

Waves and Multiscale Phenomena

John K. Hunter

Department of Mathematics
University of California at Davis
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Chapter 1

Semiclassical Quantum Mechanics

In this Chapter we discuss the Schrödinger equation of quantum mechanics, which is a fundamental example of a linear dispersive wave equation. We show how classical mechanics emerges from quantum mechanics in a high-frequency, short wave, “geometrical optics” limit, in which a classical particle corresponds to a packet of quantum mechanical waves. The velocity of a classical particle is equal to the group velocity of the corresponding quantum mechanical wave packet.

1.1 Classical mechanics

We consider, as an example of a mechanical system, the motion of a particle of mass m in \mathbb{R}^d in a potential field* $V : \mathbb{R}^d \rightarrow \mathbb{R}$. The position $\mathbf{x}(t) \in \mathbb{R}^d$ of the particle at time t satisfies Newton’s second law

$$m \frac{d^2 \mathbf{x}}{dt^2} = -\nabla V(\mathbf{x}).$$

(We will frequently abuse notation slightly and use \mathbf{x} to denote either a point in \mathbb{R}^d , or a path $t \mapsto \mathbf{x}(t)$.) The ideas we develop in the context of this basic example apply in much greater generality.

First, we briefly recall the Lagrangian and Hamiltonian formulations of the particle dynamics. As we will see, these formulations arise naturally from the semiclassical limit of quantum mechanics. The Hamiltonian formulation arises directly from short-wave asymptotics, while the Lagrangian formulation arises directly from a semiclassical approximation of Feynman’s path integral formulation of quantum mechanics.

We define the Lagrangian $L : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ of the particle by

$$L(\mathbf{x}, \mathbf{v}) = \frac{1}{2} m \mathbf{v}^2 - V(\mathbf{x}).$$

*We will assume that the potential V satisfies appropriate smoothness and regularity conditions, unless stated otherwise.

That is, L is the difference between the kinetic and potential energies of the particle. The action $\mathcal{S}(\xi)$ of any (smooth) path $\xi : [0, t] \rightarrow \mathbb{R}^d$ is the time integral of the Lagrangian,

$$\mathcal{S}(\xi) = \int_0^t L\left(\frac{d\xi}{ds}(s), \xi(s)\right) ds. \quad (1.1)$$

Newton's second law is equivalent to the Euler-Lagrange equations associated with L ,

$$-\frac{d}{dt}\left(\frac{\partial L}{\partial \mathbf{v}}\right) + \frac{\partial L}{\partial \mathbf{x}} = 0.$$

Thus, the particle paths are stationary points of the action, meaning that

$$\left.\frac{d}{d\varepsilon}\mathcal{S}(\mathbf{x} + \varepsilon\mathbf{h})\right|_{\varepsilon=0} = 0$$

for all paths $\mathbf{h} : [0, t] \rightarrow \mathbb{R}^d$ such that $\mathbf{h}(0) = \mathbf{h}(t) = 0$.

The Hamiltonian $H(\mathbf{p}, \mathbf{x})$ of the particle is defined as the Legendre transform of the Lagrangian with respect to \mathbf{v} ,

$$\mathbf{p} = \frac{\partial L}{\partial \mathbf{v}}, \quad H(\mathbf{p}, \mathbf{x}) = \mathbf{p} \cdot \mathbf{v} - L(\mathbf{x}, \mathbf{v}).$$

For the particle moving in a potential, we have

$$\mathbf{p} = m\mathbf{v}, \quad H(\mathbf{p}, \mathbf{x}) = \frac{1}{2m}\mathbf{p}^2 + V(\mathbf{x}).$$

Thus, \mathbf{p} is the momentum of the particle, and H is the total energy. The Euler-Lagrange equations may then be written as Hamilton's equations

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &= \frac{\partial H}{\partial \mathbf{p}}, \\ \frac{d\mathbf{p}}{dt} &= -\frac{\partial H}{\partial \mathbf{x}}. \end{aligned}$$

1.2 The Schrödinger Equation

The Schrödinger equation for a quantum mechanical particle of mass m moving in a potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$ is

$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\Delta\psi + V(\mathbf{x})\psi. \quad (1.2)$$

Here, \hbar is Planck's constant, which has the dimension of action (momentum \times length, or energy \times time).

The complex-valued function $\psi(\mathbf{x}, t)$ is the wavefunction of the particle, where $|\psi|^2$ is the probability density of the particle. Probability is conserved on account of the conservation law

$$\partial_t |\psi|^2 + \nabla \cdot \mathbf{J} = 0,$$

where \mathbf{J} is the probability flux,

$$\mathbf{J} = \frac{i\hbar}{2m} (\psi^* \nabla \psi - \psi \nabla \psi^*).$$

Example 1.1 Let $\Omega \subset \mathbb{R}^d$ be an open set. The classical “billiard” problem of a particle confined to a region Ω with a rigid boundary corresponds formally to the potential

$$V(\mathbf{x}) = \begin{cases} 0 & \text{if } x \in \Omega, \\ +\infty & \text{if } x \notin \Omega \end{cases},$$

The quantum mechanical problem consists of the Dirichlet problem for the free Schrödinger equation:

$$\begin{aligned} i\hbar\psi_t &= -\frac{\hbar^2}{2m}\Delta\psi & x \in \Omega, \\ \psi &= 0 & x \in \partial\Omega. \end{aligned}$$

The classical problem ranges from completely integrable to ergodic, depending on the shape of the domain Ω . Thus, this problem is a useful test case for the investigation of the quantum behavior of classically chaotic systems.

We look for a solution of (1.2) of the form

$$\psi = A(\mathbf{x}, t; \hbar) e^{iS(\mathbf{x}, t)/\hbar}, \quad (1.3)$$

where A is a complex-valued amplitude, and S is a real-valued phase.[†]

The use of (1.3) in (1.2) implies that

$$-S_t A + i\hbar A_t = \frac{1}{2m} |\nabla S|^2 A + V A - \frac{i\hbar}{2m} (2\nabla S \cdot \nabla A + \Delta S A) - \frac{\hbar^2}{2m} \Delta A. \quad (1.4)$$

We look for an asymptotic solution of this equation for A of the form

$$A(\mathbf{x}, t; \hbar) \sim \sum_{n=0}^{\infty} \hbar^n A^{(n)}(\mathbf{x}, t) \quad \text{as } \hbar \rightarrow 0. \quad (1.5)$$

Remark 1.2 Strictly speaking, the limit $\hbar \rightarrow 0$ in (1.5) does not make sense, because \hbar is a fixed dimensional number. What we really mean is that $\hbar/S_0 \rightarrow 0$ where S_0 is an action associated with the solutions that we consider. To make clear

[†]One can also consider complex-valued phases, for example in the construction of Gaussian beam solutions that are concentrated near a single ray, but we will not do so here.

sense of an asymptotic limit, we should first nondimensionalize the problem, but here it is more convenient not to do so explicitly.

We use (1.5) in (1.4) and equate coefficients of \hbar^n to zero. When $n = 0$, and assuming that $A^{(0)} \neq 0$, we find that

$$S_t + \frac{1}{2m} |\nabla S|^2 + V(\mathbf{x}) = 0. \quad (1.6)$$

This equation is the eikonal equation for the Schrödinger equation.

Remark 1.3 The local frequency and wavenumber of the solution in (1.3) are

$$\omega = -\frac{S_t}{\hbar}, \quad \mathbf{k} = \frac{\nabla S}{\hbar}.$$

These satisfy the local dispersion relation

$$\hbar\omega = \frac{\hbar^2 \mathbf{k}^2}{2m} + V(\mathbf{x}),$$

obtained by “freezing” coefficients in (1.2) and looking for Fourier mode solutions. The analogy of this dispersion relation with the classical expression for the energy,

$$E = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}),$$

suggests that we can define the energy E and momentum \mathbf{p} (or pseudo-energy and pseudo-momentum) of a wave in terms of its frequency and wavenumber by

$$E = \hbar\omega, \quad \mathbf{p} = \hbar\mathbf{k}.$$

This connection is often useful, although it has pitfalls, especially for nonlinear waves [34].

Equating coefficients of \hbar , we get the transport equation

$$A_t^{(0)} + \mathbf{v} \cdot \nabla A^{(0)} + \frac{1}{2} (\operatorname{div} \mathbf{v}) A^{(0)} = 0, \quad (1.7)$$

where the group velocity $\mathbf{v}(\mathbf{x}, t)$ is given by

$$\mathbf{v} = \frac{1}{m} \nabla S.$$

The group velocity may be written as $\mathbf{v} = \mathbf{p}/m$, so it is equal to the classical velocity of the particle. Note that although the the group velocity is orthogonal to the wavefronts $S(\cdot, t) = \text{constant}$, it is not equal in magnitude to the phase velocity $\mathbf{c} = -\nabla S/S_t$. Equation (1.7) implies the conservation of probability,

$$\partial_t |A^{(0)}|^2 + \operatorname{div} (\mathbf{v} |A^{(0)}|^2) = 0.$$

The higher order corrections $A^{(n)}$ for $n \geq 1$ satisfy similar, nonhomogeneous, transport equations,

$$A_t^{(n)} + \mathbf{v} \cdot \nabla A^{(n)} + \frac{1}{2} (\operatorname{div} \mathbf{v}) A^{(n)} = \frac{i}{2m} \Delta A^{(n-1)}.$$

The classical particle paths are called the rays, or bicharacteristics, of the Schrödinger equation. Let $\mathbf{x} = \mathbf{X}(\mathbf{x}_0, t)$ be the ray that starts at \mathbf{x}_0 , so that

$$\mathbf{X}_t = \mathbf{v}(\mathbf{X}, t), \quad \mathbf{X}(\mathbf{x}_0, 0) = \mathbf{x}_0.$$

We define the Jacobian $J(\mathbf{x}, t)$ by

$$J(\mathbf{X}(\mathbf{x}_0, t), t) = \det \left[\frac{\partial \mathbf{X}(\mathbf{x}_0, t)}{\partial \mathbf{x}_0} \right].$$

Lemma 1.4

$$\frac{1}{J} \frac{dJ}{dt} = \operatorname{div} \mathbf{v}, \tag{1.8}$$

where

$$\frac{d}{dt} = \partial_t + \mathbf{v} \cdot \nabla$$

is a derivative along a ray.

