

$$\begin{aligned} |h_{n+1}(x,k)| &\le \frac{1}{|k|^{n+1}n!}\int_x^\infty |W(y)|\ C_0(y)^n\ dy = -\frac{1}{|k|^{n+1}n!}\int_x^\infty C_0'(y)\ C_0(y)^n\ dy \\ &= -\frac{1}{|k|^{n+1}(n+1)!}\int_x^\infty \frac{d}{dy}\big(C_0(y)^{n+1}\big)\ dy = \frac{1}{|k|^{n+1}(n+1)!}C_0(x)^{n+1}, \end{aligned}$$

which implies (3.14) for $n+1$. Since $C_0(x) \le \int |W|\ dy$, we deduce the convergence of f_n.

(ii) Note that since $f^\pm$ are analytic in the upper-half, so is $\mathcal{W}(f^-, f^+)$, which depends on k only. On the other hand,

$$\begin{aligned}\mathcal{W}(f^-, f^+)(+\infty) &= \mathcal{W}(\beta(k)f^+(\cdot,-k) + \alpha(k)f^+\big(\cdot), f^+(\cdot,k)\big)(+\infty) \\ &= \beta(k)\mathcal{W}\big(f^+(\cdot,-k), f^+(\cdot,k)\big)(+\infty) \\ &= \beta(k)\mathcal{W}(e^{-ikx}, e^{ikx})(+\infty) = 2ik\beta(k).\end{aligned}$$

From this we deduce that β is analytic. Similarly, since $\mathcal{W}\big(f^+(\cdot,k), f^+(\cdot,-k)\big)$ is analytic, and

$$\begin{aligned}\mathcal{W}\big(f^+(\cdot,k), f^+(\cdot,-k)\big)(+\infty) &= \mathcal{W}(\beta(k)f^+(\cdot,-k) + \alpha(k)f^+\big(\cdot), f^+(\cdot,-k)\big)(+\infty) \\ &= \alpha(k)\mathcal{W}\big(f^+(\cdot,k), f^+(\cdot,-k)\big)(+\infty) \\ &= \alpha(k)\mathcal{W}(e^{ikx}, e^{-ikx})(+\infty) = -2ik\alpha(k),\end{aligned}$$

we deduce that α is analytic. □

Note that when $k = i\ell$ is purely imaginary, then $k^2 = -\ell^2$, and since $f^\pm(x,k)$ satisfy equation (3.8), we learn that $f^\pm$ would serve as an eigenfunction associated with the eigenvalue $-\ell^2$ provided that $f^\pm$ is in L^2. Note that $f^-(x,k) \cong e^{\ell x}$ at $-\infty$, and $f^+(x,k) \cong e^{-\ell x}$ at ∞. To have both, we need $\beta(i\ell) = 0$ because of (3.12). Hence purely imaginary zeros of the analytic function β would yield eigenvalues in the discrete spectrum. These are the poles of $b(k)$ as we will see below. Since we already know that there are only finitely many eigenvalues and they are all situated in $(-\infty, 0)$, we deduce that the only singularities of the function b (equivalently, the only zeros of β) are situated on the line $i\mathbb{R}^+$. We are now ready to give a proof of Theorem 3.2.

Proof of Theorem 3.2 *(Step 1)* We set

$$F^\pm(x,\xi) = \frac{1}{2\pi} f^\pm(x,k)e^{-ik\xi}\ dk.$$

Note that since $f^\pm(x,k) \cong e^{\pm ikx}$, as $x \to \infty$, we learn $F^\pm(x,\xi) \cong \delta_0(x \mp \xi)$, as $x \to \infty$. This suggests writing $F^\pm(x,\xi) =: \delta_0(\xi \mp x) + E^\pm(x,\xi)\ d\xi$. Integrating both sides against $(2\pi)^{-1}e^{-ik\xi})$ yields the Wave Equation

$$F^\pm_{xx} - F^\pm_{\xi\xi} = WF^\pm. \tag{3.15}$$

Substituting $\delta_0(\xi \mp x) + E^\pm(x,\xi)\ d\xi$ for $F^\pm(x, d\xi)$ yields the equation

$$E^\pm_{xx}(x,\xi) - E^\pm_{\xi\xi}(x,\xi) = W(x)E^\pm(x,\xi) + \delta_0(\xi \mp x)W(x), \tag{3.16}$$

because $\delta_0(\xi \mp x) = \eta$ satisfies the Wave Equation $\eta_{xx} - \eta_{\xi\xi} = 0$. Some care is needed for the exact meaning of (3.16). For the simplicity of our presentation, let us assume that the potential W is of compact support $[-c_0, c_0]$ so that all $\cong$ at $\pm\infty$ can be replaced with $=$ outside the interval $[-c_0, c_0]$. Observe that $E^{\pm}(x,\xi) = 0$ when $\pm x \geq c_0$. Since the right-hand side (3.16) has a delta function, we guess that $E^{\pm}_x \pm E^{\pm}_\xi$ experiences a jump discontinuity along the line $\{(x,\xi) :\ \xi \mp x = 0\}$, so that $(\partial_x \mp \partial_\xi)(E_x \pm E_\xi)$ produces $\delta_0(\xi \mp x)W(x)$. Note that if

$$2z^{\pm} = \xi \pm x, \qquad H^{\pm}(z^+, z^-) = E^{\pm}(x,\xi) = E^{\pm}\left(z^+ - z^-, z^+ + z^-\right),$$

then when $H^{\pm}$ is twice differentiable,

$$H^{\pm}_{z^+} = E^{\pm}_x + E^{\pm}_\xi, \qquad H^{\pm}_{z^-} = -E^{\pm}_x + E^{\pm}_\xi, \qquad H^{\pm}_{z^+z^-} = -E^{\pm}_{xx} + E^{\pm}_{x\xi} - E^{\pm}_{\xi x} + E^{\pm}_{\xi\xi} = -E^{\pm}_{xx} + E^{\pm}_{\xi\xi}.$$

The discontinuity of $H^{\pm}_{z^{\pm}}$ occurs at $z^{\mp} = 0$. For example,

$$-E^{+}_{xx} + E^{+}_{\xi\xi} = H^{+}_{z^+z^-} + (H^{+}_{z^-}(z^+, 0+) - H_z(z^+, 0-))\delta_0(z^-).$$

From this and (3.16) we learn

$$\begin{aligned}-(H^{+}_{z^+}(z^+, 0+) - H_{z^+}(z^+, 0-))\delta_0(z^-) &= W(x)\delta_0(\xi - x) = W(z^+ - z^-)\delta_0(2z^-)\\ &= 2^{-1}W(z^+)2\delta_0(2z^-) = 2^{-1}W(z^+)\delta_0(z^-),\end{aligned}$$

which in turn implies

$$W(z^+) = -2(H_z(0+, z^+) - H_z(0-, z^+)). \tag{3.17}$$

Regarding x as the time variable, and treating WF^+ as a source, we may use $F^+(x,\xi) = \delta_0(x-\xi),\ x \geq c_0$ and D'Alambert's formula, to write

$$\begin{aligned}F^+(x,\xi) =& \frac{1}{2}\big(F^+(c_0, \xi - x + c_0) + F^+(c_0, \xi + x - c_0)\big) + \frac{1}{2}\int_{\xi+x-c_0}^{\xi-x+c_0} F^+_x(x,\zeta)\ d\zeta\\ &+ \frac{1}{2}\int_x^{c_0}\int_{\xi+x-c_0+\theta}^{\xi-x+c_0-\theta} (WF^+)(\theta,\zeta)\ d\zeta d\theta,\end{aligned}$$

for $x \leq c_0$. This formula is formal because $F^+(c_0,\xi) = \delta_{c_0}(\xi)$. Though we can approximate δ_{c_0} by a smooth function and write the analogous formula for the corresponding solution (it would not matter for the conclusion we will get in the end). We can use this formula to setup an iteration scheme for approximating F^+. For example, if $F^{+,n} \to F^+$ in large n limit, where $F^{+,n}$ is defined inductively by

$$\begin{aligned}F^{+,n+1}(x,\xi) =& \frac{1}{2}\big(F^{+,n}(c_0, \xi - x + c_0) + F^{+,n}(c_0, \xi + x - c_0)\big) + \frac{1}{2}\int_{\xi+x-c_0}^{\xi-x+c_0} F^{+,n}_x(x,\zeta)\ d\zeta\\ &+ \frac{1}{2}\int_x^{c_0}\int_{\xi+x-c_0+\theta}^{\xi-x+c_0-\theta} (WF^{+,n})(\theta,\zeta)\ d\zeta d\theta,\end{aligned}$$

for $x \le c_0$, starting from $F^{+,0}(x,\xi) = \delta_0(\xi - x)$. Inductively we can show that for $x \le c_0$, the support of $F^{+,n}$ is contained in $[x, 2c_0 - x]$. Hence the same is true F^+. As a consequence, the support the function E^+ is contained in the set

$$\big\{(x,\xi) : \ x \le c_0, \ \xi \in [x, 2c_0 - x]\big\}.$$

In particular $H^+_z(0+, z) = 0$. From this and (3.15) we deduce

$$W(z) = 2H^+_{z^+}(z^+, 0-). \tag{3.18}$$

Similarly, we can show that the support of E^- is contained in the set

$$\big\{(x,\xi) : \ x \ge -c_0, \ \xi \in [-2c_0 - x, x]\big\}.$$

In summary we have learned two important fact about F, the Fourier transform of the Jost's solution $f^\pm$:

- $F^\pm(x,\xi) = \delta_0(x \mp \xi) + E^\pm(x,\xi)$, and we can recover the potential W from the jump discontinuity of $E^\pm$ as in (3.16).
- The function $E^\pm$ is supported in the set $\{(x,\xi) : \ \pm(\xi - x) > 0\}$.

By Fourier Inversion Formula, we may write

$$\begin{aligned} f^+(x,k) = &\int_{-\infty}^{\infty} e^{ik\xi} F^+(x,\xi)\ d\xi = e^{\pm ikx} + \int_{-\infty}^{\infty} e^{ik\xi} E^+(x,\xi)\ d\xi \\ =& e^{\pm ikx} + \int_x^{\infty} e^{ik\xi} E^+(x,\xi)\ d\xi, \end{aligned} \tag{3.19}$$

$$f^-(x,k) = = e^{-ikx} + \int_{-\infty}^{x} e^{ik\xi} E^-(x,\xi)\ d\xi. \tag{3.20}$$

(Step 2) We next define

$$\Phi(x,\xi) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik\xi} \varphi(x,k)\ dk.$$

(Note that instead of $e^{-ik\xi}$, we are integrating against $e^{ik\xi}$.) From (3.12) we can relate Φ to $F^\pm$. For example,

$$\begin{aligned} \Phi(x,\xi) =& F^+(x,\xi) + \frac{1}{2\pi} \int A(k) f^+(x,k) e^{ik\xi}\ dk \\ =& F^+(x,\xi) + \frac{1}{(2\pi)^2} \int A(k_1) f^+(x,k_2) e^{ik_1\xi} e^{i(k_1-k_2)\zeta}\ d\zeta dk_1 dk_2 \\ =& F^+(x,\xi) + \frac{1}{(2\pi)^2} \int B_c(\xi+\zeta) F^+(x,\zeta)\ d\zeta \\ =& \delta_0(\xi - x) + E^+(x,\xi) + B_c(\xi + x) + \int_x^{\infty} B_c(\xi+\zeta) E^+(x,\zeta)\ d\zeta. \end{aligned} \tag{3.21}$$

Alternatively we can write

$$\Phi(x,\xi) = \frac{1}{2\pi}\int_{-\infty}^{\infty} b(k) f^-(x,k) e^{ik\xi}\ dk. \tag{3.22}$$