Proof. If $E(t) \in M^{d \times d}$ is a smooth matrix-valued function with $E(0) = I$, then

$$\left. \frac{d}{dt} \det E(t) \right|_{t=0} = \operatorname{tr} \frac{dE}{dt}(0).$$

Hence, if $F(t)$ is invertible, we have

$$\begin{aligned} \frac{d}{dt} \det F(t) &= \left. \frac{d}{ds} \det F(t+s) \right|_{s=0} \\ &= \det F(t) \left. \frac{d}{ds} F^{-1}(t) \det F(t+s) \right|_{s=0} \\ &= \det F(t) \operatorname{tr} \left\{ F^{-1}(t) \frac{dF}{dt}(t) \right\}. \end{aligned}$$

Setting $F = \partial \mathbf{X} / \partial \mathbf{x}_0$, we get

$$\begin{aligned} \frac{dJ}{dt} &= J \operatorname{tr} \left\{ \frac{\partial \mathbf{x}_0}{\partial \mathbf{X}} \frac{d}{dt} \frac{\partial \mathbf{X}}{\partial \mathbf{x}_0} \right\} \\ &= J \operatorname{tr} \left\{ \frac{\partial \mathbf{x}_0}{\partial \mathbf{X}} \frac{\partial \mathbf{v}}{\partial \mathbf{x}_0} \right\} \\ &= J \operatorname{tr} \left\{ \frac{\partial \mathbf{v}}{\partial \mathbf{x}} \right\} \\ &= J \operatorname{div} \mathbf{v}. \end{aligned}$$

□

Since $J(\mathbf{x}_0, 0) = 1$, we have $J(\mathbf{x}_0, t) \neq 0$ for small enough t , so the function $\mathbf{x}_0 \mapsto \mathbf{x}$ is locally invertible. It follows from (1.8) that the ray density $\rho = J^{-1}$ satisfies the continuity equation

$$\rho_t + \operatorname{div}(\rho \mathbf{v}) = 0.$$

Along a ray, we have

$$\frac{dA^{(0)}}{dt} = -\frac{1}{2J} \frac{dJ}{dt} A^{(0)}.$$

Thus,

$$A^{(0)}(\mathbf{X}(\mathbf{x}_0, t), t) = J^{-1/2}(\mathbf{x}_0, t) A_0(\mathbf{x}_0).$$

This equation implies that $A^{(0)}$ increases as the rays focus. The asymptotic solution is not valid near caustics, where $J \rightarrow 0$ (*c.f.* Section 1.7).

The above construction gives an asymptotic solution

$$\psi^{(n)}(\mathbf{x}, t; \hbar) = \sum_{k=0}^n A^{(k)}(\mathbf{x}, t) e^{iS(\mathbf{x}, t)/\hbar}$$

of the Schrödinger equation, for any $n \in \mathbb{N}$, such that

$$\begin{aligned} i\hbar\psi_t^{(n)} + \frac{\hbar^2}{2m}\Delta\psi^{(n)} + V(\mathbf{x})\psi^{(n)} &= -\frac{\hbar^{n+2}}{2m}\Delta A^{(n-1)}, \\ \psi^{(n)}(\mathbf{x}, 0; \hbar) &= A_0(\mathbf{x})e^{iS_0(\mathbf{x})/\hbar}. \end{aligned}$$

The asymptotic solution is well-defined in any time interval $0 \leq t \leq T$ for which a smooth solution of the eikonal equation (1.6) with initial data $S(\mathbf{x}, 0) = S_0(\mathbf{x})$ exists (see Section 1.4).

Using standard estimates for the Schrödinger equation, we see that the asymptotic solution is an asymptotic approximation of the exact solution $\psi(\mathbf{x}, t; \hbar)$, which satisfies

$$\begin{aligned} i\hbar\psi_t + \frac{\hbar^2}{2m}\Delta\psi + V(\mathbf{x})\psi &= O(\hbar^{n+1}), \\ \psi(\mathbf{x}, 0; \hbar) &= A_0(\mathbf{x})e^{iS_0(\mathbf{x})/\hbar}, \end{aligned}$$

Theorem 1.5 If $\psi : [0, T] \rightarrow L^2(\mathbb{R}^d)$ satisfies

$$\begin{aligned} i\hbar\psi_t + \frac{\hbar^2}{2m}\Delta\psi - V(\mathbf{x})\psi &= f(\mathbf{x}, t), \\ \psi(\mathbf{x}, 0) &= 0, \end{aligned}$$

then

$$\|\psi\|_{L^\infty([0, T]; L^2)} \leq \|f\|_{L^1([0, T]; L^2)}.$$

Note that the asymptotic solution approximates the exact solution as $\hbar \rightarrow 0$ on a fixed time interval, but even if there is a global smooth solution of the eikonal equation, the asymptotic solution is not generally uniformly valid as $t \rightarrow \infty$.

1.3 Hydrodynamic form

Writing the solution of the Schrödinger equation in the form (1.3), where A is real-valued amplitude, and equating real and imaginary parts in (1.4), we get

$$\begin{aligned} \left(S_t + \frac{1}{2m} |\nabla S|^2 + V \right) A &= \frac{\hbar^2}{2m} \Delta A, \\ A_t + \frac{1}{2m} (2\nabla S \cdot \nabla A + \Delta S A) &= 0. \end{aligned}$$

We introduce the density $\rho = A^2$ and the velocity $\mathbf{v} = \nabla S/m$. Then, when $\rho \neq 0$, we may rewrite these equations as

$$\begin{aligned} \rho_t + \nabla \cdot (\rho \mathbf{v}), \\ \mathbf{v}_t + \mathbf{v} \cdot \nabla \mathbf{v} + \frac{1}{m} \nabla V &= \frac{\hbar^2}{2m^2} \nabla \left(\frac{1}{\sqrt{\rho}} \Delta \sqrt{\rho} \right). \end{aligned}$$

These equations correspond to those of a compressible, pressureless fluid, with a dispersive regularization that is neglected in the semiclassical limit.

1.4 The Hamilton-Jacobi equation

The eikonal equation (1.6) for the phase $S(\mathbf{x}, t)$ of the semiclassical solution of the Schrödinger equation (1.2) is a Hamilton-Jacobi equation of the form

$$S_t + H \left(\frac{\partial S}{\partial \mathbf{x}}, \mathbf{x} \right) = 0. \quad (1.9)$$

In the case of a particle moving in a potential V , the Hamiltonian function H is given by

$$H(\mathbf{p}, \mathbf{x}) = \frac{1}{2m} |\mathbf{p}|^2 + V(\mathbf{x}), \quad (1.10)$$

but most of the discussion in this section will apply to any smooth Hamiltonian that is a convex function of \mathbf{p} .

It is convenient to introduce a d -dimensional configuration space \mathbf{M} , with coordinates \mathbf{x} , and a $2d$ -dimensional phase space \mathbf{P} , with coordinates (\mathbf{x}, \mathbf{p}) . We also define the projection π of phase space onto configuration space by

$$\pi : \mathbf{P} \rightarrow \mathbf{M}, \quad \pi : (\mathbf{x}, \mathbf{p}) \mapsto \mathbf{x}. \quad (1.11)$$

As we will see, the solution of (1.9) by the method of characteristics leads directly to Hamilton's equations of classical mechanics, showing how quantum mechanics leads to classical mechanics through short wave asymptotics.

First, let us suppose that S is a smooth solution of (1.9). A *ray* associated with S is a curve in configuration space (whose equation, with a slight abuse of notation, we write as $t \mapsto \mathbf{x}(t)$) that satisfies the ODE

$$\frac{d\mathbf{x}}{dt} = \frac{\partial H}{\partial \mathbf{p}} \left(\frac{\partial S}{\partial \mathbf{x}}, \mathbf{x} \right).$$

Computing the derivative of $\partial S / \partial \mathbf{x}$ along a ray, we find that

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial S}{\partial \mathbf{x}} \right) &= \frac{\partial S_t}{\partial \mathbf{x}} + \frac{d\mathbf{x}}{dt} \cdot \frac{\partial^2 S}{\partial \mathbf{x}^2} \\ &= -\frac{\partial}{\partial \mathbf{x}} \left[H \left(\frac{\partial S}{\partial \mathbf{x}}, \mathbf{x} \right) \right] + \frac{\partial H}{\partial \mathbf{p}} \cdot \frac{\partial^2 S}{\partial \mathbf{x}^2} \\ &= -\frac{\partial H}{\partial \mathbf{x}} \left(\frac{\partial S}{\partial \mathbf{x}}, \mathbf{x} \right). \end{aligned}$$

Since the second derivatives of S cancel, we get a closed system of ODEs for the position $\mathbf{x}(t)$ of the ray, and the momentum $\mathbf{p}(t)$ on the ray,

$$\mathbf{p}(t) = \frac{\partial S}{\partial \mathbf{x}} (\mathbf{x}(t), t).$$

This system is Hamilton's equations:

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &= \frac{\partial H}{\partial \mathbf{p}}, \\ \frac{d\mathbf{p}}{dt} &= -\frac{\partial H}{\partial \mathbf{x}}. \end{aligned} \tag{1.12}$$

The curves $t \mapsto (\mathbf{x}(t), \mathbf{p}(t))$ in phase space are called the *characteristic curves* of (1.9) associated with S . The projections of the characteristic curves onto configuration space are rays. Thus, the rays are just the classical particle paths.

The derivative of the phase $S(\mathbf{x}(t), t)$ along a ray is given by

$$\begin{aligned} \frac{dS}{dt} &= S_t + \frac{d\mathbf{x}}{dt} \cdot \frac{\partial S}{\partial \mathbf{x}} \\ &= \mathbf{p} \cdot \frac{d\mathbf{x}}{dt} - H \\ &= L \left(\frac{d\mathbf{x}}{dt}, \mathbf{x} \right), \end{aligned} \tag{1.13}$$

where the Lagrangian $L(\mathbf{v}, \mathbf{x})$ is the Legendre transform of $H(\mathbf{p}, \mathbf{x})$ with respect to \mathbf{p} :

$$L(\mathbf{v}, \mathbf{x}) = \mathbf{p} \cdot \frac{\partial H}{\partial \mathbf{p}}(\mathbf{p}, \mathbf{x}) - H(\mathbf{p}, \mathbf{x}), \quad \mathbf{v} = \frac{\partial H}{\partial \mathbf{p}}(\mathbf{p}, \mathbf{x}).$$

Thus, from (1.13), the phase is the time integral of the Lagrangian along a classical path, or, in other words, the classical action (*c.f.* Section 1.1).