Note that the function $\varphi(x,k) = b(k)f^-(x,k)$ is analytic in the upper-half expect for the poles of b that are situated on the line $i\mathbb{R}^+$. Let us take a positively oriented contour γ that consists of the line segment $[-R,R]$, and a half circle C of radius R and center 0 in the upper-half plane. By the Residue Theorem

$$\frac{1}{2\pi}\int_C \varphi(x,k)e^{ik\xi}\ dk = i\sum_{j=1}^n Res(i\ell_j),$$

where the sum is over j with $-\ell_j^2$ representing the j-th eigenvalue, and $Res(i\ell_j)$ is the residue of $\varphi(x,k)e^{ik\xi}$ at $k = i\ell_j$. We can show that the circular part of C does not contribute. As a result,

$$\Phi(x,\xi) = i\sum_{j=1}^n Res(i\ell_j). \tag{3.23}$$

(Step 3) We wish to calculate $Res(i\ell_j)$. We certainly have

$$\begin{aligned}
Res(i\ell_j) =& \lim_{k\to i\ell_j}(k-i\ell_j)\varphi(x,k)e^{ik\xi} = \lim_{k\to i\ell_j}(k-i\ell_j)b(k)f^-(x,k)e^{ik\xi} \\
=& f^-(x,i\ell_j)e^{-k\ell_j}\lim_{k\to i\ell_j}(k-i\ell_j)\beta(k)^{-1} = f^-(x,i\ell_j)e^{-k\ell_j}\beta'(i\ell_j)^{-1},
\end{aligned}$$

where $\beta = b^{-1}$. On the other hand,

$$\mathcal{W}(f^+,f^-) = \mathcal{W}\big(f^+,\beta\bar{f}^+ + \alpha f^+\big) = \beta\mathcal{W}\big(f^+,\bar{f}^+\big) = \beta\mathcal{W}\big(f^+,\bar{f}^+\big)(\infty) = -2ik\beta(k).$$

Differentiating both sides with respect to k yields

$$-\big(2i\beta(k) + 2ik\beta'(k)\big) = \frac{d}{dk}\mathcal{W}(f^+,f^-) = \mathcal{W}(\dot{f}^+,f^-) + \mathcal{W}(f^+,\dot{f}^-), \tag{3.24}$$

where by $\dot{g}$ we mean g'. From (3.11) we deduce

$$\dot{f}^{\pm}_{xx} + k^2\dot{f}^{\pm} + 2kf^{\pm} = W\dot{f}^{\pm}.$$

This and (3.11) again yield

$$\begin{aligned}
\frac{d}{dx}\mathcal{W}(f^+,\dot{f}^-) &= \frac{d}{dx}\det\begin{bmatrix} f^+ & \dot{f}^- \\ f^+_x & \dot{f}^-_x\end{bmatrix} = \det\begin{bmatrix} f^+ & \dot{f}^- \\ f^+_{xx} & \dot{f}^-_{xx}\end{bmatrix} \\
&= \det\begin{bmatrix} f^+ & \dot{f}^- \\ (W-k^2)f^+ & (W-k^2)\dot{f}^- - 2kf^-\end{bmatrix} = -2kf^-f^+.
\end{aligned}$$

Similarly
$$\frac{d}{dx}\mathcal{W}(\dot{f}^+, f^-) = 2kf^-f^+.$$
Equivalently,
$$\mathcal{W}(f^+, \dot{f}^-)(x) - \mathcal{W}(f^+, \dot{f}^-)(-\infty) = -2\int_{-\infty}^{x} kf^-f^+ \, dy,$$
$$\mathcal{W}(\dot{f}^+, f^-)(x) - \mathcal{W}(\dot{f}^+, f^-)(+\infty) = -2\int_{x}^{+\infty} kf^-f^+ \, dy.$$
Adding these equations up yields
$$2\int_{-\infty}^{\infty} kf^-(y,k)f^+(y,k)\, dy = \mathcal{W}(\dot{f}^-, f^+)(+\infty) + \mathcal{W}(\dot{f}^-, f^+)(-\infty) - \big[\mathcal{W}(\dot{f}^-, f^+) + \mathcal{W}(\dot{f}^-, f^+)\big](x).$$
Imagine that we can show
$$\mathcal{W}(\dot{f}^-, f^+)(+\infty) + \mathcal{W}(\dot{f}^-, f^+)(-\infty) = 0, \tag{3.25}$$
so that
$$2\int_{-\infty}^{\infty} kf^-(y,k)f^+(y,k)\, dy = -\big[\mathcal{W}(\dot{f}^-, f^+) + \mathcal{W}(\dot{f}^-, f^+)\big](x).$$
Note that the right-hand side is independent of x, because the left-hand side of (3.24) is independent of x.) Then when$k = \bar{k} = -i\ell$, with $\bar{k}^2$ an eigenvalue, we have $\beta(\bar{k}) = 0$, and (3.24) yields
$$2i\bar{k}\beta'(\bar{k}) = -\big[\mathcal{W}(\dot{f}^-, f^+) + \mathcal{W}(\dot{f}^-, f^+)\big](x, \bar{k}) = 2\bar{k}\int_{-\infty}^{\infty} f^-(y,\bar{k})f^+(y,\bar{k})\, dy.$$
Hence
$$i\beta'(i\ell) = \int_{-\infty}^{\infty} f^-(y,i\ell)f^+(y,i\ell)\, dy = \int_{-\infty}^{\infty} \alpha(i\ell)f^+(y,i\ell)^2\, dy.$$
Recall that $f^+(x, i\ell_j)$ is the bound state associated with $-\ell_j^2$:
$$\psi(x,\ell) = a(\ell_j)f^+(x, i\ell_j).$$
Since $\int \psi^2 \, dy = 1$, we learn
$$\int f^+(y,k_0)^2\, dy = a(\ell_j)^{-2}.$$
As a result,
$$iRes(i\ell_j) = ia(\ell_j)^2 f^-(x, i\ell_j)e^{-k\ell_j}A()^{-1}b(k_0) = ia(\ell_j)^2 f^+(x, i\ell_j)e^{-k\ell_j}.$$

$\square$

3.2 Fredholm-Volterra Integral Equation

For our IST, we need to solve (3.6), which is an example of a *Fredholm-Volterra Integral Equation*. More generally, we wish to find a function $E(\xi)$ that solve the equation

$$E(\xi) + \int K(\xi, \zeta)E(\zeta)\ d\zeta = C(\xi). \tag{3.26}$$

For our application, $\lambda = 1,\ K(\xi, \zeta) = B(\xi + \zeta)\mathbb{1}(\zeta \geq x),\ C(\xi) = -B(\xi + x)$. Writing

$$\mathcal{K}E(\xi) = \int K(\xi, \zeta)E(\zeta)\ d\zeta,$$

we wish to invert the operator $I + \mathcal{K}$. An integral operator $\mathcal{K}$ is an infinite dimensional analog of a matrix multiplication where the sums are replace with integrals. According to the *Fredholm Theory*, one can define the determinant of $I + \mathcal{K}$ under some natural conditions on K. Indeed, if $\mathcal{K}$ is symmetric with eigenvalues $\{\lambda_i :\ i \in \mathbb{N}\}$, then a candidate for the determinant $\det(I + \mathcal{K})$ is simply $\prod_i(1 + \lambda_i)$, which is well-defined when $\sum_i |\lambda_i| < \infty$. When such a condition is met, we say that the operator $I + \mathcal{K}$ is of the *trace class*. Moreover, the operator $I + \mathcal{K}$ is invertible iff $\det(I + \mathcal{K}) \neq 0$, and $(I + \mathcal{K})^{-1}$ can be represented by a formula that is a generalization of the Cramer's formula for the inverse of a matrix. Before presenting the work of Fredholm, let us review some basic facts about matrices:

(i) Given a $d \times d$ matrix $A = [a_{ij}]_{i,j=1}^d$, recall that its minor $M(A) = [M_{ij}]_{i,j=1}^d$ is the matrix with $M_{ij} = \det \hat{A}_{ij}$, where $\hat{A}_{ij}$ is the $(d-1) \times (d-1)$ matrix that is obtain from A by removing its i-th row and j-column. The cofactor $Cof(A) = [C_{ij}]_{i,j=1}^d$ is the matrix with $C_{ij} = (-1)^{i+j}M_{ij}$. The transpose of $Cof(A)$ is the adjoint of A and is denoted by $Adj(A)$. According to Cramer's formula $A^{-1} = (\det A)^{-1}Adj(A)$. If we regard $\det : \mathbb{R}^{d\times d} \to \mathbb{R}^{d\times d}$, then

$$\nabla \det(A) = Cof(A). \tag{3.27}$$

Here we are using a matrix notation to represent $\nabla \det(A)$ (as opposed to a vector in $\mathbb{R}^{d^2}$). The proof of (3.27) is an immediate consequence of

$$\det A = \sum_j a_{ij}C_{ij},$$

which implies that $\partial \det / \partial a_{ij}(A) = C_{ij}$, because C_{ij} is independent of a_{ij}. The equation (3.27) allows us to rewrite Cramer's formula as

$$\left[A^{-1}\right]^t = \nabla \log \det(A). \tag{3.28}$$

The moral of this formula is that if we have a good candidate for the determinant in an infinite dimensional setting, we might be able to use it to find a formula for the inverse.

(ii) We next assume that $A = I + K$ for a $d \times d$ matrix $K = [k_{ij}]_{i,j=1}^{d}$. Our hope is that the formula (3.28) in terms of K has a chance to be meaningful even when $d \to \infty$. First we study $\det(I+K)$. Let us write $[d]$ for the set $\{1, \dots, d\}$. Given $\mathbf{a} = (a_1, \dots, a_r)$, $\mathbf{b} = (b_1, \dots, b_r)$, and and $s \in [d]$, we set

$$K_{\mathbf{a}} := [K_{a_i a_j}]_{i,j=1}^{r}, \qquad K_{\mathbf{a},\mathbf{b}} := [K_{a_i b_j}]_{i,j=1}^{r}.$$

We have

$$\Delta(K) := \det(I+K) = 1 + \sum_{r=1}^{d} \sum_{1 \le a_1 < \dots < a_r \le d} \det \left[k_{a_s a_t}\right]_{s,t=1}^{r} = 1 + \sum_{r=1}^{d} \frac{1}{r!} \sum_{a_1, \dots, a_r \in [d]} \det \left[k_{a_s a_t}\right]_{s,t=1}^{r}.$$

Here we have the facts that if $a_1, \dots, a_r$ are not distinct, then the determinant is 0, and that a permutation of $a_1, \dots, a_r$ does not alter the corresponding determinant. We also define $R = [R_{ij}]$, with

$$\begin{aligned}
R_{ij} :=& k_{ij} + \sum_{r=1}^{d} \sum_{1 \le a_1 < \dots < a_r \le d} \det K_{(i,a_1,\dots,a_r),(j,a_1,\dots,a_r)} \\
=& k_{ij} + \sum_{r=1}^{d} \sum_{1 \le a_1 < \dots < a_r \le d} k_{ij} \det K_{(a_1,\dots,a_r)} \\
&+ \sum_{r=1}^{d} \sum_{s=1}^{r} \sum_{1 \le a_1 < \dots < a_r \le d} (-1)^s k_{ia_s} \det K_{(a_1,\dots,a_r),(j,a_1,\dots,a_{s-1},a_{s+1},\dots,a_r)} \\
=& k_{ij} + k_{ij} \sum_{r=1}^{d} \sum_{1 \le a_1 < \dots < a_r \le d} \det K_{(a_1,\dots,a_r)} \\
&- \sum_{r=1}^{d} \sum_{s=1}^{r} \sum_{1 \le a_1 < \dots < a_r \le d} k_{ia_s} \det K_{(a_s,a_1,\dots,a_{s-1},a_{s+1},\dots,a_r),(j,a_1,\dots,a_{s-1},a_{s+1},\dots,a_r)} \\
=& k_{ij}\Delta(K) - (KR)_{ij}.
\end{aligned}$$

In other words, $R = K(\Delta(K)I - R)$. As a result,

$$(I+K)^{-1} = K - \Delta(K)^{-1}R. \tag{3.29}$$

□

Fredholm observed that the operator R has an extension to infinite dimension, namely the integral operator associated with a kernel K, we may define an operator $\mathcal{R}$ associated with a kernel R the is defined by

$$R(x,y) = K(x,y) + \sum_{r=1}^{\infty} \int \cdots \int_{x_1<\cdots<x_r} \det K_{(x,x_1,\ldots,x_k),(y,x_1,\ldots,x_k)}\ dx_1 \ldots dx_k. \tag{3.30}$$

As before, if $\mathbf{a} = (a_1, \ldots, a_\ell)$, $\mathbf{b} = (b_1, \ldots, b_\ell)$, then by $K_{\mathbf{a},\mathbf{b}}$ we mean the matrix

$$[K(a_i, b_j)]_{i,j=1}^{\ell}.$$

Moreover, the formula (3.29) holds provided that $\Delta(K) \neq 0$, with

$$\Delta(K) = 1 + \sum_{r=1}^{\infty} \int \cdots \int_{x_1<\cdots<x_r} \det K_{(x_1,\ldots,x_k),(x_1,\ldots,x_k)}\ dx_1 \ldots dx_k. \tag{3.31}$$

3.3 Exercise

(i) Verify (3.10), and show directly that $f^{\pm}$ of (3.9) satisfy (3.8).