Next, we reverse the above discussion, and use integration along characteristics to piece together a local solution of (1.9) subject to the initial condition

$$S(\mathbf{x}, 0) = S_0(\mathbf{x}). \quad (1.14)$$

Theorem 1.6 Suppose that $H : \mathbf{P} \rightarrow \mathbb{R}$ and $S_0 : \mathbf{M} \rightarrow \mathbb{R}$ are smooth functions, and $\bar{\mathbf{x}} \in \mathbf{M}$. There is a neighborhood $U \subset \mathbf{M}$ of $\bar{\mathbf{x}}$ and a neighborhood $W \subset \mathbf{M} \times \mathbb{R}$ of $(\bar{\mathbf{x}}, 0)$ such that there is a unique smooth solution $S : W \rightarrow \mathbb{R}$ of the IVP

$$\begin{aligned} S_t + H\left(\frac{\partial S}{\partial \mathbf{x}}, \mathbf{x}\right) &= 0 & (\mathbf{x}, t) \in W, \\ S(\mathbf{x}, 0) &= S_0(\mathbf{x}) & \mathbf{x} \in U. \end{aligned}$$

Proof. We will only sketch the proof. (For the analytical details, see *e.g.* §3.2 of [11].) Standard ODE theorems imply that for every $\mathbf{x}_0 \in \mathbf{M}$, there is a unique local solution of Hamilton's equations (1.12) with the initial data

$$\mathbf{x}(0) = \mathbf{x}_0, \quad \mathbf{p}(0) = \frac{\partial S_0}{\partial \mathbf{x}}(\mathbf{x}_0). \quad (1.15)$$

We write this solution as

$$\mathbf{x}(t) = \mathbf{X}(t; \mathbf{x}_0), \quad \mathbf{p}(t) = \mathbf{P}(t; \mathbf{x}_0). \quad (1.16)$$

Since $\det[\partial \mathbf{X} / \partial \mathbf{x}_0] \neq 0$ when $t = 0$, the implicit function theorem implies that the map $\mathbf{x}_0 \rightarrow \mathbf{x}(t)$ is locally invertible for sufficiently small t . Thus there is an open interval $I \subset \mathbb{R}$ containing the origin, a neighborhood $U \subset \mathbf{M}$ of $\bar{\mathbf{x}}$, and a neighborhood $W \subset \mathbf{M} \times I$ of $(\bar{\mathbf{x}}, 0)$, such that for every point $(\mathbf{x}_1, t_1) \in W$ there exists a unique point $\mathbf{x}_0 = \mathbf{X}_0(t_1; \mathbf{x}_1) \in U$ with

$$\mathbf{x}_1 = \mathbf{X}(t_1; \mathbf{x}_0).$$

We then define $S : W \rightarrow \mathbb{R}$ by (*c.f.* equation (1.13))

$$S(\mathbf{x}_1, t_1) = S_0(\mathbf{X}_0(t_1; \mathbf{x}_1)) + \int_{C(\mathbf{x}_1, t_1)} \{\mathbf{p} \cdot d\mathbf{x} - H dt\},$$

where $C(\mathbf{x}_1, t_1)$ is the characteristic curve (1.16) with $\mathbf{x}(t_1) = \mathbf{x}_1$ and $0 \leq t \leq t_1$ (or $t_1 \leq t \leq 0$ if $t_1 < 0$).

One can verify directly that this function satisfies the Hamilton-Jacobi equation (1.9) in W . Uniqueness follows from the method of characteristics described above. \square

Although the IVP for (1.9) has a unique local solution, the global structure of the solution is usually more complicated. We denote the flow of the Hamiltonian vector field in (1.9) by $g^t : \mathbf{P} \rightarrow \mathbf{P}$. For simplicity, we suppose that the solutions of (1.9) exist globally in time, so that g^t is defined for all $t \in \mathbb{R}$.

The initial data (1.14) defines a d -dimensional submanifold Λ^0 of $2d$ -dimensional phase space, with equation

$$\mathbf{p} = \frac{\partial S_0}{\partial \mathbf{x}}(\mathbf{x}).$$

The phase flow maps Λ^0 to a submanifold

$$\Lambda^t = g^t \Lambda^0.$$

For sufficiently small t , Λ^t projects locally onto \mathbf{M} under π in (1.11), and we obtain a unique local solution. For larger times, Λ^t may “fold over,” so that several points on it project to the same point of space.

An image of a singularity of the projection $\pi : \Lambda^t \rightarrow \mathbf{M}$, where the derivative $d\pi$ is singular, is called a *caustic*. The structure of generic caustics may be classified by the use of singularity theory [2]. Once caustics form, the method of characteristics gives a multivalued solution $S(\cdot, t)$ of the Hamilton-Jacobi equation.

It is often useful, instead, to regard the phase as a single-valued phase function $\tilde{S}(\cdot, t)$ defined on Λ^t . From (1.13), the variation in the phase \tilde{S} along a characteristic curve is given by

$$\frac{d\tilde{S}}{dt} = \mathbf{p} \cdot \frac{d\mathbf{x}}{dt} - H, \quad (1.17)$$

which implies that, for $(\mathbf{x}_1, \mathbf{p}_1) \in \Lambda^{t_1}$,

$$\tilde{S}(\mathbf{x}_1, \mathbf{p}_1, t_1) = S_0(\mathbf{x}_0) + \int_C \{\mathbf{p} \cdot d\mathbf{x} - H dt\},$$

where C is the characteristic curve $t \mapsto (\mathbf{x}(t), \mathbf{p}(t))$ that satisfies $\mathbf{x}(0) = \mathbf{x}_0$, $\mathbf{p}(0) = \partial S_0 / \partial \mathbf{x}(\mathbf{x}_0)$, and $\mathbf{x}(t_1) = \mathbf{x}_1$, $\mathbf{p}(t_1) = \mathbf{p}_1$.

Remark 1.7 We may also consider \tilde{S} as defined on the $(d+1)$ -dimensional submanifold

$$\Lambda = \bigcup_{t \in \mathbb{R}} \Lambda^t$$

of the $2(d+1)$ -dimensional phase space with coordinates $(\mathbf{x}, t, \mathbf{p}, E)$, where $H(\mathbf{p}, \mathbf{x}) = -E$.

Away from the caustics, there are finitely many[†] phase functions S_j , each of which is a local solution of (1.9), such that

$$S_j(\mathbf{x}, t) = \tilde{S}(\mathbf{x}, \mathbf{p}_j, t), \quad (\mathbf{x}, \mathbf{p}_j) \in \Lambda^t.$$

Each phase is associated with a ray, and several rays reach the same point with different momenta. As we explain below (*c.f.* Section 1.7), near the caustics, the

[†]there may be none at all

amplitude of the wave is larger than elsewhere, as a result of the focusing of the rays. Moreover, there is a phase shift of $-\pi/2$ in the wave amplitude each time a ray passes through a simple caustic.

Thus, when caustics are present, the semiclassical solution away from the caustics has the form

$$\psi \sim \sum_j A_j e^{iS_j/\hbar - i\pi\mu_j/2},$$

where the integer μ_j is the Morse index of the j th ray, which is equal to the number of caustics (counted according to their multiplicity) that the ray passes through (see Section 1.5).

1.5 The calculus of variations and conjugate points

Let us consider all (smooth) paths $\xi : [t_0, t_1] \rightarrow \mathbb{R}^d$ such that $\xi(t_0) = \mathbf{x}_0$, and $\xi(t_1) = \mathbf{x}_1$. Let $t \mapsto \mathbf{x}(t)$ be a stationary point of the action

$$\mathcal{S}(\xi) = \int_{t_0}^{t_1} L\left(\xi, \frac{d\xi}{dt}\right) dt.$$

Then we define the classical action (or Hamilton's principal function) S by

$$S(\mathbf{x}_1, t_1; \mathbf{x}_0, t_0) = \mathcal{S}(\mathbf{x}).$$

Thus, S is the action associated with the classical particle path. In general, there may be several stationary paths, and then S is multi-valued. (It is single valued when $t_1 - t_0$ is sufficiently small.)

Example 1.8 Consider the simple harmonic oscillator, with equation of motion

$$m \frac{d^2 x}{dt^2} + m\omega^2 x = 0,$$

and action

$$\mathcal{S}(x) = \int_{t_0}^{t_1} \left\{ \frac{1}{2} m \left(\frac{dx}{dt} \right)^2 - \frac{1}{2} m \omega^2 x^2 \right\} dt.$$

Then, provided that $\omega(t_0 - t_1) \neq n\pi$, the classical path with $x(t_0) = x_0$ and $x(t_1) = x_1$ is given by

$$x(t) = x_0 \cos \omega(t - t_0) + \left[\frac{x_1 - x_0 \cos \omega(t_1 - t_0)}{\sin \omega(t_1 - t_0)} \right] \sin \omega(t - t_0).$$

Evaluating the action on this path, we find that the classical action is given by

$$S(x_1, t_1; x_0, t_0) = \frac{m\omega}{2 \sin \omega(t_1 - t_0)} [(x_0^2 + x_1^2) \cos \omega(t_1 - t_0) - 2x_0 x_1].$$

Theorem 1.9 The classical action $S(\mathbf{x}, t; \mathbf{x}_0, t_0)$ is a solution of the Hamilton-Jacobi equation

$$S_t + H\left(\frac{\partial S}{\partial \mathbf{x}}, \mathbf{x}\right) = 0.$$

Proof. First, consider a stationary path $\mathbf{x}(t)$ such that $\mathbf{x}(t_0) = \mathbf{x}_0$ and $\mathbf{x}(t_1) = \mathbf{x}_1$. We consider a nearby stationary path $\mathbf{x}(t) + \mathbf{h}(t)$ with $\mathbf{h}(t_0) = 0$ and $\mathbf{h}(t_1) = \mathbf{h}_1$. Then

$$\begin{aligned} & S(\mathbf{x}_1 + \mathbf{h}_1, t_1; \mathbf{x}_0, t_0) - S(\mathbf{x}_1, t_1; \mathbf{x}_0, t_0) \\ &= \int_{t_0}^{t_1} \left\{ L\left(\mathbf{x} + \mathbf{h}, \frac{d\mathbf{x}}{dt} + \frac{d\mathbf{h}}{dt}\right) - L\left(\mathbf{x}, \frac{d\mathbf{x}}{dt}\right) \right\} dt \\ &= \int_{t_0}^{t_1} \left\{ \frac{\partial L}{\partial \mathbf{x}}\left(\mathbf{x}, \frac{d\mathbf{x}}{dt}\right) \cdot \mathbf{h} + \frac{\partial L}{\partial \mathbf{v}}\left(\mathbf{x}, \frac{d\mathbf{x}}{dt}\right) \cdot \frac{d\mathbf{h}}{dt} \right\} dt + O(\mathbf{h}^2) \\ &= \left[\frac{\partial L}{\partial \mathbf{v}} \cdot \mathbf{h} \right]_{t_0}^{t_1} + \int_{t_0}^{t_1} \left\{ \frac{\partial L}{\partial \mathbf{x}} - \frac{d}{dt} \frac{\partial L}{\partial \mathbf{v}} \right\} \cdot \mathbf{h} dt + O(\mathbf{h}^2) \\ &= \frac{\partial L}{\partial \mathbf{v}}\left(\mathbf{x}(t_1), \frac{d\mathbf{x}}{dt}(t_1)\right), \end{aligned}$$

where we have used the fact that $\mathbf{x}(t)$ satisfies the Euler-Lagrange equations associated with L . It follows that

$$\frac{\partial S}{\partial \mathbf{x}_1}(\mathbf{x}_1, t_1; \mathbf{x}_0, t_0) = \frac{\partial L}{\partial \mathbf{v}}(\mathbf{x}_1, \mathbf{v}_1), \quad (1.18)$$

where \mathbf{v}_1 is the velocity of the stationary path at $t = t_1$,

$$\mathbf{v}_1 = \frac{d\mathbf{x}}{dt}(t_1).$$

Next, we consider how S changes with time. Let $\mathbf{x}(t)$ be a stationary path such that $\mathbf{x}(t_0) = \mathbf{x}_0$ and $\mathbf{x}(t_1) = \mathbf{x}_1$, and $\mathbf{x}(t_1 + k) = \mathbf{x}_1 + \mathbf{h}_1$. Then

$$\begin{aligned} & S(\mathbf{x}_1 + \mathbf{h}_1, t_1 + k; \mathbf{x}_0, t_0) - S(\mathbf{x}_1, t_1; \mathbf{x}_0, t_0) \\ &= \int_{t_1}^{t_1+k} L\left(\mathbf{x}, \frac{d\mathbf{x}}{dt}\right) dt \\ &= L(\mathbf{x}_1, \mathbf{v}_1)k + O(k^2). \end{aligned}$$

We have $\mathbf{h}_1 = k\mathbf{v}_1 + O(k^2)$, so dividing by k and letting $k \rightarrow 0$, we obtain that

$$S_{t_1}(\mathbf{x}_1, t_1; \mathbf{x}_0, t_0) + \mathbf{v}_1 \cdot \frac{\partial S}{\partial \mathbf{x}_1}(\mathbf{x}_1, t_1; \mathbf{x}_0, t_0) = L(\mathbf{x}_1, \mathbf{v}_1).$$

Hence, from (1.18), we get

$$S_{t_1}(\mathbf{x}_1, t_1; \mathbf{x}_0, t_0) + \mathbf{v}_1 \cdot \frac{\partial L}{\partial \mathbf{v}}(\mathbf{x}_1, \mathbf{v}_1) - L(\mathbf{x}_1, \mathbf{v}_1) = 0.$$

Since the Hamiltonian is the Legendre transform of the Lagrangian, and $\mathbf{p}_1 = \partial S / \partial \mathbf{x}_1$, the result follows. \square

1.6 Symplectic geometry

From a mathematical point of view, classical mechanics is part of symplectic geometry. A symplectic structure arises naturally from short wave asymptotics, which explains how the symplectic structure of classical mechanics arises from quantum mechanics. In this section, we make a few brief remarks about the geometry of phase space.

A *symplectic manifold* is a manifold equipped with a closed nondegenerate two-form [1]. The phase space \mathbf{P} considered in the previous section is a symplectic manifold with the canonical two-form [1]

$$\omega = d\mathbf{p} \wedge d\mathbf{x} = dp_i \wedge dx^i. \quad (1.19)$$

Here, $\mathbf{x} = (x^1, \dots, x^d)$, $\mathbf{p} = (p_1, \dots, p_d)$, and summation is implied over repeated upper and lower indices. (If X and Y are vectors in \mathbf{P} , then $\omega(X, Y)$ is the sum of the areas of the parallelograms formed by the projections of X and Y onto the (x^i, p_i) coordinate planes.) We have $\omega = d\theta$, where θ is the canonical one-form

$$\theta = \mathbf{p} \cdot d\mathbf{x} = p_i dx^i.$$

The symplectic form (1.19) arises naturally on the cotangent bundle $T^*\mathbf{M}$ of any manifold \mathbf{M} . If $S : \mathbf{M} \rightarrow \mathbb{R}$ is a function defined on configuration space, then the differential

$$dS = \left(\frac{\partial S}{\partial x^i} \right) dx^i$$

is a covector field $dS : \mathbf{M} \rightarrow T^*\mathbf{M}$. (Here we use the notation of differential forms, instead of the less geometrical partial derivative notation $\partial S / \partial \mathbf{x}$.)

The function defines a d -dimensional submanifold Λ of $\mathbf{P} = T^*\mathbf{M}$, with the equation

$$\mathbf{p} = dS(\mathbf{x}).$$

An important geometrical property of such a submanifold is that it is Lagrangian.

Definition 1.10 A *Lagrangian submanifold* of a symplectic manifold (\mathbf{P}, ω) of dimension $2d$ is a submanifold Λ of dimension d such that

$$\omega|_{\Lambda} = 0.$$

Example 1.11 The coordinate planes $\mathbf{x} = 0$ and $\mathbf{p} = 0$ are Lagrangian submanifolds of $\mathbf{P} = \mathbb{R}^{2d}$ with respect to the canonical two-form $d\mathbf{p} \wedge d\mathbf{x}$ (all areas project to

zero). More generally, if $\{\alpha_1, \dots, \alpha_r\}$ and $\{\beta_1, \dots, \beta_s\}$ is any disjoint partition of $\{1, \dots, d\}$ (so $r + s = d$), then the coordinate plane

$$x^{\alpha_1} = 0, \dots, x^{\alpha_r} = 0, \quad p_{\beta_1} = 0, \quad \dots, p_{\beta_s} = 0$$

is Lagrangian.

Lemma 1.12 If Λ is a submanifold of $\mathbf{P} = T^*\mathbf{M}$, and $\pi : U \subset \Lambda \rightarrow \mathbf{M}$ is a diffeomorphism, where U is a simply connected open set, then Λ is Lagrangian if and only if there is a function $\varphi : U \rightarrow \mathbb{R}$ such that

$$U = \{(\mathbf{x}, \mathbf{p}) \in P \mid \mathbf{p} = d\varphi(\mathbf{x})\}.$$

Proof. If U is given by (1.12), then

$$\begin{aligned} \omega|_U &= d\mathbf{p} \wedge d\mathbf{x}|_U \\ &= \left(\frac{\partial^2 \varphi}{\partial x^i \partial x^j} \right) dx^i \wedge dx^j \\ &= 0. \end{aligned}$$

Conversely, suppose that Λ is Lagrangian. Since ω is closed, we may write it locally as $\omega = d\theta$ for a suitable one-form θ , and $d\theta|_U = 0$. Hence, $\theta|_U$ is closed, so we may write it locally as $\theta|_U = dS$. If \mathbf{x} provides local coordinates on Λ , then this implies that $\mathbf{p} = dS(\mathbf{x})$ is a local expression for Λ . \square

The initial manifold Λ^0 has equation $\mathbf{p} = dS_0(\mathbf{x})$, so it is Lagrangian. Since the flow map g^t is symplectic [1], it follows that Λ^t is Lagrangian for all t even after it folds over.

We may introduce a topological invariant associated with a Lagrangian submanifold called the Maslov index.

1.7 Caustics

The straightforward short wave solution described in the previous section breaks down near caustics. We will show that the passage of a ray through a simple caustic (or turning point) leads to a phase shift of $-\pi/2$ in the wave, and that the wave amplitude is of the order $\hbar^{-1/6}$ larger near the caustic than away from it.

A simple caustic separates a classically allowed region from a classically forbidden region, which the classical particle has insufficient energy to penetrate. In quantum mechanics, diffraction effects are important near a caustic, and the normal dependence of the wave function is described by an Airy function, which makes a transition from oscillatory behavior in the classically allowed region, to exponentially decaying behavior in the classically forbidden region. The fact that the wave

function is nonzero (though small) in the classically forbidden region has important physical consequences, such as the quantum tunneling of a particle through a potential barrier. We will not consider this effect here, however.

There are various ways to motivate the asymptotic form of the solution near a caustic, such as the method of stationary phase for a Fourier integral with coalescing stationary phase points,

$$\psi(\mathbf{x}, t; \hbar) = \int A(\mathbf{x}, t; \xi) e^{iS(\mathbf{x}, t; \xi)/\hbar} d\xi.$$

Here we obtain a uniform asymptotic solution by use of the method of multiple scales ([33]). These ideas have extensive further developments in the theory of microlocal analysis (see [10], for example).

We look for a solution of (1.2) of the form

$$\psi(\mathbf{x}, t; \hbar) = \hbar^\nu F\left(\frac{\rho(\mathbf{x}, t)}{\hbar^{2/3}}, \mathbf{x}, t; \hbar\right) e^{i\varphi(\mathbf{x}, t)/\hbar}, \quad (1.20)$$

where ν is an arbitrary exponent which we introduce for later convenience. This solution satisfies (1.2) if and only if $F(\eta, \mathbf{x}, t; \hbar)$ satisfies the PDE

$$\begin{aligned} & \left(\varphi_t + \frac{1}{2m} |\nabla \varphi|^2 + V \right) F - \frac{1}{2m} \hbar^{2/3} |\nabla \rho|^2 F_{\eta\eta} \\ &= i \hbar^{1/3} \left(\rho_t + \frac{1}{m} \nabla \varphi \cdot \nabla \rho \right) F_\eta \\ &+ i \hbar \left(F_t + \frac{1}{m} \nabla \varphi \cdot \nabla F + \frac{1}{2m} \Delta \varphi F \right) \\ &+ \frac{1}{m} \hbar^{4/3} \left(\nabla \rho \cdot \nabla F_\eta + \frac{1}{2} \Delta \rho F_\eta \right) + \frac{1}{2m} \hbar^2 \Delta F. \end{aligned} \quad (1.21)$$

on $\eta = \rho(\mathbf{x}, t)/\hbar^{2/3}$.