(ii) Let W be a potential function such that $A^W(k) = 0$ (reflectionless) for all k, and $\sigma_d(\mathcal{L}^W) = \{-\ell^2\}$ consists of a single eigenvalue. Use Theorem 3.2 to find the form of W. (*Hint:* Search for a solution of (3.6) of the form $E(x,\xi) = M(x)e^{-\ell\xi}$.)

(iii) Let W be a potential function such that $A^W(k) = 0$ (reflectionless) for all k, and $\sigma_d(\mathcal{L}^W) = \{-\ell_1^2, -\ell_2^2\}$ consists of exactly two eigenvalues. Use Theorem 3.2 to find the form of W. (*Hint:* Search for a solution of (3.6) of the form $E(x,\xi) = M_1(x)e^{-\ell_1\xi} + M_2(x)e^{-\ell_2\xi}$.)

4 Burgers Equation and Hamilton-Jacobi PDE

Hamilton-Jacobi equation (in short HJE) is a PDE of the form

$$u_t + H(x, u_x, t) = 0, \quad u(x, 0) = g(x). \tag{4.1}$$

Here $H : \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}$ is known as the Hamiltonian function, and $u : \mathbb{R}^d \times [0, \infty) \to \mathbb{R}$ is a function of the position x and time t. Here are two applications of HJEs;

(i) *(Classical Mechanics)* If $x = (x_1, \dots, x_d)$ and $p = (p_1, \dots, p_d)$ represent the positions and momenta of moving bodies in a system, then the evolution of (x, p) is given by a Hamiltonian ODE of the form

$$\dot{x} = H_p(x, p, t), \quad \dot{p} = -H_x(x, p, t), \tag{4.2}$$

where $H(x, p, t)$ represents the total energy of the pair (x, p) at time t. The system (4.2) is completely integrable, if there exists a change of coordinates $(x, p) \mapsto (X, P)$ such that the system (4.2) in new coordinates reads as

$$\dot{X} = \nabla \bar{H}(P), \quad \dot{P} = 0. \tag{4.3}$$

In other words, in (X, P) the system is a Hamiltonian ODE associated with the Hamiltonian function $\bar{H}$ that is independent of X. The momentum P is conserved in (4.3). To guarantee that our change of coordinates preserves the Hamiltonian form of our system, the map $(x, p) \mapsto (X, P)$ must be *canonical (symplectic)*. For canonical maps we can find a *generating function* S such that

$$(P \cdot dX - H dt) - (p \cdot dx - \bar{H} dt) = dS.$$

We may rewrite this as

$$X \cdot dP + p \cdot dx - (H - \bar{H})dt = du,$$

where $w = X \cdot P - S$. Regarding w as a function of (x, t, P), we can assert $w_x = p,\ w_P = X,\ w_t = \bar{H} - H$. Hence,

$$w_t(x, t; P) + H\big(x, t, w_x(x, t; P)\big) = \bar{H}(P),$$

which is a HJE for u, for every P. Note that the volume measure $dX_1 \wedge \dots \wedge dX_d$ is invariant for the flow of the first equation of(4.3) for fixed P. Since $X = w_P$, we can write

$$dX_1 \wedge \dots \wedge dX_d = \det(w_{Px})\ dx_1 \wedge \dots \wedge dx_d.$$

This gives an invariant measure for the flow of the ODE

$$\dot{x} = H_p\big(x, t, w_x(x, t; P)\big),$$

for every P.

(ii) *(Classical Mechanics)* When the Hamiltonian function $H(x,t,p)$ is convex in the momentum variable, then we can define the Lagrangian function $L(x,v,t)$ by

$$H_p(x,t,p) = v \quad \Leftrightarrow \quad L_v(x,t,v) = p. \tag{4.4}$$

The action of a path $x : [s,t] \to \mathbb{R}^d$ is defined by

$$A(x(\cdot),s,t) = \int_s^t L\big(x(\theta),\theta,\dot{x}(\theta)\big)\; d\theta.$$

Minimizing the action yields the function

$$w(x,t) = w(x,t;y,s) = \inf\left\{A(x(\cdot),s,t):\; x \in C^1([s,t],\mathbb{R}^d),\; x(s)=y, x(t)=x\right\}.$$

It turns out that w, as a function of (x,t), satisfies the HJE (4.1) so long as $t > s$. In fact the minimizing path $x(\cdot)$ solves the Hamiltonian ODE (4.2). This is a solution that additionally satisfies

$$p(t) = w_x(x(t),t). \tag{4.5}$$

In other words, the pair $(x(t),p(t))$ lies on the graph of w_x.

(iii) *(Quantum Mechanics)* The wave function $\psi : \mathbb{R}^d \times [0,\infty) \to \mathbb{C}$ in quantum mechanics satisfies the Schrödinger Equation

$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\Delta\psi + V\psi. \tag{4.6}$$

If we write $\psi = ae^{i\frac{u}{\hbar}}$, for a pair of function $a,u : \mathbb{R}^d \times [0,\infty) \to \mathbb{R}$, then $\rho = |\psi|^2 = a^2$ is the probability density for the position. Moreover,

$$\begin{aligned}
\frac{\psi_t}{\psi} &= \frac{a_t}{a} + \frac{i}{\hbar}u_t, \qquad \psi = a_x e^{i\frac{u}{\hbar}} + \frac{i}{\hbar}u_x\psi,\\
\frac{\Delta\psi}{\psi} &= \frac{\Delta a}{a} + 2\frac{i}{\hbar}\frac{a_x\cdot u_x}{a} + \frac{i}{\hbar}\Delta u - \frac{1}{\hbar^2}|u_x|^2.
\end{aligned}$$

In terms of (a,u), the equation (4.6) is equivalent

$$u_t + \frac{1}{2m}|u_x|^2 + V = \frac{\hbar^2}{2m}\frac{\Delta a}{a}, \tag{4.7}$$

$$\rho_t + \nabla\cdot\Big(\frac{\rho}{m}u_x\Big) = 0. \tag{4.8}$$

If we replace the right-hand side of (4.7) with 0, then u satisfies a HJE associated with the Hamiltonian function

$$H(x,t,p) = \frac{1}{2m}|p|^2 + V(x,t), \tag{4.9}$$

and the corresponding wave function yields a *semi-classical approximation* of quantum mechanics. On account of (4.5), the term $m^{-1}\nabla u$ represents the velocity, and the equation (4.9) is the continuity (Liouville) equation for the probability density. If we take a family of solutions $u(x,t;P)$ of the HJE

$$u_t + \frac{1}{2m}|u_x|^2 + V = 0,$$

then $\rho = \det u_{xP}$ provides a solution to (4.8) as in our discussion in **(i)**. This in quantum mechanics is known as Van Vleck's theorem. □

In the third application, we learned how to turn the Schrödinder equation (4.6) to a pair of equations (4.7) and (4.8). A similar idea of Cole and Hopf would allow us to go from a diffusion equation to a variant of (4.7), namely the *viscous HJE*

$$u_t + \frac{1}{2m}|u_x|^2 + V = \alpha\Delta u, \qquad u(x,0) = g(x). \tag{4.10}$$

More precisely if we set $\psi = e^{-\frac{u}{2m\alpha}}$, then

$$\frac{\psi_t}{\psi} = -\frac{u_t}{2m\alpha}, \qquad \nabla\psi = -\frac{u_x}{2m\alpha}\ \psi, \qquad \frac{\Delta\psi}{\psi} = -\frac{\Delta u}{2m\alpha} + \frac{|u_x|^2}{(2m\alpha)^2} = \frac{1}{2m\alpha^2}\left(-\alpha\Delta u + \frac{1}{2m}|u_x|^2\right).$$

This in turn implies

$$u_t + \frac{1}{2m}|u_x|^2 + V - \alpha\Delta u = -2m\alpha\left[\frac{1}{\psi}\left(\psi_t - \alpha\Delta\psi - \frac{1}{2m\alpha}V\psi\right)\right]. \tag{4.11}$$

In particular, if u satisfies (4.11), then ψ satisfies the diffusion equation

$$\psi_t = \alpha\Delta\psi + (2m\alpha)^{-1}\ V\psi, \quad \psi(x,0) = e^{-\frac{g}{2m\alpha}}. \tag{4.12}$$

Based on our experience with (4.12), we can study the behavior of (4.11) as $\alpha \to 0$. As a warm-up, let use first assume that $V = 0$. In this case, $u = u^\alpha$ is given by

$$u^\alpha(x,t) = -2m\alpha\ \log \int ((4\pi\alpha t)^{-d/2} \exp\left[-(2m\alpha)^{-1}\left(g(y) + \frac{m|x-y|^2}{2t}\right)\right]\ dy. \tag{4.13}$$

Let us write $\varepsilon = 2m\alpha$, and assume that α (equivalently ε) is small. If we assume that (for example) g is a Lipschitz function, then

$$g(y) + \frac{m|x-y|^2}{2t} \geq g(x) - c|x-y| + \frac{m|x-y|^2}{2t} \geq g(x) - \frac{tc^2}{2m} + \frac{m}{2t}\left[|x-y| - \frac{ct}{m}\right]^2,$$

which is large of order $O(|y|^2)$, when $|y|$ is large. (Here c is the Lipschitz constant of g.) From this, we learn

$$\min_y \left(g(y) + \frac{m|x-y|^2}{2t}\right) \geq g(x) - \frac{tc^2}{2m} > -\infty,$$

and that large y's contribute very little to the integral (4.13). From this, it is not hard to deduce

$$\lim_{\alpha \to 0} u^\alpha(x,t) = w(x,t) = \min_y \left(g(y) + \frac{m|x-y|^2}{2t}\right).$$

In summary, we have a candidate for the (unique) solution of the PDE

$$w_t + \frac{1}{2m}|w_x|^2 = 0, \qquad u(x,0) = g(x), \tag{4.14}$$

namely

$$w(x,t) = \min_y \left(g(y) + \frac{m|x-y|^2}{2t}\right). \tag{4.15}$$

We now turn our attention to the equation (4.11) for general V. We already know that by the Feynman-Kac formula, the solution $u = u^\alpha$ can be expressed as

$$u^\alpha(x,t) = -2m\alpha \ \log \mathbb{E} \exp\left[-(2m\alpha)^{-1}\left(g\big(x + \sqrt{2\alpha}B(t)\big) + \int_0^t V\big(x + \sqrt{2\alpha}B(s), s\big)\ ds\right)\right].$$

As our formula right after (2.40) suggests, the right-hand side can be interpreted as

$$-\varepsilon\ \log \int Z([0,t])^{-1} \exp\left[-\varepsilon^{-1}\left(g(y(t)) + \int_0^t \left(\frac{m}{2}|\dot{y}(s)|^2 - V(y(s),s)\right)\ ds\right)\right] \mathcal{D}(dy(\cdot)),$$

where $\varepsilon = 2m\alpha$, and $y(t) = x + \sqrt{2\alpha}B(t)$. This suggests that the solution w of the PDE

$$w_t + \frac{1}{2m}|w_x|^2 + V = 0, \qquad u(x,0) = g(x), \tag{4.16}$$

has a representation as

$$w(x,t) = \inf\left\{g(y(t)) + \int_0^t L(y(s), s, \dot{y}(s))\ ds :\ y(0) = x,\ y \in C^1([0,t];\mathbb{R}^d)\right\}. \tag{4.17}$$

where $L(x,t,v) = \frac{m}{2}|v|^2 - V(x,t)$. If we set $z(s) = y(t-s)$, then (4.17) reads as

$$w(x,t) = \inf\left\{ g(z(0)) + \int_0^t L(z(s), s, \dot{z}(s))\ ds :\ z(t) = x,\ z \in C^1([0,t];\mathbb{R}^d) \right\}. \tag{4.18}$$

Indeed this formula offers a solution to (4.1) whenever H is convex in p, and L is the Legendre transform of H:

$$L(x,t,v) = \sup_p \big(v \cdot p - H(x,t,p)\big). \tag{4.19}$$

Note that at the maximizing $p = p(x,t,v)$, we have $H_p(x,t,p) = v$, and

$$\begin{aligned} L_v(x,t,v) &= \big(v \cdot p(x,t,v) - H(x,t,p(x,t,v))\big)_v \\ &= \big(v \cdot p - H(x,t,p)\big)_p\ p_v(x,t,v) + p(x,t,v) = p(x,t,v), \end{aligned}$$

which is consistent with (4.4).