We suppose that

$$F(\eta, \mathbf{x}, t; \hbar) = A(\mathbf{x}, t; \hbar) \text{Ai}(\eta) + i \hbar^{1/3} B(\mathbf{x}, t; \hbar) \text{Ai}'(\eta), \quad (1.22)$$

where the prime denotes differentiation with respect to η , $A(\mathbf{x}, t; \hbar)$ and $B(\mathbf{x}, t; \hbar)$ are complex-valued functions, and $\text{Ai}(\eta)$ is the solution of the Airy equation

$$\text{Ai}'' = \eta \text{Ai},$$

that decays as $\eta \rightarrow +\infty$, normalized so that

$$\text{Ai}(0) = \frac{1}{3^{2/3}} \Gamma\left(\frac{2}{3}\right).$$

(See e.g. <http://mathworld.wolfram.com/AiryFunctions.html> for graphs.) This solution decays exponentially as $\eta \rightarrow +\infty$ (corresponding to the classical forbidden

region) and oscillates, with algebraic decay, as $\eta \rightarrow -\infty$. Specifically [29],

$$\text{Ai}(\eta) \sim \begin{cases} \frac{1}{2}\pi^{-1/2}\eta^{-1/4} \exp[-2\eta^{3/2}/3] & \text{as } \eta \rightarrow +\infty, \\ \pi^{-1/2}(-\eta)^{-1/4} \sin[2(-\eta)^{3/2}/3 + \pi/4] & \text{as } \eta \rightarrow -\infty. \end{cases}$$

We have

$$\begin{aligned} F &= AAi + i\hbar^{1/3}BAi', \\ F_\eta &= i\hbar^{1/3}\eta BAi + AAi', \\ F_{\eta\eta} &= (\eta A + i\hbar^{1/3}B)Ai + i\hbar^{1/3}\eta BAi'. \end{aligned}$$

Using (1.22) in (1.21), simplifying the result, and setting $\eta = \rho(\mathbf{x}, t)/\hbar^{2/3}$, we find that

$$-i\hbar\psi_t - \frac{\hbar^2}{2m}\Delta\psi + V\psi = PAi + i\hbar^{1/3}QAi',$$

where

$$\begin{aligned} P &= \left\{ \varphi_t + \frac{1}{2m}|\nabla\varphi|^2 - \rho|\nabla\rho|^2 + V \right\} A + \rho \left\{ \rho_t + \frac{1}{m}\nabla\varphi \cdot \nabla\rho \right\} B \\ &\quad - i\hbar \left\{ A_t + \frac{1}{m}\nabla\varphi \cdot \nabla A + \frac{1}{2m}\Delta\varphi A \right. \\ &\quad \left. + \frac{1}{m}\rho\nabla\rho \cdot \nabla B + \frac{1}{2m}\rho\Delta\rho B + \frac{1}{2m}|\nabla\rho|^2 B \right\} - \frac{\hbar^2}{2m}\Delta A, \\ Q &= \left\{ \varphi_t + \frac{1}{2m}|\nabla\varphi|^2 - \rho|\nabla\rho|^2 + V \right\} B - \left\{ \rho_t + \frac{1}{m}\nabla\varphi \cdot \nabla\rho \right\} A \\ &\quad - i\hbar \left\{ B_t + \frac{1}{m}\nabla\varphi \cdot \nabla B + \frac{1}{2m}\Delta\varphi B + \frac{1}{m}\rho\nabla\rho \cdot \nabla A + \frac{1}{2m}\rho\Delta\rho A \right\} - \frac{\hbar^2}{2m}\Delta B. \end{aligned}$$

Thus, a sufficient condition for (1.20) and (1.22) to give a solution of the Schrödinger equation (1.2) is that

$$P = 0, \quad Q = 0.$$

We look for an asymptotic solution of these equations for A and B of the form

$$\begin{aligned} A &= A^{(0)} + \hbar^{1/3}A^{(1)} + \hbar^{2/3}A^{(2)} + O(\hbar), \\ B &= B^{(0)} + \hbar^{1/3}B^{(1)} + \hbar^{2/3}B^{(2)} + O(\hbar), \end{aligned}$$

where $A^{(0)}$ and $B^{(0)}$ are assumed to be nonzero. Using these expansion in the equations, and equating coefficients of powers of $\hbar^{1/3}$ to zero, we find that

$$\begin{aligned} \varphi_t + \frac{1}{2m}(|\nabla\varphi|^2 - \rho|\nabla\rho|^2) + V &= 0, \\ \rho_t + \frac{1}{m}\nabla\varphi \cdot \nabla\rho &= 0, \end{aligned}$$

$$\begin{aligned}
& A_t^{(0)} + \frac{1}{m} \nabla \varphi \cdot \nabla A^{(0)} + \frac{1}{2m} \Delta \varphi A^{(0)} + \frac{1}{m} \rho \nabla \rho \cdot \nabla B^{(0)} \\
& + \frac{1}{2m} (\rho \Delta \rho + |\nabla \rho|^2) B^{(0)} = 0, \\
& B_t^{(0)} + \frac{1}{m} \nabla \varphi \cdot \nabla B^{(0)} + \frac{1}{2m} \Delta \varphi B^{(0)} + \frac{1}{m} \nabla \rho \cdot \nabla A^{(0)} + \frac{1}{2m} \Delta \rho A^{(0)} = 0.
\end{aligned}$$

The solutions of these equations provide a uniform asymptotic solution of the Schrödinger equation in a region that contains a simple caustic.

In $\rho < 0$, we define

$$S^\pm = \varphi \pm \frac{2}{3} (-\rho)^{3/2}.$$

Then we have

$$S_t^\pm + \frac{1}{2m} |\nabla S^\pm|^2 + V = 0,$$

meaning that each S^\pm satisfies the eikonal equation. We interpret S^- as the phase of an incoming wave, since the corresponding group velocity

$$\frac{1}{m} \nabla \varphi + \frac{1}{m} (-\rho)^{1/2} \nabla \rho$$

is directed towards the caustic $\rho = 0$ from the side $\rho < 0$ where the solution is oscillatory, and S^+ as the phase of an outgoing wave.

As $\eta \rightarrow -\infty$, we find that (1.20) has the form

$$F \sim \frac{\hbar^{\nu+1/6}}{2\pi^{1/2}(-\rho)^{1/4}} A \left\{ e^{iS^-/\hbar+i\pi/4} + e^{iS^+/\hbar-i\pi/4} \right\}.$$

Thus, away from the caustic, the solution is a superposition of two waves, with the phase of the outgoing wave retarded by $\pi/2$ from the phase of the incoming wave. This loss of phases may be interpreted as the result of the diffraction of the wave into the shadow region in a layer of the order of its wavelength. The ray density J is proportional to $(-\rho)^{-1/2}$.

If the wave amplitudes are $O(1)$ as $\hbar \rightarrow 0$ away from the caustic, we see that we must take $\nu = -1/6$. Thus the wave amplitude is larger by a factor of $\hbar^{-1/6}$ in a layer of width $\hbar^{2/3}$ near the caustic (where, again, it is convenient not to nondimensionalize the problem).

1.8 Eigenvalue problems

Eigenvalue problems are harder to analyse than the wavepacket problems we have considered so far, because the semiclassical limit $\hbar \rightarrow 0$ does not commute with the large time limit $t \rightarrow \infty$. There is a consistent semiclassical quantization method (EBK quantization) when the classical system is completely integrable, but the

behavior of the spectrum of quantum systems that correspond to chaotic classical systems is still not well understood.

The $2d$ -dimensional phase space of a completely integrable system with compact energy surfaces is foliated into d -dimensional tori. The basic principle of EBK-quantization is that the phase function of a semiclassical eigenfunction should be single-valued on one of these tori. This picks out tori whose actions are integer multiples of 2π . When caustics are taken into account, this condition leads to corrected Bohr-Sommerfeld conditions.

Even for integrable systems, some difficulties may arise when quantum mechanical tunneling between different tori is possible, typically leading to an exponentially small splitting of eigenvalues. For nonintegrable systems, the problem is much more difficult. Mixing systems have spectra that resemble those of random matrices. For KAM type systems, whose phase space contains a complex fractal structure of invariant tori and stochastic layers, the problem is harder still.

1.9 Path integrals

Every quantum event is associated with a complex number, called the *amplitude* of the event. The probability of the event is proportional to the square of its amplitude. If an event can occur as the result of several different outcomes, then its amplitude is the sum of the amplitudes of each outcome. The amplitude of each outcome is proportional to $e^{iS/\hbar}$ where S is the action of the event.

Remark 1.13 The fact that amplitudes, rather than probabilities, add leads to the interference effects that are characteristics of quantum mechanics.

Feynman used this formulation of quantum mechanics to give a beautiful expression for the solution of the Schrödinger equation in terms of path integrals [12], [13]. In particular, semiclassical quantum mechanics is obtained from the path integral by a stationary phase approximation, so that classical events are ones for which the cancellation between the amplitudes of nearby quantum fluctuations is minimal.

The Green's function, or "propagator," $G(\mathbf{x}, t; \mathbf{y})$, of the Schrödinger equation (1.2) is the solution of

$$\begin{aligned} i\hbar G_t &= -\frac{\hbar^2}{2m}\Delta G + V(\mathbf{x})G, \\ G(\mathbf{x}, 0; \mathbf{y}) &= \delta(\mathbf{x} - \mathbf{y}), \end{aligned}$$

where δ is the delta function. The solution of the initial value problem

$$\begin{aligned} i\hbar\psi_t &= -\frac{\hbar^2}{2m}\Delta\psi + V(\mathbf{x})\psi, \\ \psi(\mathbf{x}, 0) &= \psi_0(\mathbf{x}), \end{aligned}$$

has the Green's function representation

$$\psi(\mathbf{x}, t) = \int_{\mathbb{R}^d} G(\mathbf{x}, t; \mathbf{y}) \psi_0(\mathbf{y}) d\mathbf{y}. \quad (1.23)$$

Feynman's expression for the Green's function as a path integral is

$$G(\mathbf{x}, t; \mathbf{y}) = \frac{1}{Z} \int_{(\mathbf{y}, 0)}^{(\mathbf{x}, t)} e^{i\mathcal{S}(\xi)/\hbar} d\xi. \quad (1.24)$$

Here, $\xi : [0, t] \rightarrow \mathbb{R}^d$ denotes a continuous curve, or “path,” $d\xi$ is supposed to denote a translation-invariant measure on the infinite-dimensional space of paths, and Z is a suitable normalization factor. The integral $\int_{(\mathbf{y}, 0)}^{(\mathbf{x}, t)}$ denotes an integral over the set of paths from \mathbf{y} at time 0 to \mathbf{x} at time t

$$\{\xi \in C([0, t]; \mathbb{R}^d) \mid \xi(0) = \mathbf{y}, \quad \xi(t) = \mathbf{x}\}.$$

As in classical mechanics, the action $\mathcal{S}(\xi, t)$ of a path ξ on the time-interval $[0, t]$ is the time-integral of the difference between the kinetic and potential energies

$$\mathcal{S}(\xi, t) = \int_0^t \left\{ \frac{1}{2} m \left| \frac{d\xi}{ds} \right|^2 - V(\xi) \right\} ds. \quad (1.25)$$

Suppose that a particle is located at the point \mathbf{y} at time 0. The event of observing the particle at the point \mathbf{x} time t can occur in many different ways: the particle can move along any path connecting \mathbf{y} to \mathbf{x} . Formally summing the amplitudes of these paths, we get (1.24).

Despite the intuitive appeal of (1.24), we cannot define the Feynman integral directly as an integral. There are no translationally-invariant measures on infinite-dimensional spaces, analogous to Lebesgue measure on finite-dimensional spaces (see [36] for an interesting discussion of this fact), so “ $d\xi$ ” cannot be interpreted as a measure. Moreover, the integrand in (1.24) is a highly oscillatory function of ξ , since $\mathcal{S}(\xi)$ is large for non-smooth paths, and is not even defined for paths whose derivative does not belong to $L_{\text{loc}}^2(\mathbb{R}_+)$.