Let us study the minimizing path $z(s) = z(s;x)$ in (4.18). Define

$$\Gamma(a) = g(a(0)) + \int_0^t L(a(s), s, \dot{a}(s))\ ds.$$

Given $w \in C^1$ with $w(t) = 0$, set $\varphi(\tau) = \Gamma(z + \tau w)$. We have

$$\begin{aligned} 0 =& \dot{\varphi}(0) = \nabla g(z(0)) \cdot w(0) + \int_0^t \big[L_x(z(s), s, \dot{z}(s)) \cdot w(s) + L_v(z(s), s, \dot{z}(s)) \cdot \dot{w}(s)\big]\ ds \\ =& \big[\nabla g(z(0)) - L_v(z(0), 0, \dot{z}(0))\big] \cdot w(0) + \int_0^t \left[L_x(z(s), s, \dot{z}(s)) = \frac{d}{ds}\big(L_v(z(s), s, \dot{z}(s))\big)\right] \cdot w(s)\ ds. \end{aligned}$$

As we vary w, we deduce

$$\nabla g(z(0)) = L_v(z(0), 0, \dot{z}(0)), \qquad \frac{d}{ds}\big(L_v(z(s), s, \dot{z}(s))\big) = L_x(z(s), s, \dot{z}(s)). \tag{4.20}$$

We may use these to evaluate w_x:

$$\begin{aligned} w_x(x,t) =& \frac{\partial}{\partial x}\left[g(z(0;x)) + \int_0^t L(z(s;x), s, z_s(s;x))\ ds\right] \\ =& \nabla g(z(0;x)) \cdot z_x(0;x) \\ &+ \int_0^t \big[L_x(z(s;x), s, z_s(s;x)) \cdot z_x(s;x) + L_v(z(s;x), s, z_s(s;x)) \cdot z_{sx}(s;x)\big]\ ds \\ =& \big[\nabla g(z(0;x)) - L_v(z(0;x), 0, \dot{z}(0;x)) \cdot z_x(0;x) + L_v(z(t;x), t, z(t;x)) \\ &+ \int_0^t \left[L_x(z(s;x), s, z_s(s;x)) - \frac{d}{ds}\big(L_v(z(s), s, \dot{z}(s))\big)\right] \cdot z_x(s;x)\ ds \\ =& L_v(z(t;x), t, \dot{z}(t;x)) = L_v(x, t, \dot{z}(t;x)). \end{aligned}$$

where we have used $z_x(t;x) = id$ for the second equality. Since the minimizing $z(s;x)$ is also a minimizer at earlier times i.e.

$$s_1 < s_2 < t \quad \Longrightarrow \quad z\big(s_1; z(s_2;x), s_2\big) = z(s_1;x,t),$$

we learn

$$w_x\big(z(s;x,t),s\big) = L_v\big(z(s;x,t),s,\dot{z}(s;x,t)\big). \tag{4.21}$$

Also, if we write $x(s) = z(s;x,t),\ p(s) = L_v(x(s),s,\dot{x}(s))$, then (x,s) satisfies (4.2). From (4.4), we certainly have $\dot{x}(s) = H_p(x(s),s,p(s))$. On the other hand,, from

$$L(x,t,v) = v \cdot p(x,t,v) - H(x,t,p(x,t,v)),$$

we deduce

$$L_x(x,t,v) = \big(v - H_p(x,t,p(x,t,v))\big)\cdot p_x(x,t,v) - H_x(x,t,p(x,t,v)) = -H_x(x,t,p(x,t,v)).$$

This and the second equation in (4.20) imply that $\dot{p}(s) = -H_x(x(s),s,p(s))$.

In the above calculation, we assume that there exists a unique minimizer. When there is more that one minimizer, w is not differentiable at (x,t). Note that if $\rho = w_x$, then ρ satisfies

$$\rho_t + H(x,t,\rho)_x = 0. \tag{4.22}$$

We already have a representation for ρ in terms of the minimizing path $z(\cdot;x,t)$:

$$\rho(x,t) = L_v\big(x,t,\dot{z}(t;x,t)\big). \tag{4.23}$$

When there more than one minimizers, $\rho(x,t)$ is discontinuous. When $d = 1$, and H is of the form (4.9), the corresponding PDE, namely

$$\rho_t + m^{-1}\rho\rho_x = f, \tag{4.24}$$

is known as the *forced Burgers' equation*. Here $f = -V_x$ represents the force.

Remark 4.1 A rigorous derivation of (4.17) from the Feynman-Kac's formula of u^α can be carried out with the aid of the so-called *Large Deviation Theory*. More specifically a large deviation principle holds for $\sqrt{2\alpha}B$ by a result of Schilder. This and the celebrated Varadhan's lemma can be used to derive (4.17). See for example [R] for details. □

4.1 Exercise

(i) Prove that for any continuous function h, and any ℓ,

$$\lim_{\varepsilon \to 0} \varepsilon \log \int_{|x| \le \ell} e^{-\frac{1}{\varepsilon} h(x)} \, dx = - \min_{|x| \le \ell} h(x).$$

(ii) Let L be a convex function. Show that the minimizing path $(z(s), s),\ s \in [0, t]$ in the variational problem

$$\min \left\{ \int_0^t L(\dot{z}(s)) \, ds : \ z(0) = a, \ z(t) = b \right\},$$

is the straight line connecting $(a, 0)$ to (b, t). *(Hint: Use Jensen's inequality.)*

(iii) Assume that the map $\Phi(x, p) = (X(x, p), P(x, p))$ is a canonical map with a generating function $w(x, P)$, so that $w_x(x, P) = p, \ w_P(x, P) = X$. Assume that the matrix

$$w_{xP} = [w_{x_i P_j}]_{i,j=1}^d,$$

is invertible. The function $P(x, p)$ may be defined implicitly by $w_x(x, P) = p$. Use this to find P_x and P_p in terms of the second derivatives of w. Verify that the matrix $P_p P_x^T$ is symmetric. (By A^T we mean the transpose of A.)

(iv) Let $P(x, t) = \big(P^1(x, t), \ldots, P^d(x, t)\big)$. Show that $\{P^i, P^j\} = 0$ for all i and j.

(v) Consider the viscous Burgers' equation

$$\rho_t + \rho \rho_x = \alpha \rho_{xx},$$

in dimension one. Find solutions of the form $\rho(x, t) = \varphi(x - vt)$ for a function φ that is decreasing, and $\varphi(\pm\infty) = \rho_\pm$, $\varphi'(\pm\infty) = 0$, where ρ_- and ρ_+ are two given constants. Show that such a solution exists if and only if $v = (\rho_- + \rho_+)/2$.

5 Completely Integrable Hamiltonian PDEs

In Chapter 2, we discussed Hamiltonian ODEs. In this chapter we discuss two examples of completely integrable Hamiltonian PDEs. For this, we first describe a robust generalization of Hamiltonian ODEs of the form (3.2). An infinite dimensional extension of our formalism would allow us to recast our two examples as Hamiltonian PDEs.

Observe that if we use complex numbers, we may regard a solution $z(t) = (x(t), p(t))$ of (3.2) as a path $z(t) = x(t) + ip(t)$ as a solution $\dot{z} = -i\nabla H(z, t)$. Also, if we set

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix},$$

then we can rewrite (3.2) as

$$\dot{z} = J\nabla H(z, t) =: X_{H(\cdot,t)}(t). \tag{5.1}$$

We refer to X_H as the *Hamiltonian vector field* associated with the Hamiltonian function H. We also write ϕ_t^H for the flow of the vector field X_H. Given any C^1 function $f : \mathbb{R}^{2d} \to \mathbb{R}$, we have

$$\frac{d}{dt} f(z(t)) = J\nabla H(z(t), t) \cdot \nabla f(z(t)) =: \{H(\cdot, t), f\}(z(t)). \tag{5.2}$$

We refer to $\{H, f\}$ as the *Poisson bracket* of H and f. If we set

$$\bar{\omega}(a, b) = Ja \cdot b, \tag{5.3}$$

then we always have

$$\{H, f\} = \bar{\omega}(X_H, X_f). \tag{5.4}$$

Recall that for a completely integrable Hamiltonian ODE, we can find a change of coordinates $(x, p) \mapsto (X, P)$ that turns (3.2) to (3.3). Since P is conserved for (3.3), we deduce that that each coordinate of $P(x, p)$ is conserved for (3.2). In other words $\{H, P_i\} = 0$ for $i = 1, \dots, d$. By Exercise **(v)** of Chapter 3 twe know that $\{P_i, P_j\} = 0$ for all i and j. In fact the converse is also true by a result of Liouville. More precisely, if we have d conserved functions $f_1, \dots, f_d$ such that $\{f_i, f_j\} = 0$ for $i, j \in \{1, \dots, d\}$, and the vectors $\nabla f_1, \dots, \nabla f_d$ are linearly independent at every point, then the ODE (3.2) is completely integrable.

Moreover, Poincare discovered that if $\gamma : [0, T] \to \mathbb{R}^{2d}$ is a closed curve, then

$$\int_{\phi_t^H(\gamma)} p \cdot dx = \int_\gamma p \cdot dx. \tag{5.5}$$

This invariance principle of Poincare is a fundamental property of Hamiltonian flows, and we extend our notation of Hamiltonian ODEs by replacing the one form $p \cdot dx$ with more general one forms.

Given a 1-form $\lambda := w(z) \cdot dz$, and its exterior derivative $\omega = d\lambda$, we have

$$\omega_z(a, b) = C(w)(z)a \cdot b,$$

where $C(w)$ is the curl of $w = (w^1, \dots, w^{2d})$:

$$C(w) = \left[w^j_{z_i} - w^i_{z_j}\right]^{2d}_{i,j=1}.$$

When $C(w)$ is invertible, we say that the form ω is *symplectic*. The associated Hamiltonian vector field and Poisson bracket are defined by

$$X_H = -C(w)^{-1}\nabla H, \qquad \{H, f\} = -C(w)^{-1}\nabla H \cdot \nabla f. \tag{5.6}$$

To explain the reason behind our definition, let us state and prove the analog of (5.5).

Proposition 5.1 . *Let γ be a closed curve and write ϕ^H_t for the flow of the Hamiltonian vector field X_H of* (5.6). *Then*

$$\int_{\phi^H_t(\gamma)} w(z) \cdot dz = \int_\gamma w(z) \cdot dz. \tag{5.7}$$

Proof Let us parametrize γ by a C^1 function $z : \mathbb{R} \to \mathbb{R}^{2d}$, which T-periodic. Write $z = (z^1, \dots, z^{2d})$, and define $z(\theta, t) = (\phi^H_t z)(\theta)$. We have

$$\begin{aligned}
\big(w(z) \cdot z_\theta\big)_t =& \frac{d}{dt}\sum_i w^i z^i_\theta = \sum_i \left(\frac{dw^i}{dt} z^i_\theta + w^i z^i_{t\theta}\right) = \sum_i \left(\frac{dw^i}{dt}\ z^i_\theta - \frac{dw^i}{d\theta}\ z^i_t\right) + (w \cdot z_t)_\theta \\
=& \sum_{i,j} w^i_{z^j}\left(z^j_t z^i_\theta - z^j_\theta z^i_t\right) + (w \cdot z_t)_\theta = -C(w) z_t \cdot z_\theta + (w \cdot z_t)_\theta \\
=& \nabla H(z) \cdot z_\theta + (w \cdot z_t)_\theta = \big(H(z) + w(z) \cdot z_t)_\theta.
\end{aligned}$$

As a result,

$$\frac{d}{dt}\int_0^T \big(w(z) \cdot z_\theta\big)\ d\theta = 0,$$

which implies (5.7). $\square$

We now explain how our formalism can be carried out in infinite dimension in the case of two examples.

(i) *(Nonlinear Schrödinger (NSL) equation)* NLS arises in various physical settings for the description of wave propagation in plasma and nonlinear optics. It also arises in quantum field theory as a mean field equation for a system of large number of bosons weakly interacting via a pair potential. The statistical dynamics of such a system is governed by the *Gross-Pitaevskii equation*

$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\Delta\psi + V\psi + \frac{4\pi\hbar^2 a_s}{2m}|\psi|^2\psi, \tag{5.8}$$

where a_s is a wave scattering length associated with the pair potential. Here V is the external potential, and $\frac{4\pi\hbar^2 a_s}{2m}|\psi|^2$ represents a statistical average of the pair potential (which is a multiple of the density $|\psi|^2$). Let us assume $V = 0$, and to simplify our notation, let us replace some of the constants by one. Nonlinear Schrödinger equation (NLS) is the PDE

$$i\psi_t = -\Delta\psi + \kappa|\psi|^{r-1}\psi. \tag{5.9}$$

This equation is equivalent to (5.8) when $r = 3$ (in the case of $V = 0$). We refer to (5.8) as the *defocusing NLS* (respectively *focusing NLS*) when $\kappa > 0$ (respectively $\kappa < 0$). If we write $\psi = q + ip$, then (5.9) can be rewritten as

$$\begin{aligned} q_t &= -\Delta p + \kappa|\psi|^{r-1}p, \\ p_t &= \Delta q - \kappa|\psi|^{r-1}q. \end{aligned} \tag{5.10}$$

To interpret (5.9) as a Hamiltonian PDE, we define two bilinear forms on $\mathcal{X} = L^2(\mathbb{R}^d)$ by

$$\begin{aligned} \langle\psi, \psi'\rangle &= \int Re(\psi\bar{\psi}')\ dx = \int (qq' + pp')\ dx, \\ \omega(\psi, \psi') &= \int Im(\psi\bar{\psi}')\ dx = \int (pq' - qp')\ dx, \end{aligned}$$

where $\psi = q + ip,\ \psi' = q' + ip'$. The form ω is a symplectic form and can be written as

$$\omega(\psi, \psi') = \langle J\psi, \psi'\rangle := -\langle i\psi, \psi'\rangle.$$

We define $\mathcal{H} : H^1 \to \mathbb{R}$, by

$$\mathcal{H}(\psi) = \int \left[\frac{1}{2}|\nabla\psi|^2 + \frac{\kappa}{r+1}|\psi(x)|^{r+1}\right]\ dx. \tag{5.11}$$

(For this to be well-defined, we assume that $r + 1 \le 2^* = 2d/(d-2)$ so that by Gagliardo-Nirenberg-Sobolev inequality, $\mathcal{H}(\psi) < \infty$ for every $\psi \in H^1$.) We note that in the defocusing case, the Hamiltonian $\mathcal{H}$ is convex and nonnegative. This is no longer the case in the focusing case. We can readily calculate the functional derivative of $\mathcal{H}$; given a C^2 functions ψ and ζ, the directional derivative of $\mathcal{H}$ at ψ, in the direction of ζ is defined as

$$\partial_\zeta \mathcal{H}(\psi) := \frac{d}{d\theta}\mathcal{H}(\psi+\theta\zeta)|_{\theta=0}.$$

The functional derivative of $\mathcal{H}$ with respect to the inner product $\langle\cdot,\cdot\rangle$ is defined to be the function $\partial H(\psi)$ such that

$$\partial_\zeta \mathcal{H}(\psi) = \langle \partial\mathcal{H}(\psi), \zeta\rangle.$$

We certainly have

$$\partial_\zeta \mathcal{H}(\psi) = \langle \nabla\psi, \nabla\zeta\rangle + \kappa\left\langle |\psi|^{r-1}\psi, \zeta\right\rangle.$$

After an integration by parts we deduce

$$\partial\mathcal{H}(\psi) = -\Delta\psi + \kappa|\psi|^{r-1}\psi. \tag{5.12}$$

From this we conclude that (5.9) can be written as

$$\psi_t = J\partial\mathcal{H}(\psi). \tag{5.13}$$

In accordance with Symplectic Geometry, we expect to have a Poincare-type invariance. More precisely, if we take a family of solutions $(\psi(x,t;\theta) = q(x,t;\theta) + ip(x,t;\theta) : \theta\in\mathbb{R})$ of NLS that is T-periodic in θ, then

$$\frac{d}{dt}\int_0^T\int p(x,t;\theta)q_\theta(x,t;\theta)\ dx\ d\theta = 0. \tag{5.14}$$

Indeed, from

$$\begin{aligned}\left(pq_\theta\right)_t &= p_t q_\theta + pq_{\theta t} = p_t q_\theta - p_\theta q_t + \left(pq_t\right)_\theta = Re(J\psi_t\bar{\psi}_\theta) + \left(pq_t\right)_\theta\\ &= -Re(\partial\mathcal{H}(\psi)\bar{\psi}_\theta) + \left(pq_t\right)_\theta = \left(pq_t - \mathcal{H}(\psi)\right)_\theta,\end{aligned}$$

we can deduce (5.14). This implies that if we take a family of solutions

$$(\psi(x,t;\theta_1,\theta_2) = q(x,t;\theta_1,\theta_2) + ip(x,t;\theta_1,\theta_2) : (\theta_1,\theta_2)\in U),$$

for a region U in the plane, then

$$\frac{d}{dt}\iint_U\int (p_{\theta_1}q_{\theta_2} - p_{\theta_2}q_{\theta_1})(x,t;\theta_1,\theta_2)\ dx\ d\theta_1\ d\theta_2 = 0,$$

by Green's theorem, because if

$$\alpha = \alpha(x,t;\cdot) = p\ q_{\theta_2}\ d\theta_2 + p\ q_{\theta_1}\ d\theta_1,$$

is regarded as a 1-form in $\mathbb{R}^2$, then

$$d\alpha = (p_{\theta_1}q_{\theta_2} - p_{\theta_2}q_{\theta_1})\ d\theta_1 \wedge\ d\theta_2.$$

Needless to say that the Hamiltonian $\mathcal{H}(\psi)$ is conserved for NLS solution. It turns out that the L^2 norm

$$\mathcal{M}(\psi) = \int |\psi(x)|^2\ dx,$$

is also conserved. This is an immediate consequence of (5.10). Zakharov and Shabat in 1972 showed that NLS equation is completely integrable in dimension one.

We can construct explicit traveling wave solutions to focusing NSL equation when $d = 1$. To ease the notion, we assume that $\kappa = -2$. Note that if $\psi(x,t)$ is a solution, so is $\hat{\psi}(x,t) = a\psi(ax, a^2t)$. As a warm-up, let us search for a stationary solution of the form $\psi(x,t) = ae^{ia^2t}f(ax)$, where f, and f' vanish at $\pm\infty$. Substituting this in

$$i\psi_t + \psi_{xx} + 2|\psi|^2\psi = 0,$$

yields $-f + f'' + 2f^3 = 0$. Multiplying both sides by $2f'$ yields $(f')^2 + f^4 - f^2 = 0$, which has a solution of the form $f(x) = \cosh^{-1}(x)$. More generally, we can find solutions of the form

$$\psi(x,t) = ae^{i(bx+ct)}f\big(a(x - x_0 - \sigma t)\big). \tag{5.15}$$

(ii) *(Korteweg–De Vries (KdV) equation)* The KdV equation describes the evolution of surface waves in narrow canals. If the surface wave elevation at position $x \in \mathbb{R}$ and time t is denotes by $V(x,t)$, then according to KdV equation, V satisfies

$$V_t + 6VV_x + V_{xxx} = 0. \tag{5.16}$$

More generally we may consider

$$V_t + \kappa\big(V^r\big)_x + V_{xxx} = 0. \tag{5.17}$$

We refer to (5.17) as KdV(r). To represent (5.17) as a Hamiltonian PDE, we use the standard inner product

$$\langle V, V'\rangle = \int_{\mathbb{R}} VV'\ dx.$$

We define a Hamiltonian function

$$\mathcal{H}(V) = \int \left(\frac{1}{2}\left(\frac{dV}{dx}\right)^2 - \frac{\kappa}{r+1}V^{r+1}\right)\ dx, \tag{5.18}$$

for a C^1 function $V : \mathbb{R} \to \mathbb{R}$, such that V and $\frac{dV}{dx}$ decays sufficiently fast at infinity. We can readily show

$$\partial\mathcal{H}(V) = -V_{xx} - \kappa V^r. \tag{5.19}$$

As a result, we may rewrite (5.17) as

$$V_t = \mathcal{J}\partial\mathcal{H}(V), \tag{5.20}$$

where $\mathcal{J} = \frac{d}{dx}$ is the differentiation operator. Note that if $\mathcal{J}(V) = W$, then $\int W\ dx = 0$. For such W, we define the inverse of $\mathcal{J}$ by

$$\mathcal{I}(W)(x) = \int_{-\infty}^{x} W(y)\ dy.$$

We also define

$$\omega(W, W') = \int \mathcal{I}(W)W'\ dx.$$

Evidently $\mathcal{H}(V)$ is conserved for solutions of (5.17). It is not hard to show that the mass and momentum

$$\mathcal{M}(V) = \int V\ dx, \quad \mathcal{P}(V) = \int V^2\ dx,$$

are also conserved. Kruskal, Zabusky, Mirua and Gardner discovered infinitely many conservation laws when $r = 3$ or 2. They also showed that these PDEs are completely integrable. Moreover, Mirua found a transformation that maps a solution of KdV(3) equation to a solution of KdV(2).

Given a function $\psi = e^w$, observe

$$w_x = \frac{\psi_x}{\psi}, \quad w_{xx} = \frac{\psi_{xx}}{\psi} - w_x^2, \quad w_t - 2w_x^3 + w_{xxx} = \frac{\psi_t}{\psi} - 2\big(w_{xx} + w_x^2\big)\frac{\psi_x}{\psi} + \big(w_{xx} + w_x^2\big)_x.$$

Hence we can write

$$\mathcal{L}(\psi) := -\psi_{xx} + V\psi = 0, \quad \mathcal{C}(w) := w_t - 2w_x^3 + w_{xxx} = \psi^{-1}\big(\psi_t - 2V\psi_x + V_x\psi\big), \tag{5.21}$$

where $V = -(w_{xx} + w_x^2)$ is the potential. The transformation $w \mapsto V$ was introduced by Miura to study KdV equation. Indeed

$$\begin{aligned}
-\big(V_t + 6VV_x + V_{xxx}\big) =& (w_{xx} + w_x^2)_t - 3\big[(w_{xx} + w_x^2)^2\big]_x + (w_{xx} + w_x^2)_{xxx} \\
=& (w_{txx} + 2w_x w_{tx}) - 3\big(w_{xx}^2 + 2w_{xx}w_x^2 + w_x^4\big)_x \\
& + (w_{xxxxx} + 2w_x w_{xxxx} + 6w_{xx}w_{xxx}) \\
=& (w_{txx} + 2w_x w_{tx}) - \big(3\big(w_{xx}^2\big)_x + (2w_x^3)_{xx} + 12w_x^3 w_{xx}\big) \\
& + (w_{xxxxx} + 2w_x w_{xxxx} + 6w_{xx}w_{xxx}) \\
=& \big(w_t - 2w_x^3 + w_{xxx}\big)_{xx} + 2w_x\big(w_t - 2w_x^3 + w_{xxx}\big)_x.
\end{aligned}$$

In summary,

$$V_t + 6VV_x + V_{xxx} = -\mathcal{C}(w)_{xx} - 2w_x\mathcal{C}(w)_x. \tag{5.22}$$

To develop a better understanding for (5.16), let us first examine its scaling property. In other words, assume that V is a solution, and given a scalar λ, set $W(x,t) = \lambda^\alpha V(\lambda x, \lambda^\beta t)$. We wish to find α and β so that W is also a solution. Since

$$W_t + 6WW_x + W_{xxx} = \lambda^{\alpha+\beta}V_t + 6\lambda^{2\alpha+1}VV_x + \lambda^{\alpha+3}V_{xxx},$$

we need $\alpha + \beta = 2\alpha + 1 = 3 + \alpha$, which leads to $\alpha = 2,\ \beta = 3$.