We therefore have to define the path integral in some other way, for example, as a limit of finite dimensional integrals on \mathbb{R}^n as $n \rightarrow \infty$, or by analytic continuation from integration with respect to Wiener measure. Unfortunately, these definitions, and others, lack the direct intuitive appeal of the heuristic path-integral formulation.

1.10 Trotter product formula

The definition of the Feynman path integral as a limit of finite-dimensional integrals is based on the Trotter product formula. Every self-adjoint operator A on a Hilbert space is associated with a unitary group e^{-itA} [8], where $u(t) = e^{-itA}u_0$ is the

solution of

$$iu_t = Au, \quad u(0) = u_0.$$

The Trotter product formula (which we consider here only for unitary groups) provides an expression for the solution operator of

$$iu_t = Au + Bu$$

in terms of the solution operators of

$$iu_t = Au, \quad iu_t = Bu.$$

If A and B commute, then

$$e^{-it(A+B)} = e^{-itA} e^{-itB}.$$

If they do not commute, we can still obtain $e^{-i(A+B)t}$ by means of a fractional step method.

Theorem 1.14 (Trotter product) Let

$$A : D(A) \subset \mathcal{H} \rightarrow \mathcal{H}, \quad B : D(B) \subset \mathcal{H} \rightarrow \mathcal{H}$$

be unbounded, self-adjoint operators on a complex Hilbert space \mathcal{H} . Suppose that $A + B$ is essentially self-adjoint on $D(A) \cap D(B)$, and let $C = \overline{A + B}$. Then, for each $u_0 \in \mathcal{H}$,

$$e^{-itC} u_0 = \lim_{n \rightarrow \infty} \left[e^{-itA/n} e^{-itB/n} \right]^n u_0,$$

where the limit exists uniformly in t on bounded intervals $|t| \leq T$.

In other words, $e^{-it(A+B)}$ is the strong limit of $[e^{-itA/n} e^{-itB/n}]^n$. We write the Schrödinger equation (1.2) as an abstract evolution equation on $\mathcal{H} = L^2(\mathbb{R}^d)$,

$$i\hbar\psi_t = H\psi \quad H = \overline{T + V},$$

where the kinetic and potential energy operators T and V , respectively, are given by

$$\begin{aligned} T\psi &= -\frac{\hbar^2}{2m}\Delta\psi, & D(T) &= H^2(\mathbb{R}^d), \\ V\psi &= V \cdot \psi, & D(V) &= \{\psi \in L^2(\mathbb{R}^d) \mid V \cdot \psi \in L^2(\mathbb{R}^d)\}. \end{aligned}$$

Here, with a slight abuse of notation, we use the same symbol V to denote both the potential function and the associated multiplication operator.

The solution of

$$i\hbar\psi_t = V\psi \tag{1.26}$$

is given by

$$\psi(\mathbf{x}, t) = e^{-itV(\mathbf{x})/\hbar} \psi_0(\mathbf{x}),$$

where $\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x})$. The solution of

$$i\hbar\psi_t = T\psi \tag{1.27}$$

is given by

$$\psi(\mathbf{x}, t) = \int_{\mathbb{R}^d} E(\mathbf{x} - \mathbf{y}, t) \psi_0(\mathbf{y}) d\mathbf{y},$$

where E is the Green's function of the free Schrödinger equation

$$E(\mathbf{x}, t) = \left(\frac{m}{2\pi i\hbar t} \right)^{d/2} \exp \left(\frac{im|\mathbf{x}|^2}{2\hbar t} \right).$$

Assuming that V is sufficiently regular[§] for the hypotheses of Theorem 1.14 to hold, we find from the Trotter product formula that

$$\begin{aligned} \psi(\mathbf{x}, t) &= \lim_{n \rightarrow \infty} \left(\frac{mn}{2\pi i\hbar t} \right)^{nd/2} \int_{\mathbb{R}^d} \dots \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} e^{iS_n(\mathbf{x}, \mathbf{y}_{n-1}, \dots, \mathbf{y}_1, \mathbf{y}; t/n)/\hbar} \\ &\quad \psi_0(\mathbf{y}) d\mathbf{y}_{n-1} \dots d\mathbf{y}_1 d\mathbf{y}, \end{aligned} \tag{1.28}$$

where the limit is with respect to the $L^2(\mathbb{R}^d)$ -norm, and

$$S_n(\mathbf{y}_n, \mathbf{y}_{n-1}, \dots, \mathbf{y}_1, \mathbf{y}_0; t) = \frac{t}{n} \sum_{k=0}^{n-1} \left\{ \frac{1}{2} m \frac{|\mathbf{y}_{k+1} - \mathbf{y}_k|^2}{t/n} - V(\mathbf{y}_k) \right\}. \tag{1.29}$$

This expression is a discretization of the action integral (1.25) for a path $\xi : [0, t] \rightarrow \mathbb{R}^d$, with time-step $\Delta t = t/n$ and $\xi(k\Delta t) = \mathbf{y}_k$ for $0 \leq k \leq n$. Thus, (1.28)–(1.29) provides a definition of the path integral representation (1.23)–(1.24) as a limit of finite-dimensional integrals.

Example 1.15 The path integral may be evaluated exactly for a quadratic potential.

1.11 Wiener measure

Feynman's path integral representation of the solutions of the Schrödinger equation inspired Kac to obtain an analogous expression for solutions of a diffusion equation. Kac's path integral is a genuine integral with respect to Wiener measure on the function space of continuous paths. The Feynman integral for the Schrödinger

[§]A sufficient condition for $-\Delta + V$ to be essentially self-adjoint is that $V \geq 0$ pointwise and $V \in L^2_{\text{loc}}(\mathbb{R}^d)$; see [25].

equation may be defined by analytic continuation from the Kac integral for the diffusion equation.

Let

$$\Omega = C(\mathbb{R}_+; \mathbb{R}^d)$$

denote the space of continuous functions $\beta : \mathbb{R}_+ \rightarrow \mathbb{R}^d$, where $\mathbb{R}_+ = [0, \infty)$. Let \mathcal{C} be the σ -algebra on Ω generated by the cylinder sets

$$\{\beta \in \Omega \mid \beta(t_1) \in A_1, \beta(t_2) \in A_2, \dots, \beta(t_n) \in A_n\},$$

where $0 \leq t_1 < t_2 < \dots < t_n$, and A_1, A_2, \dots, A_n are Borel subsets of \mathbb{R}^d .

We denote the Gaussian density with mean zero and variance tI on \mathbb{R}^d by

$$p(\mathbf{x}, t) = \frac{1}{(2\pi t)^{d/2}} \exp\left(-\frac{|\mathbf{x}|^2}{2t}\right).$$

Definition 1.16 Let $\mathbf{x} \in \mathbb{R}^d$. *Wiener measure*, starting at \mathbf{x} , is the probability measure $P^{\mathbf{x}}$ on \mathcal{C} such that $P^{\mathbf{x}}(\beta(0) = \mathbf{x}) = 1$, and

$$\begin{aligned} & P^{\mathbf{x}}(\beta(t_1) \in A_1, \beta(t_2) \in A_2, \dots, \beta(t_n) \in A_n) \\ &= \int_{A_1} \int_{A_2} \dots \int_{A_n} p(\mathbf{y}_1 - \mathbf{x}, t_1) p(\mathbf{y}_2 - \mathbf{y}_1, t_2 - t_1) \dots p(\mathbf{y}_n - \mathbf{y}_{n-1}, t_n - t_{n-1}) \\ & \quad d\mathbf{y}_1 d\mathbf{y}_2 \dots d\mathbf{y}_n. \end{aligned}$$

for all $0 < t_1 < t_2 < \dots < t_n$, and all Borel subsets A_1, A_2, \dots, A_n of \mathbb{R}^d .

It is not clear from the definition that Wiener measure exists, or that it is unique. There are many ways to construct it (for example, by approximation by random walks, or by random Fourier series [26]), but we will take its existence for granted. We denote the expected value of a functional $f : \Omega \rightarrow \mathbb{R}$ that is integrable with respect to $P^{\mathbf{x}}$ by

$$\mathbf{E}^{\mathbf{x}}[f] = \int_{\Omega} f(\beta) dP^{\mathbf{x}}(\beta).$$

For functions that depend only on the values of β at finitely many times $0 < t_1 < t_2 < \dots < t_n$, we have

...

In view of this formula, we write the density of Wiener measure formally as

$$dP^{\mathbf{x}} = \exp\left(-\frac{1}{2} \int_0^t \dot{\beta}^2(s) ds\right) d\beta, \quad (1.30)$$

where $d\beta$ is supposed to denote a suitably normalized translation invariant measure on Ω . This equality is purely heuristic, however, since there is no such translation invariant measure on Ω . Moreover, it is possible to prove that β is nowhere

differentiable almost surely with respect to Wiener measure [26], so that $\dot{\beta}$ is not well-defined. Nevertheless, (1.30) is useful in connecting Wiener and Feynman integrals.

Remark 1.17 We may define a stochastic process[¶]

$$\{B_t : \Omega \rightarrow \mathbb{R}^d \mid t \in \mathbb{R}_+\}$$

on the probability space $(\Omega, \mathcal{C}, P^{\mathbf{x}})$ that consists of the coordinate maps

$$B_t(\beta) = \beta(t).$$

This definition gives a canonical representation of *Brownian motion*, which is a Gaussian, Markov process with the properties that:

- (a) $B_0 = \mathbf{x}$ and $t \mapsto B_t$ is continuous almost surely;
- (b) for all $0 \leq s < t$, the increment $B_t - B_s$ is a Gaussian random variable with mean zero and variance $(t - s)I$ that is independent of B_r for $0 \leq r \leq s$.

The Feynman-Kac formula provides a representation of the solution $u(\mathbf{x}, t)$ of the parabolic IVP

$$\begin{aligned} u_t &= \frac{1}{2} \Delta u - V(\mathbf{x})u & t > 0, \mathbf{x} \in \mathbb{R}^d, \\ u(\mathbf{x}, 0) &= u_0(\mathbf{x}) & \mathbf{x} \in \mathbb{R}^d, \end{aligned} \tag{1.31}$$

in terms of an integral with respect to Wiener measure.

Theorem 1.18 (Feynman-Kac formula) For a sufficiently regular potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$ and initial data $u_0 : \mathbb{R}^d \rightarrow \mathbb{R}$, the solution of (1.31) is given by

$$u(\mathbf{x}, t) = \mathbf{E}^{\mathbf{x}} \left[u_0(\beta(t)) \exp \left\{ - \int_0^t V(\beta(s)) ds \right\} \right]. \tag{1.32}$$

Formally, we may use (1.30) to write (1.32) as

$$u(\mathbf{x}, t) = \int_{\mathbf{x}, 0} \exp \left\{ - \int_0^t \left(\frac{1}{2} \dot{\beta}^2(s) + V(\beta(s)) \right) ds \right\} u_0(\beta(t)) d\beta,$$

where $\int_{\mathbf{x}, 0}$ denotes an integral over the paths $\{\beta \in \Omega \mid \beta(0) = \mathbf{x}\}$. It is possible to prove under suitable assumptions on V that the right hand side of (1.32) can be continued analytically from real t to imaginary t , and that the resulting analytic continuation provides a solution of the Schrödinger equation

$$\begin{aligned} iu_t &= -\frac{1}{2} \Delta u + V(\mathbf{x})u & t > 0, \mathbf{x} \in \mathbb{R}^d, \\ u(\mathbf{x}, 0) &= u_0(\mathbf{x}) & \mathbf{x} \in \mathbb{R}^d, \end{aligned}$$

that results formally from the transformation $t \mapsto it$ to imaginary time in (1.31).