An early evidence of the complete integrabilty of KdV equation was observed by Kruskal and Zabusky in their simulations of solutions. To explain their discovery, let us first consider traveling wave solutions of (5.16). These are solutions of the form $V(x,t) = f(x - \sigma t)$ where f is a C^3 functions such that $f,\ f'$ and f'' are vanishing at $\pm\infty$. Substituting such a wave function V in (5.16) yields $-\sigma f' + 6ff' + f''' = 0$. Integrating once leads to $-\sigma f + 3f^2 + f'' = 0$. We now multiply both sides by $2f'$, and integrate again to arrive at the equation

$$-\sigma f^2 + 2f^3 + (f')^2 = 0.$$

If we assume $\sigma > 0$, then we can write

$$f(x) = \frac{\sigma}{2} g\left(\frac{\sqrt{\sigma}}{2}(x - x_0)\right),$$

with g satisfying $(g')^2 = 4g^2(1-g)$, which has a solution of the form

$$g(x) = \cosh^{-2}(x).$$

This yields traveling wave solutions of (5.16) that are known as *solitons*. When $x_0 = 0$, the corresponding solution

$$V^\sigma(x,t) = \frac{\sigma}{2} g\left(\frac{\sqrt{\sigma}}{2}(x - \sigma t)\right) = \sigma V^1\big(\sigma^{1/2}x, \sigma^{3/2}t\big),$$

has the scaling property that was discussed before. Kruskal and Zabusky observed the stability of solitons in the following sense: If the initial data has two solitons V^0 and V^1 of centers x_0 and x_1, and speeds σ_0 and σ_1 with $s_0 < s_1,\ x_0 >> x_1$, then after a nonlinear interaction, the two solitons emerge unscathed (with some shift of the traveled centers due to the interaction). $\square$

We now describe a robust method of Lax that offers a recipe for finding conservation laws for certain PDEs.

Proposition 5.2 **(i)** *Let $\mathcal{L}(t), \mathcal{A}(t) : \mathcal{X} \to \mathcal{X}$ be two families of operators on a Hilbert space $\mathcal{X}$ such that*

$$\dot{\mathcal{L}} = [\mathcal{A}, \mathcal{L}] := \mathcal{A}\mathcal{L} - \mathcal{L}\mathcal{A}. \tag{5.23}$$

Then

$$\mathcal{L}(t) = \mathcal{U}(t)\mathcal{L}(0)\mathcal{U}(t)^{-1}, \tag{5.24}$$

where $\mathcal{U}(t)$ defined by

$$\dot{\mathcal{U}}(t) = \mathcal{A}(t)\mathcal{U}(t), \quad \mathcal{U}(0) = id. \tag{5.25}$$

We refer to $(\mathcal{L}, \mathcal{A})$ as a Lax pair.

(ii) *For a Lax pair $(\mathcal{L}, \mathcal{A})$, the spectrum of the operator $\mathcal{L}(t)$ is independent of t. Moreover, if λ is an eigenvalue of $-\mathcal{L}$, and $\psi(0)$ is the corresponding eigenfunction of $-\mathcal{L}(0)$, then $\psi(t) = \mathcal{U}(t)\psi(0)$ is a corresponding eigenfunction of $-\mathcal{L}(t)$.*

(iii) *Let $\mathcal{L}, \mathcal{A} : \mathcal{X} \to \mathcal{X}$ be two linear operators. Assume that there exist functions $\lambda : \mathbb{R} \to \mathbb{R}$ and $\psi : \mathcal{X} \to \mathbb{R}$ such that*

$$\dot{\lambda} = 0, \quad -\mathcal{L}\psi = \lambda\psi, \quad \dot{\psi} = \mathcal{A}\psi. \tag{5.26}$$

Then $\big(\dot{\mathcal{L}} + [\mathcal{L}, \mathcal{A}]\big)\psi = 0$.

Proof(i) From (5.23) and (5.25) we learn

$$\begin{aligned}\frac{d}{dt}\big(\mathcal{U}(t)^{-1}\mathcal{L}(t)\mathcal{U}(t)\big) &= -\mathcal{U}(t)^{-1}\dot{\mathcal{U}}(t)\mathcal{U}(t)^{-1}\mathcal{L}(t)\mathcal{U}(t) + \mathcal{U}(t)^{-1}\dot{\mathcal{L}}(t)\mathcal{U}(t) + \mathcal{U}(t)^{-1}\mathcal{L}(t)\dot{\mathcal{U}}(t) \\ &= -\mathcal{U}(t)^{-1}\mathcal{A}(t)\mathcal{L}(t)\mathcal{U}(t) + \mathcal{U}(t)^{-1}\mathcal{L}(t)\mathcal{A}(t)\mathcal{U}(t) \\ &\quad + \mathcal{U}(t)^{-1}\big(\mathcal{A}(t)\mathcal{L}(t) - \mathcal{L}(t)\mathcal{A}(t)\big)\mathcal{U}(t) = 0.\end{aligned}$$

This immediately implies (5.24).

(iii) From differentiating $(\mathcal{L} + \lambda)\psi = 0$ we deduce

$$0 = \dot{\mathcal{L}}\psi + \mathcal{L}\dot{\psi} + \lambda\mathcal{A}\psi = \dot{\mathcal{L}}\psi + \mathcal{L}\mathcal{A}\psi + \mathcal{A}\mathcal{L}\psi = \big(\dot{\mathcal{L}} + [\mathcal{L}, \mathcal{A}]\big)\psi.$$

□

Example 5.2(i) We note that when $\mathcal{A}$ is anti-selfadjoint, then $\mathcal{U}$ is unitary because

$$\begin{aligned}\frac{d}{dt}\|\mathcal{U}(t)\psi\|^2 &= \langle\dot{\mathcal{U}}(t)\psi, \mathcal{U}(t)\psi\rangle + \langle\mathcal{U}(t)\psi, \dot{\mathcal{U}}(t)\psi\rangle \\ &= \langle\mathcal{A}(t)\mathcal{U}(t)\psi, \mathcal{U}(t)\psi\rangle + \langle\mathcal{U}(t)\psi, \mathcal{A}(t)\mathcal{U}(t)\psi\rangle = 0.\end{aligned}$$

Moreover if $\mathcal{L}(0)$ is self-adjoint, then $\mathcal{L}(t)$ is also self-adjoint by (5.24). Let $\mathcal{X}$ be the space of wave functions $\psi : \mathbb{R}^d \to \mathbb{C}$, and let

$$\mathcal{A} = \frac{i}{\hbar}\mathcal{H} = \frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\Delta + V\right),$$

for a potential $V(x)$. Then $U(t)^{-1} = U(-t) = e^{-\frac{i}{\hbar}t\mathcal{H}}$ is the fundamental solution of the Schrodinger's equation. The corresponding $\mathcal{L}(t)$ is the observable at time t, and (5.23) yields the evolution of the observable as in Heisenberg's description of quantum mechanics.

(ii) Given a function $V(x,t)$, and a constant c, set

$$\big(\mathcal{L}(t)\psi\big)(x) = \psi''(x) + V(x,t)\psi(x), \qquad \mathcal{A}\psi(x) = -c\psi'(x).$$

We have

$$\begin{aligned}\big(\dot{\mathcal{L}} + [\mathcal{L},\mathcal{A}]\big)\psi &= V_t\psi - a\left[\frac{d^2}{dx^2} + V, \frac{d}{dx}\right]\psi = V_t\psi - c\left[V, \frac{d}{dx}\right]\psi \\ &= V_t\psi - cV\psi' + c(V\psi)_x = (V_t + cV_x)\psi.\end{aligned}$$

Hence (5.23) is satisfied iff V satisfies the PDE $V_t + cV_x = 0$. A solutions to this PDE is of the form $V(x,t) = V^0(x-ct)$. We have the same form for the eigenfunction equation $\psi_t + c\psi_x = 0$, namely $\psi(x,t) = \psi^0(x-ct)$. □

5.1 KdV Equation

Given a C^3 function $V(x,t)$, let $\mathcal{L}$ be as in **(ii)**, but now

$$\mathcal{A} = -\left(a\frac{d^3}{dx^3} + bV\frac{d}{dx} + cV_x\right).$$

From

$$\begin{aligned}\left[\mathcal{L}, \frac{d^3}{dx^3}\right] &= \left[V, \frac{d^3}{dx^3}\right] = -\left(V_{xxx} + 3V_{xx}\frac{d}{dx} + 3V_x\frac{d^2}{dx^2}\right), \\ \left[\mathcal{L}, V\frac{d}{dx}\right] &= \left[V, V\frac{d}{dx}\right] + \left[\frac{d^2}{dx^2}, V\frac{d}{dx}\right] = -VV_x + V_{xx}\frac{d}{dx} + 2V_x\frac{d^2}{dx^2}, \\ [\mathcal{L}, V_x] &= \left[\frac{d^2}{dx^2}, V_x\right] = V_{xxx} + 2V_{xx}\frac{d}{dx}.\end{aligned}$$

we deduce

$$[\mathcal{L},\mathcal{A}] = (a-c)V_{xxx} + bVV_x + (3a-b-2c)V_{xx}\,\frac{d}{dx} + (3a-2b)V_x\,\frac{d^2}{dx^2}.$$

This operator is a multiplication if $a = 4, b = 6, c = 3$. For such choices,

$$\dot{\mathcal{L}} + [\mathcal{L}, \mathcal{A}] = V_t + 6VV_x + V_{xxx}. \tag{5.27}$$

If we write $\lambda(V)$ for an eigenvalue of $\mathcal{L} = \mathcal{L}^V$, then $\lambda(V)$ is conserved for a solution of KdV equation (5.17). □

Remark 5.1 We could have started from a general $\mathcal{A}$ of the form

$$\mathcal{A} = -\left(a\frac{d^3}{dx^3} + B\frac{d}{dx} + C\right),$$

with a a scalar, and B, C two functions of (x, t). Then the requirement that operator $\dot{\mathcal{L}} + [\mathcal{L}, \mathcal{A}]$ is a multiplication would lead to an ODE for (B, C). From this ODE we can readily deduce that B and C are constant multiples of V and V_x. □

As we have seen in Proposition 5.2, (5.23) can be recast as a compatibility equation for the over-determined system (5.26). In our examples, the operators $\mathcal{L}$ and $\mathcal{A}$ depend on a function V, and if we require isospectral property for $\mathcal{L}(t)$, as we vary t, then the compatibility of the equation we have for the eigenfuncton ψ is the PDE we try to solve. In other words, we have turned our (nonlinear) PDE to a compability condition for two linear PDEs. As we have seen in the case of KdV, the operators $\mathcal{L}$ and $\mathcal{A}$ are differential operators of order 2 and 3. There is a way of turning our system (5.26) to a system of first order PDEs provided we switch from scalar-valued function to a vector valued function. Let us explain this in the setting of KdV equation first. Note that if we set $\Psi = \begin{bmatrix} \psi \\ \psi_x \end{bmatrix}$, then the equation $(\mathcal{L} + \lambda)\psi = 0$ can be rewritten as

$$\Psi_x = X\Psi, \quad \text{where} \quad X = \begin{bmatrix} 0 & 1 \\ -(V+\lambda) & 0 \end{bmatrix} \tag{5.28}$$

On the other hand, the equation $\psi_t = \mathcal{A}\psi$ would lead to

$$\begin{aligned}
\psi_t &= -3V_x\psi - 6V\psi_x - 4\psi_{xxx} = -3V_x\psi - 6V\psi_x + 4\big[(V+\lambda)\psi_x + V_x\psi\big] \\
&= V_x\psi + 2\big(2\lambda - V\big)\psi_x, \\
\psi_{xt} &= V_{xx}\psi + V_x\psi_x - 2V_x\psi_x + 2\big(2\lambda - V\big)\psi_{xx} = V_{xx}\psi - V_x\psi_x - 2\big(2\lambda - V\big)(V+\lambda)\psi \\
&= \big[V_{xx} - 2\big(2\lambda - V\big)(V+\lambda)\big]\psi - V_x\psi_x.
\end{aligned}$$

Hence

$$\Psi_t = T\Psi, \quad \text{where} \quad T = \begin{bmatrix} V_x & 2\big(2\lambda - V\big) \\ V_{xx} - 2\big(2\lambda - V\big)(V+\lambda) & -V_x \end{bmatrix}. \tag{5.29}$$

In other words, Ψ satisfies

$$\Psi_x = X\Psi, \qquad \Psi_t = T\Psi. \tag{5.30}$$

The compatibility of these equations lead to

$$X_t - T_x + [X, T] = 0, \tag{5.31}$$

which is the analog of (5.23). A direct computation yields

$$[X, T] = \begin{bmatrix} V_{xx} & -2V_x \\ -2(V+\lambda)V_x & -V_{xx} \end{bmatrix}.$$

From this we can readily deduce

$$X_t - T_x + [X, T] = -\begin{bmatrix} 0 & 0 \\ V_t + 6VV_x + V_{xxx} & 0 \end{bmatrix}.$$

So far we know that V is a solution iff the linear equations in (5.26) hold for a wave function ψ that serves as an eigenfunction ψ of the linear operator $\mathcal{L}$. The question now is whether this connection can be used to completely integrate (5.16). Recall that for a completely integrable Hamiltonian ODE we have a change variable $\Phi(x,p) = (X, P)$ such that P is conserved and the evolution of X is linear in t. For the complete integrability of (5.16), we wish to come up with such a transformation. The rough description of our strategy for constructing such a transformation has 3 steps:

- **(i)** We define a set $\mathcal{V}$ of potential functions $W(x)$ that vanishes sufficiently fast at infinity. We write $\Phi(W)$ for a collection of spectral/scattering data that are associated with $W \in \mathcal{V}$.
- **(ii)** We describe the linear evolution of $\Phi\big(V(\cdot,t)\big)$ when V solves the KdV equation.
- **(iii)** We determine the inverse operator Φ^{-1}. In other words, we learn how to recover a potential W from its spectral/scattering data.