[¶]Here, the subscript t denotes dependence on the time variable t , and not a partial derivative.

1.12 Semiclassical quantum mechanics

Semiclassical mechanics may be obtained as a stationary phase approximation of the path integral. A rigorous justification of a stationary phase argument for the Feynman path integral is more technical than in the finite-dimensional case, and the justification depends on how the path integral is defined. Here, we consider a formal argument.

We can give an alternative expression for the Jacobian J as a *Van Vleck determinant*.

Proposition 1.19

$$J = \det \left(\frac{\partial^2 S}{\partial \mathbf{x} \partial \mathbf{y}} \right).$$

1.13 Wigner transforms

Suppose, for simplicity, that $\varphi : \mathbb{R}^d \rightarrow \mathbb{C}$ is a Schwartz function. We define the Wigner transform $W : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ of φ by

$$\begin{aligned} W(\mathbf{x}, \mathbf{p}) &= \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} \varphi \left(\mathbf{x} - \frac{1}{2}\mathbf{y} \right) \overline{\varphi \left(\mathbf{x} + \frac{1}{2}\mathbf{y} \right)} e^{i\mathbf{p} \cdot \mathbf{y}/\hbar} d\mathbf{y} \\ &= \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} \widehat{\varphi} \left(\mathbf{p} - \frac{1}{2}\mathbf{q} \right) \overline{\widehat{\varphi} \left(\mathbf{p} + \frac{1}{2}\mathbf{q}/\hbar \right)} e^{-i\mathbf{q} \cdot \mathbf{x}} d\mathbf{q}, \end{aligned}$$

where $\widehat{\varphi}$ is the Fourier transform of φ ,

$$\widehat{\varphi}(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{d/2}} \int_{\mathbb{R}^d} \varphi(\mathbf{x}) e^{-i\mathbf{p} \cdot \mathbf{x}/\hbar} d\mathbf{x}.$$

The Wigner transform has the property that

$$\int_{\mathbb{R}^d} W(\mathbf{x}, \mathbf{p}) d\mathbf{p} = |\varphi(\mathbf{x})|^2, \quad \int_{\mathbb{R}^d} W(\mathbf{x}, \mathbf{p}) d\mathbf{x} = |\widehat{\varphi}(\mathbf{p})|^2.$$

Thus, in some respects, W is similar to a phase space density of φ . It may, however, be negative.

Example 1.20 Find the Wigner transform of a function

$$\varphi(\mathbf{x}) = A(\mathbf{x}) e^{iS(\mathbf{x})/\hbar},$$

and compute its limit as $\hbar \rightarrow 0$.

Remark 1.21 A nonnegative density function, the *Husimi transform*, may be obtained by convolution of W with a Gaussian in both variables. One may also construct H -measures (Tartar) or Wigner measures (Gerard). The nonnegativity of W is recovered in the limit $\hbar \rightarrow 0$.

If $\psi(\mathbf{x}, t)$ satisfies the Schrödinger equation (1.2), and

$$W(\mathbf{x}, \mathbf{p}, t) = \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} \psi\left(\mathbf{x} - \frac{1}{2}\mathbf{y}, t\right) \overline{\psi\left(\mathbf{x} + \frac{1}{2}\mathbf{y}, t\right)} e^{i\mathbf{p}\cdot\mathbf{y}/\hbar} d\mathbf{y},$$

is the Wigner transform of ψ , then it follows that

$$\begin{aligned} & W_t(\mathbf{x}, \mathbf{p}, t) + \frac{\mathbf{p}}{m} \cdot \frac{\partial W}{\partial \mathbf{x}}(\mathbf{x}, \mathbf{p}, t) \\ & - \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} \left[\frac{V\left(\mathbf{x} - \frac{1}{2}\mathbf{y}\right) - V\left(\mathbf{x} + \frac{1}{2}\mathbf{y}\right)}{i\hbar} \right] \psi\left(\mathbf{x} - \frac{1}{2}\mathbf{y}\right) \overline{\psi\left(\mathbf{x} + \frac{1}{2}\mathbf{y}\right)} e^{i\mathbf{p}\cdot\mathbf{y}/\hbar} d\mathbf{y} = 0. \end{aligned}$$

Hence as $\hbar \rightarrow 0$, we find that W satisfies a Liouville equation,

$$W_t + \frac{\mathbf{p}}{m} \cdot \frac{\partial W}{\partial \mathbf{x}} - \frac{\partial V}{\partial \mathbf{x}} \cdot \frac{\partial W}{\partial \mathbf{p}} = 0.$$

The characteristics of this PDE are

$$\frac{d\mathbf{x}}{dt} = \frac{\mathbf{p}}{m}, \quad \frac{d\mathbf{p}}{dt} = -\frac{\partial V}{\partial \mathbf{x}}$$

These are the classical equations corresponding to the Hamiltonian

$$H(\mathbf{x}, \mathbf{p}) = \frac{|\mathbf{p}|^2}{2m} + V(\mathbf{x}).$$

1.14 References

For semiclassical mechanics, see... For path integrals, see [13], [25], and [45]. For quantum chaos, see..

Chapter 2

Linear Dispersive Waves

In this Chapter, we describe some basic ideas about dispersive wave propagation, such as group velocity.

2.1 Dispersion relations

We consider a linear wave equation in d -dimensional Euclidean space, whose solution depends on a space variable $\mathbf{x} \in \mathbb{R}^d$ and a time variable $t \in \mathbb{R}$. If the wave equation is invariant under space and time translations (corresponding to wave propagation in a uniform medium), then it has solutions proportional to the Fourier modes (the eigenfunctions of space and time translations)

$$e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)}. \quad (2.1)$$

The constants $\mathbf{k} \in \mathbb{R}^d$ and $\omega \in \mathbb{R}$ are called the *wavenumber* and (angular) *frequency* of the wave, respectively. The *phase velocity* $\mathbf{c} \in \mathbb{R}^d$ of the wave (2.1) is the normal velocity of the phase fronts $\mathbf{k} \cdot \mathbf{x} - \omega t = \text{constant}$, or

$$\mathbf{c} = \frac{\omega}{k} \frac{\mathbf{k}}{k}, \quad (2.2)$$

where $k = |\mathbf{k}|$ is the Euclidean norm of \mathbf{k} .

We suppose that the Fourier modes (2.1) are solutions of the wave equation if the frequency is related to the wavenumber by

$$\omega = W(\mathbf{k}), \quad (2.3)$$

where $W : \mathbb{R}^d \rightarrow \mathbb{R}$. Equation (2.3) is called the *dispersion relation* of the wave. More generally, the dispersion relation may have the form

$$P(-i\omega, i\mathbf{k}) = 0,$$

where P is the symbol of the operator that defines the wave equation. Different roots of this equation for ω give the dispersion relation of different wave-modes.

For waves modeled by a PDE in (\mathbf{x}, t) , the function P is a polynomial. For waves modeled by an integro-differential equation, a pseudo-differential equation, or an IBVP (such as waves in a waveguide, see Exercise 2.2), the function P may be algebraic or transcendental. In some cases, a wave equation may have no dispersion relation. If W is complex-valued, then the wave is damped or unstable with $\text{Im } \omega$ giving the growth rate. We will assume that W is real-valued, unless we state explicitly otherwise.

We define the *group velocity* $\mathbf{C} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ of the wave by

$$\mathbf{C} = \frac{\partial W}{\partial \mathbf{k}}. \quad (2.4)$$

The *dispersion tensor* of the wave is

$$D = \frac{\partial^2 W}{\partial \mathbf{k}^2}. \quad (2.5)$$

A wave is *dispersive* if the dispersion tensor is nonsingular, meaning that

$$\det \left(\frac{\partial^2 W}{\partial k_i \partial k_j} \right) \neq 0,$$

otherwise the wave is *nondispersive*.

Example 2.1 (Given by Stokes in an 1876 exam question at Cambridge University.) Consider a superposition of two waves with wavenumbers $\mathbf{k} + \Delta \mathbf{k}$ and $\mathbf{k} - \Delta \mathbf{k}$, where $|\Delta \mathbf{k}| \ll |\mathbf{k}|$:

$$u(\mathbf{x}, t) = ae^{i(\mathbf{k} + \Delta \mathbf{k}) \cdot \mathbf{x} - iW(\mathbf{k} + \Delta \mathbf{k})t} + ae^{i(\mathbf{k} - \Delta \mathbf{k}) \cdot \mathbf{x} - iW(\mathbf{k} - \Delta \mathbf{k})t}.$$

Taylor expanding this expression in $\Delta \mathbf{k}$, and using the definition (2.4) of the group velocity, we obtain that

$$\begin{aligned} u(\mathbf{x}, t) &= A(\mathbf{x}, t)e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} + O(\Delta \mathbf{k}), \\ A(\mathbf{x}, t) &= 2a \cos [\Delta \mathbf{k} \cdot (\mathbf{x} - \mathbf{C}(\mathbf{k})t)]. \end{aligned}$$

Thus, the “beats” in the envelope of the wave train propagate at the group velocity.

The general solution of a wave equation for a scalar wave-field $u(\mathbf{x}, t)$ with a single mode and a dispersion relation (2.3) is

$$u(\mathbf{x}, t) = \int f(\mathbf{k}) e^{i(\mathbf{k} \cdot \mathbf{x} - W(\mathbf{k})t)} d\mathbf{k},$$

where $f(\mathbf{k})$ is the Fourier transform of the initial data $u(\mathbf{x}, 0)$. For definiteness, we suppose that $f \in C_c^\infty(\mathbb{R}^d)$ is a smooth function with compact support. This solution may be written as

$$u(\mathbf{x}, t) = \int f(\mathbf{k}) e^{it\varphi(\mathbf{x}/t, \mathbf{k})} d\mathbf{k}, \quad (2.6)$$

where

$$\varphi(\mathbf{v}, \mathbf{k}) = \mathbf{k} \cdot \mathbf{v} - W(\mathbf{k}).$$

We consider the limit of (2.6) as $t \rightarrow \infty$ with $\mathbf{x}/t = \mathbf{v}$, where \mathbf{v} is fixed. The asymptotic behavior of the integral in (2.6) is dominated by contributions from a neighborhood of the stationary phase points such that

$$\frac{\partial \varphi}{\partial \mathbf{k}}(\mathbf{v}, \mathbf{k}) = 0.$$

Thus, $\mathbf{k} = \mathbf{k}'(\mathbf{v})$ is a stationary phase point if

$$\mathbf{C}(\mathbf{k}'(\mathbf{v})) = \mathbf{v}, \quad (2.7)$$

meaning that the group velocity of $\mathbf{k}'(\mathbf{v})$ is equal to \mathbf{v} .