We start with Step **(i)**. Given a potential W that vanishes sufficiently fast at $\pm\infty$, $\Phi(W)$ is roughly the *full spectrum* of the operator $\mathcal{L}^W = -\frac{d^2}{dx^2} - W$, and the behavior of the corresponding eigenfunctions at $\pm\infty$. By a full spectrum we mean the set of eigenvalues plus the continuous spectrum that will be defined below. The reason we consider only the behavior of the eigenfunctions at $\pm\infty$ is because the eigenfuctions are equal to the eigenfunctions of $-\frac{d^2}{dx^2}$ asymptotically, and as a result the dynamics of their coefficients simplify to a linear ODE. This is exactly what we advertise for in **(ii)** above.

We wish to define a map Φ that assigns to a potential W its certain spectral data. In fact our map is of the form $\Phi(W) = (P(W), X(W))$, with $P(W) = \sigma(\mathcal{L}^W)$, where

$\mathcal{L}^W = -\frac{d^2}{dx^2} - W$. Note that if (5.24) holds, then $\rho(\mathcal{L}(t))$ is independent of t. From this and (5.27) we learn that if $V^t(x) = V(x,t)$ satisfies the KdV equation (5.16), then

$$\frac{d}{dt}P(V^t) = 0. \tag{5.32}$$

We are now ready to define $X(W)$.

Definition 5.4(i) Let $\lambda = -\ell^2 \in \sigma_d(\mathcal{L}^W),\ \ell > 0$. Then there exists a unique C^2 function $\psi^\ell : \mathbb{R} \to \mathbb{R}$ such that

$$\int (\psi^\ell(x))^2\ dx = 1, \quad (\mathcal{L}^W + \ell^2)\psi^\ell = 0,$$

and $\psi^\ell \cong a_\pm(\ell)e^{-\ell|x|}$ as $x \to \pm\infty$, for constants $a_\pm(\ell) = a^W_\pm(\ell) \in \mathbb{R}$.

(ii) Let $\lambda = k^2 \in \sigma_{ess}(\mathcal{L}^W) = [0,\infty)$. Then there exists a unique C^2 function φ^k such that $(\mathcal{L}^W - k^2)\varphi^k = 0$, and $\varphi \cong b(k)e^{-ikx}$ as $x \to -\infty$, and $\varphi \cong e^{-ikx} + A(k)e^{ikx}$ as $x \to \infty$, for constants $b(k) = b^W(k), A(k) = A^W(k) \in \mathbb{R}$.

(ii) Define $X(W) : P(W) \to \mathbb{R}$ by $X(W)(-\ell^2) = a_+(\ell),\ X(W)(k^2) = A(k)$.

We are now ready for our step **(ii)**.

Theorem 5.1 *Let a^W_+, b^W, A^W be as above. If V satisfies the KdV equation* (5.16)*, $V \cong 0$, and $V_x \cong 0$ at $\pm\infty$, and write $a(t,\ell) := a^{V^t}_+(\ell)$, $b(t,k) := b^{V^t}(k)$, and $A(t,k) := A^{V^t}(k)$. Then*

$$a_t(t,\ell) = 4\ell^3 a(t,\ell), \quad A_t(t,k) = -8ik^3 A(t,k), \quad b_t(t,k) = 0. \tag{5.33}$$

Moreover,

$$\varphi_t = \mathcal{A}\varphi - 4ik^3\varphi.$$

Proof Assume V satisfies the KdV equation (5.16). Recall that if $\psi(t) = \psi^\ell(t)$ is the eigenfunction of the operator $\mathcal{L}(t) = -\mathcal{L}^{-V^t}$ associated with the eigenvalue $\lambda = -\ell^2$, then by Proposition 5.2, and Example 5.2**(iii)**,

$$\psi_t = \mathcal{A}\psi = V_x\psi + 2(2\lambda - V)\psi_x \cong 4\lambda\psi_x = -4\ell^2\psi_x, \tag{5.34}$$

by (5.28). On the other hand,

$$\psi_t \cong a_t e^{-\ell x}, \quad \psi_x \cong -a\ell e^{-\ell x},$$

as $x \to \infty$. From this and (5.34) we deduce the first equation of (5.33).

For the other two equations in (5.33), we no longer have $\varphi_t = \mathcal{A}\varphi$ because $\varphi \notin \mathcal{X} = L^2(\mathbb{R})$. In other words even though (5.23) and (5.24) hold, the third equation of (5.26) does not hold for φ (φ is not in the domain of the definition of $\mathcal{U}^{-1}$). Nonetheless we can derive an equation of φ_t. To this end, let us write $h = \varphi_t - \mathcal{A}\varphi$. From (5.23), and $\mathcal{L}\varphi = \lambda\varphi = -k^2\varphi$ we learn

$$
\begin{aligned}
0 =& \frac{d}{dt}\big[(\mathcal{L}-\lambda)\varphi\big] = \dot{\mathcal{L}}\varphi + (\mathcal{L}-\lambda)\varphi_t = \mathcal{A}\mathcal{L}\varphi - \mathcal{L}\mathcal{A}\varphi + (\mathcal{L}-\lambda)\varphi_t \\
=& \lambda\mathcal{A}\varphi - \mathcal{L}\mathcal{A}\varphi + (\mathcal{L}-\lambda)\varphi_t = (\mathcal{L}-\lambda)h.
\end{aligned}
$$

From this, $(\mathcal{L}-\lambda)\varphi = 0$, and Proposition 5.5 we deduce that $\mathcal{W}(\varphi, h) = c$ is constant. Note,

$$
\begin{aligned}
h &= \varphi_t - V_x\varphi - 2(2\lambda - V)\varphi_x \cong \varphi_t - 4\lambda\varphi_x \cong (b_t + 4i\lambda kb)e^{-ikx}, && \text{as } \ x \to -\infty, \\
h &\cong \varphi_t - 4\lambda\varphi_x \cong (A_t - 4i\lambda kA)e^{ikx} + 4ik\lambda e^{-ikx}, && \text{as } \ x \to +\infty, \\
h_x &= \varphi_{tx} - (\mathcal{A}\varphi)_x = \varphi_{tx} - \big[V_x\varphi + 2(2\lambda - V)\varphi_x\big]_x \cong \varphi_{tx} - 4\lambda\varphi_{xx} \\
&\cong \varphi_{tx} - 4\lambda^2\varphi \cong -(ikb_t + 4\lambda^2 b)e^{-ikx}, && \text{as } \ x \to -\infty, \\
h_x &\cong \varphi_{tx} - 4\lambda^2\varphi \cong (ikA_t - 4\lambda^2 A)e^{ikx} - 4\lambda^2 e^{-ikx}. && \text{as } \ x \to +\infty,
\end{aligned}
$$

From this and $\lambda = k^2$ we learn

$$
\mathcal{W}(\varphi, h) = \varphi h_x - \varphi_x h \cong -b(ikb_t + 4\lambda^2 b)e^{-2ikx} + ikb(b_t + 4i\lambda kb)e^{-2ikx} = 0,
$$

as $x \to -\infty$. Similarly

$$
\begin{aligned}
\mathcal{W}(\varphi, h) \cong& \big[(ikA_t - 4\lambda^2 A)e^{ikx} - 4\lambda^2 e^{-ikx}\big]\big[e^{-ikx} + Ae^{ikx}\big], \\
&- ik\big[-e^{-ikx} + Ae^{ikx}\big]\big[(A_t - 4i\lambda kA)e^{ikx} + 4ik\lambda e^{-ikx}\big] \\
=& \; ikA_t - 8\lambda^2 A + ik(A_t - 4i\lambda kA) + 4k^2\lambda A \\
&+ \big[A(ikA_t - 4\lambda^2 A) - ikA(A_t - 4i\lambda kA)\big]e^{2ikx} - \big[4k^2\lambda + 4k^2\lambda\big]e^{-2ikx} \\
=& \; 2ikA_t - 16\lambda^2 A,
\end{aligned}
$$

as $x \to -\infty$. Since $\mathcal{W}(\varphi, h)$ is independent of x, we must have $2ikA_t - 16\lambda^2 A = 0$. This implies the second equation in (5.33).

For the last equation, observe that since $\mathcal{W}(\varphi, h) = 0$, we know that h/φ is independent of x. On the other hand,

$$
\begin{aligned}
\frac{h}{\varphi} &\cong \frac{b_t + 4i\lambda kb}{b} && \text{as } \ x \to -\infty, \\
\frac{h}{\varphi} &\cong \frac{(A_t - 4i\lambda kA)e^{ikx} + 4ik\lambda e^{-ikx}}{e^{-ikx} + Ae^{ikx}} = \frac{-4ik^3 Ae^{ikx} + 4ik\lambda e^{-ikx}}{e^{-ikx} + Ae^{ikx}} = -4ik^3, && \text{as } \ x \to +\infty,
\end{aligned}
$$

Matching the right-hand sides would yield the third equation in (5.33). Moreover, $h/\varphi = -4ik^3$, which implies the last claim of the Theorem. $\square$

5.2 NLS Equation

For KdV equation, we learned that the stationary Schrodingar equation can be recast as a first order vector equation (5.28). Alternatively, the factorization

$$\frac{d^2}{dx^2} + k^2 = \left(\frac{d}{dx} + ik\right)\left(\frac{d}{dx} - ik\right),$$

suggests setting $\phi^2 = \phi$, $\phi^1 = \phi^2_x - ik\phi^2$, to recast $\phi_{xx} + k^2\phi = W\phi$, as $\phi^1_x + ik\phi^1 = W\phi^2$. As a result, we can write $\Phi_x = X\Phi$, where

$$\Phi = \begin{bmatrix} \phi^1 \\ \phi^2 \end{bmatrix}, \qquad X = \begin{bmatrix} -ik & W \\ 1 & ik \end{bmatrix}.$$

Zakharov and Shabat proposes a generalization of the form

$$\Phi_x = X\Phi, \quad \text{where} \quad X = \begin{bmatrix} -ik & \psi \\ \xi & ik \end{bmatrix}, \tag{5.35}$$

$$\Phi_t = T\Phi, \quad \text{where} \quad X = \begin{bmatrix} A & B \\ C & -A \end{bmatrix}.$$

5.3 Exercise

(i) Find solutions of the form (5.15) to (5.9) when $d = 1$, $\kappa = -2$, and $r = 3$.

(ii) Show that the derivative of the map $f(U) = U^{-1}$ is given by $Df(U)(Z) = -U^{-1}ZU^{-1}$. More precisely, given a bounded invertible linear operator U, show that there exists a constant $c_0 = c_0(U)$ such that

$$\left\|(U+Z)^{-1} - U^{-1} + U^{-1}ZU^{-1}\right\| \le c_0\|Z\|^2,$$

for every bounded operator Z of sufficiently small norm.

(iii) Let $G : \mathbb{R} \to \mathbb{R}$ be a C^1 function. Write $\mathcal{F}$ for the set of C^1 functions $u : \mathbb{R} \to \mathbb{R}$ such that u and its derivative u_x vanish at $\pm\infty$. Given a pair of functions $q, p \in \mathcal{F}$, define its Hamiltonian

$$\mathcal{H}(q,p) = \int_{-\infty,\infty} \left[\frac{1}{2}\big(q_x(x)^2 + p(x)^2\big) + G(q(x))\right] dx.$$

What PDE $q(x,t)$ satisfies if $\psi(x,t) = (q(x,t), p(x,t))$ satisfies $\psi_t = J\partial\mathcal{H}(\psi)$? (The matrix J was defined right before (5.1).)

(iv) Let V be a solution of KdV equation with $V(x,0) = -W(x)$. Assume that W is as in Exercise **(ii)** and **(iii)** of Chapter 3. Find $V(x,t)$.

6 Incompressible Fluid Equations

In this chapter we study the incompressible Euler equation (1.11). It is possible to write (1.11) as an equation for u only (getting ride of P) by projecting $(u\cdot\nabla)u$ onto its divergence free part. For this, we recall that by a result of Holmholtz, we can always decompose a vector field w into a gradient vector field , and a divergence free vector field. More precisely $w=-\nabla\phi+Z$, for a C^1 function $\varphi:\mathbb{R}^d\to\mathbb{R}$ and divergence free vector field Z. It is not hard to find ϕ by taking the divergence of both sides to obtain $-\Delta\phi=\nabla\cdot w$, which suggests a candidate for ϕ of the form

$$\phi(x)=\int\bar{G}(x,y)(\nabla\cdot w)(y)\ dy,$$

where $\bar{G}$ is the Green's function of $-\Delta$ in $\mathbb{R}^d$ (see section 2.3). When $d=3$, we may express $Z=\nabla\times A$ for a vector field A. We may choose A divergence free so that

$$\nabla\times(\nabla\times A)=\nabla(\nabla\cdot A)-\Delta A=-\Delta A.$$

Because of this, we may choose A by

$$A(x)=\int\bar{G}(x,y)(\nabla\times w)(y)\ dy,\qquad \mathbb{P}(w):=\nabla\times A.$$

With the aid of the projection operator $\mathbb{P}$, we may write (1.11) as

$$u_t+\mathbb{P}\big[(u\cdot\nabla)u\big]=0. \tag{6.1}$$

We now give a dynamical/geometric description of the equation (1.11). For this, let us consider the classical Hamiltonian function

$$H(x,U)=\frac{1}{2}|U|^2+P(x,t),$$

and consider the corresponding Hamiltonian ODE

$$\dot{x}=U,\qquad \dot{U}=-P_x(x,t), \tag{6.2}$$

which is the Newton's equation associated with the potential P. We write Φ^t for the flow of this ODE. Now imagine that the momentum $U(t)$ is related to the position $x(t)$ as

$$U(t)=u(x(t),t), \tag{6.3}$$

for a suitable vector field $u(x,t)$. We now claim that (6.2) and (6.3) are compatible if and only if u satisfies the first equation in (1.11). In fact if we write $X^t(x)=X(x,t)$ for the flow of the vector field u, i.e.,

$$X_t(x,t)=u(X(x,t),t),\qquad X(x,0)=x, \tag{6.4}$$

Then (6.3) means

$$\Phi^t(x, u(x,0)) = \big(X(x,t), u(X(x,t),t)\big). \tag{6.5}$$

If we set $U(x,t) := u(X(x,t),t)$, then

$$0 = U_t(x,t) + P_x(X(x,t),t) = (u_t + u_x u + P_x)(X(x,t),t).$$

Then if both (6.3) and (6.5) hold for every initial x, we must have $u_t + u_x u + P_x = 0$. For the ODE (6.2), the invariance (5.5) is valid:

$$\frac{d}{dt}\int_{\Phi^t(\gamma)} U \cdot dx = 0, \tag{6.6}$$

for a closed curve $\gamma : [0, t_0] \to \mathbb{R}^{2d}$. Given a closed curve $\eta : [0, t_0] \to \mathbb{R}^{2d}$, we lift it to a curve in $\mathbb{R}^{2d}$ by

$$\gamma(\theta) = \big(\eta(\theta), u(\eta(\theta), 0)\big).$$

From (6.5) we learn

$$\Phi^t(\gamma)(\theta) = \big(X^t(\eta)(\theta), u(X^t(\eta)(\theta), t)\big).$$

This and (6.6) imply

$$\frac{d}{dt}\int_{X^t(\eta)} u(x,t) \cdot dx = 0. \tag{6.7}$$

This invariance principle is due to Kelvin.

We may apply Stokes formula to rewrite (6.7) as

$$\int_{X^t(\Gamma)} (\nabla \times u)(x,t) \cdot d\mathbf{S}(x) = \int_\Gamma (\nabla \times u)(x,0) \cdot d\mathbf{S}(x), \tag{6.8}$$

where Γ is a surface with $\partial\Gamma = \gamma$, and $d\mathbf{S} = \mathbf{n}\ dS$, with $\mathbf{n}$ the unit normal to the surface. (Here the direction of $\mathbf{n}$ must be compatible with the orientation of γ.) If $x(\theta_1, \theta_2)$ is a parametrization of Γ, then

$$\mathbf{n} = x_{\theta_1} \times x_{\theta_2}.$$

If we write $\xi = \delta \times u$, and $[\xi, v_1, v_2] := \xi \cdot (v_1 \times v_2)$, then (6.8) is equivalent to saying

$$\big[\xi \circ X, (DX)v_1, (DX)v_2\big] = \big[\xi^0, v_1, v_2\big],$$

where $\xi^0(x) = \xi(x,0)$. Since $\nabla \cdot u = 0$, we have

$$\big[\xi^0, v_1, v_2\big] = \big[(DX)\xi^0, (DX)v_1, (DX)v_2\big].$$

Hence (6.8) is equivalent to

$$\xi(X(x,t),t) = X_x(x,t)\xi(x,0). \tag{6.9}$$

If we differentiate both sides with respect to t, we obtain

$$\xi_t \circ X + (\xi_x \circ X)X_t = X_{xt}\xi^0.$$

From this, and $X_t = u \circ X$ we learn

$$\xi_t \circ X + (\xi_x \circ X)(u \circ X) = (u_x \circ X)X_x\xi^0 = (u_x \circ X)(\xi \circ X).$$

In summary

$$\xi_t + \xi_x u - u_x \xi = 0. \tag{6.10}$$

A Spectral Theory

Definition A.1(i) Let $\mathcal{X}$ be a Hilbert space. Given a linear operator $\mathcal{L} : Dom(\mathcal{L}) \to \mathbb{X}$, we write $\rho(\mathcal{L})$ for the set of $\lambda \in \mathbb{C}$ such that the operator $\mathcal{L} - \lambda$ is invertible, and the inverse $(\mathcal{L} - \lambda)^{-1} : \mathcal{X} \to \mathcal{X}$ is bounded (continuous). The set $\rho(\mathcal{L})$ is called the *resolvent* of $\mathcal{L}$. Its complement $\sigma(\mathcal{L}) = \mathbb{C} \setminus \rho(\mathcal{L})$ is called the *spectrum* of $\mathcal{L}$.

(ii) We say λ is an eigenvalue of $\mathcal{L}$ if $\ker(\mathcal{L} - \lambda) \neq \{0\}$. Obviously any eigenvalue of $\mathcal{L}$ belongs to $\sigma(\mathcal{L})$.

(iii) Let $\mathcal{L} : Dom(\mathcal{L}) \to \mathbb{X}$ be a linear operator, and assume that $Dom(\mathcal{L})$ is dense in $\mathcal{X}$. We call the operator $\mathcal{L}$ closed if its graph is a closed set. That is, if x_n is a sequence in $Dom(\mathcal{L})$ such that $(x_n, \mathcal{L}x_n) \to (x, y)$ in large n limit, then $x \in Dom(\mathcal{L})$, and $y = \mathcal{L}x$. □

When $Dom(\mathcal{L}) \neq \mathcal{X}$, the a closed densely defined operator that cannot be extended to the whole space $\mathcal{X}$ must be *unbounded* by the following *closed graph theorem* of Banach:

Proposition A.1 *A closed linear operator $\mathcal{L} : \mathcal{X} \to \mathcal{X}$ is bounded (continuous).*

Definition A.2 We define the *discrete (point) spectrum* $\sigma_d(\mathcal{L})$ as the set $\lambda \in \mathbb{C}$ such that λ is an isolated point of $\sigma(\mathcal{L})$, $\ker(\mathcal{L} - \lambda) \neq \{0\}$, and $\dim\ker(\mathcal{L} - \lambda) < \infty$. The *essential (continuous) spectrum* $\sigma_{ess}(\mathcal{L})$ of $\mathcal{L}$ is defined as $\sigma_{ess}(\mathcal{L}) = \sigma(\mathcal{L}) \setminus \sigma_d(\mathcal{L})$. When $\lambda \in \sigma_d(\mathcal{L})$, we refer to it as an eigenvalue of $\mathcal{L}$. □

Proposition A.2 *Suppose that $\mathcal{L}$ is a self-adjoint operator. If λ is an isolated point of $\sigma(\mathcal{L})$, then λ is an eigenvalue. Moreover $\mathcal{L} - \lambda$ restricted to $\ker(\mathcal{L} - \lambda)^{\perp}$ has a bounded inverse.*

Theorem A.1 *(Weyl) Suppose $\mathcal{L} : Dom(\mathcal{L}) \to \mathcal{X}$ is a self-adjoint operator. Then $\lambda \in \sigma_{ess}(\mathcal{L})$ iff there exists a sequence $x_n \in Dom(\mathcal{L})$ such that*

$$\|x_n\| = 1, \qquad \lim_{n\to\infty} (\mathcal{L} - \lambda)x_n = 0, , \qquad x_n \rightharpoonup 0. \tag{A.1}$$

Proof We only show how (A.1) implies that $\lambda \in \sigma_{ess}(\mathcal{L})$. First we argue that if such a sequence exists, then $\lambda \in \sigma(\mathcal{L})$. Suppose to the contrary, $(\mathcal{L} - \lambda)^{-1}$ is a bounded operator. Then for $y_n = (\mathcal{L} - \lambda)x_n$ we have

$$\lim_{n\to\infty} y_n = 0, \qquad 1 = \|x_n\| = \left\|(\mathcal{L} - \lambda)^{-1} y_n\right\| \leq \left\|(\mathcal{L} - \lambda)^{-1}\right\| \; \|y_n\|,$$

which is impossible. Hence we must have $\lambda \in \sigma(\mathcal{L})$.

It remains to show that $\lambda \notin \sigma_d(\mathcal{L})$. Suppose to the contrary, $\lambda \in \sigma_d(\mathcal{L})$, and $\{e_1, \dots, e_k\}$ is an orthonormal basis for $\ker(\mathcal{L} - \lambda)$. Write $\mathcal{Y}$ for $\ker(\mathcal{L} - \lambda)^\perp$ and $\mathcal{P}$ for the orthogonal projection onto $\mathcal{Y}$. Set $z_n = (\mathcal{P}x_n)/\|\mathcal{P}x_n\|$. Then $\|z_n\| = 1$, and

$$\|\mathcal{P}x_n\|^2 = \|x_n\|^2 - \sum_{j=1}^{k} \langle x_n, e_j \rangle^2 = 1 - \sum_{j=1}^{k} \langle x_n, e_j \rangle^2 \to 1,$$
$$\|(\mathcal{L} - \lambda)z_n\| = \|(\mathcal{L} - \lambda)\mathcal{P}x_n\| \, \|\mathcal{P}x_n\|^{-1} = \|(\mathcal{L} - \lambda)x_n\| \, \|\mathcal{P}x_n\|^{-1} \to 0,$$

in large n limit. This implies that the restriction of $\mathcal{L} - \lambda$ to $\mathcal{Y}$ is not invertible by repeating the argument in the previous paragraph. When then use Proposition 4.4 to deduce that λ is not isolated in $\sigma(\mathcal{L})$. This contradicts $\lambda \in \sigma_d(\mathcal{L})$. $\square$

Remark A.1 If $\mathcal{L}$ is a densely defined closed operator, then $\lambda \in \rho(\mathcal{L})$ iff $\mathcal{L} - \lambda$ is one-to-one and onto. The reason is that if $(\mathcal{L} - \lambda)^{-1}$ is well-defined as a linear function on $\mathcal{X}$, then it is also closed, and hence bounded by Proposition 4.2. $\square$

Example A.1 Let $\mathcal{X}$ be an infinite dimensional separable Hilbert space with an orthonormal basis $\{e_n : \; n \in \mathbb{N}\}$. If $\mathcal{L} = I$ is the identity operator, then $\sigma(\mathcal{L}) = \sigma_{ess}(\mathcal{L}) = \{1\}$.

A.1 Exercise

(i) Show that the resolvent set $\rho(\mathcal{L})$ is open.

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