The Taylor expansion of φ in \mathbf{k} at a stationary phase point is

$$\varphi(\mathbf{v}, \mathbf{k}) = \varphi(\mathbf{v}, \mathbf{k}') - \frac{1}{2} D(\mathbf{k}') \cdot (\mathbf{k} - \mathbf{k}', \mathbf{k} - \mathbf{k}') + O(|\mathbf{k} - \mathbf{k}'|^3),$$

where D is the dispersion tensor defined in (2.5).

It follows that (Exercise 2.4)

$$u(\mathbf{v}t, t) \sim \left(\frac{2\pi}{t}\right)^{d/2} \sum' \frac{1}{\sqrt{\det D}} f(\mathbf{k}') e^{i\pi\sigma/4} e^{i\varphi(\mathbf{v}, \mathbf{k}')t} \quad \text{as } t \rightarrow \infty, \quad (2.8)$$

where the sum is taken over all wavenumbers $\mathbf{k}'(\mathbf{v})$ in the support of f that satisfy (2.7), and σ is the index of the dispersion tensor D , that is the number of its negative eigenvalues.

The energy in a wave packet propagates at the group velocity, rather than the phase velocity, and it is the group velocity that is of fundamental importance. The group velocity of a dispersive wave has nonsingular derivative with respect to \mathbf{k} . As a result, the initial data spreads out, or disperses, into an oscillatory wave train.

Example 2.2 The dispersion relation of the wave equation,

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

is

$$\omega^2 = c_0^2 k^2,$$

where the parameter $c_0 > 0$ is a wave speed. This equation has two roots,

$$\omega = \pm c_0 k.$$

We consider the positive root for definiteness. The phase and group velocities $\mathbf{c} = \mathbf{C} = c_0 \mathbf{k}/k$ are equal. The dispersion tensor,

$$D = \frac{c_0}{k} \left(I - \frac{\mathbf{k} \otimes \mathbf{k}}{k^2} \right),$$

has \mathbf{k} as a null vector, so the wave equation is nondispersive. Waves that propagate in the same direction have the same group (and phase) velocities so they do not disperse. Nevertheless, waves that propagate in different directions have different phase velocities, so they do spread out; this directionally dependent dispersion is called *diffraction*.

Example 2.3 The water wave equations are..

The dispersion relation of gravity water waves in deep water is given by

$$\omega^2 = gk, \quad (2.9)$$

where g is the acceleration due to gravity. Here, “deep water” means that the depth of the water is much greater than the wavelength of the water wave. Dimensional arguments imply that if the only parameter appearing in the equations modeling the waves is an acceleration g , with dimensions LT^{-2} , where L denotes a dimension of length and T denotes a dimension of time, then ω^2 , with dimensions of T^{-2} , must depend linearly on gk . If the wave equation is isotropic (that is, invariant under rotations and reflections), as is the case for water waves which propagate horizontally but are acted on by a vertical gravitational force, then ω can depend only on the norm k . This argument determines the dispersion relation in (2.9) up to a constant of proportionality.

The dispersion relation of water waves in water of depth h is

$$\omega^2 = gk \tanh kh.$$

This relation reduces to (2.9) as $kh \rightarrow \infty$.

Equation (2.9) implies that the group velocity $\mathbf{C} = \mathbf{c}/2$ is parallel to the phase velocity \mathbf{c} , but has half its magnitude: As a result, wave packets move slower than wave crests, and the crests move through a packet of waves. This phenomenon can be observed in the circular ring of water waves created by throwing a stone into a pond.

The generation of waves by a ship in a wedge of half-angle $\tan^{-1} 1/(2\sqrt{2})$, or approximately 19.5° can also be explained by a group velocity argument. This problem is the one that led Kelvin to develop the method of stationary phase.

By contrast, the dispersion relation for deep water, capillary waves, whose restoring forcing is dominated by surface tension instead of gravity, is

$$\omega^2 = \tau k^3,$$

where τ is the coefficient of surface tension (with dimensions L^2T^{-2}). In this case the group velocity $\mathbf{C} = 3\mathbf{c}/2$ has a larger magnitude than the phase velocity, explaining why capillary waves appear upstream of a moving source.

Example 2.4 The Boussinesq equations for the motion of a stratified fluid are...

Consider a dispersion relation of the form

$$\omega = \omega_0 \frac{\mathbf{k} \cdot \mathbf{n}}{k},$$

where the frequency depends on the direction of the wavenumber vector but not its magnitude. Here, the parameter ω_0 is a constant frequency, and \mathbf{n} is a constant unit vector. This dispersion relations arises for internal waves in a stratified fluid, where ω_0 the Väisälä-Brunt frequency, and \mathbf{n} is in the direction of gravity. The phase and group velocities,

$$\mathbf{c} = \omega_0 \frac{\mathbf{k} \cdot \mathbf{n}}{k} \frac{\mathbf{k}}{k}, \quad \mathbf{C} = \frac{\omega_0}{k} \left(\mathbf{n} - \frac{\mathbf{n} \cdot \mathbf{k}}{k} \frac{\mathbf{k}}{k} \right),$$

are orthogonal, and wave packets propagate in a direction orthogonal to their wave crests.

A striking effect of the orthogonality of the phase and group velocities is the generation of a cross-shaped pattern of internal waves by an oscillating cylinder in a stratified fluid (see [30], [53] for pictures of this “St. Andrew’s cross”). As this example illustrates, waves with different phase and group velocities often behave in unexpected ways based on ones familiarity with the wave equation, where the phase and group velocities coincide.

2.2 Wave trains and ray tracing

A *wave train* is a function of the form

$$u(\mathbf{x}, t) = A(\mathbf{x}, t) e^{i\theta(\mathbf{x}, t)}. \quad (2.10)$$

We call $A(\mathbf{x}, t) \in \mathbb{C}$ the *amplitude* and $\theta(\mathbf{x}, t) \in \mathbb{R}$ the *phase*. The uniqueness of the decomposition of u in (2.10) into an amplitude and a phase arises in an asymptotic, or “geometrical optics,” limit in which the amplitude and phase are slowly varying functions, in the sense that we explain below (2.11). When A is compactly supported, or rapidly decaying, in \mathbf{x} then we often call a wave train a *wave packet*.

We consider a scalar-valued wave-field for simplicity. More generally, the amplitude A may be vector-valued (as for electromagnetic or elastic waves, which introduces the phenomenon of polarization), tensor-valued (as for gravitational waves in general relativity), spinor-valued, or it may take values in some other space. A real-valued wave-field is given by the sum of (2.10) and its complex conjugate,

$$u(\mathbf{x}, t) = A(\mathbf{x}, t) e^{i\theta(\mathbf{x}, t)} + \text{c.c.}$$

For linear waves, we may instead take the real part of (2.10), to get

$$u(\mathbf{x}, t) = a(\mathbf{x}, t) \cos(\theta(\mathbf{x}, t) + \delta(\mathbf{x}, t)),$$

where $A = ae^{i\delta}$, with $a, \delta \in \mathbb{R}$.

Taylor expanding the solution (2.10) about $(\mathbf{x}, t) = (\mathbf{x}_0, t_0)$, we get a local plane wave solution

$$u(\mathbf{x}, t) \sim A(\mathbf{x}_0, t_0) e^{i\mathbf{k}_0 \cdot (\mathbf{x} - \mathbf{x}_0) - i\omega_0(t - t_0) + i\theta(\mathbf{x}_0, t_0)},$$

where $\mathbf{k}_0 = \nabla\theta(\mathbf{x}_0, t_0)$ and $\omega_0 = -\theta_t(\mathbf{x}_0, t_0)$. We therefore define the local wavenumber $\mathbf{k}(\mathbf{x}, t)$ and frequency $\omega(\mathbf{x}, t)$ of the wave train (2.10) by

$$\mathbf{k} = \nabla\theta, \quad \omega = -\theta_t. \quad (2.11)$$

It follows from (2.11) that

$$\mathbf{k}_t + \nabla\omega = 0.$$

This equation states the number of wave crests is conserved, a natural result when the variations in the phase are slow enough that crests cannot appear or disappear within a single period.

Example 2.5 The Fourier mode (2.1) corresponds to a wave train with constant wavenumber and frequency.

Example 2.6 The stationary phase approximation (2.8) is a wave train (Exercise 2.5).

Suppose that the local frequency and wave number are related by a local dispersion relation of the form

$$\omega = W(\mathbf{k}, \mathbf{x}, t). \quad (2.12)$$

This equation arises in the limit of slowly varying wave trains, in the sense that the frequency, wavenumber, and the amplitude change by a small fraction over a single period. For example, if $\mathbf{k} \neq 0$, then

$$\frac{|\nabla\mathbf{k}|}{k^2} \ll 1, \quad \frac{|\nabla A|}{k|A|} \ll 1.$$

Here, we take (2.12) as an assumption, and explore its consequences. The explicit dependence of W on \mathbf{x} and t describes a nonuniform and nonstationary medium whose properties may vary in space and time. Using the definitions of the local frequency and wavenumber (2.11) in the local dispersion relation (2.12), we see that the phase θ satisfies a Hamilton-Jacobi equation, called the *eikonal equation*,

$$\theta_t + W(\nabla\theta, \mathbf{x}, t) = 0. \quad (2.13)$$

The characteristic curves of (2.13) satisfy Hamilton's equations

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &= \frac{\partial W}{\partial \mathbf{k}}, \\ \frac{d\mathbf{k}}{dt} &= -\frac{\partial W}{\partial \mathbf{x}}, \end{aligned} \quad (2.14)$$

in which the wavenumber (the normal to the wavefronts $\theta = \text{constant}$) corresponds to the momentum, and the dispersion function W corresponds to the Hamiltonian. The projections $t \mapsto \mathbf{x}(t)$ of the characteristic curves onto space are called *rays*. The velocity of a ray is the group velocity \mathbf{C} .

Remark 2.7 The appearance of Hamilton’s equations and a symplectic structure is a general feature of geometrical optics, or microlocal analysis, and is one of the main ways in which symplectic structures arise in physics (*c.f.* classical mechanics and quantum mechanics).

As in the case of the Schrödinger equation, the rays may focus and form caustics, after which the solution of the Hamilton-Jacobi equation may become multivalued, meaning that several waves with different initial wave numbers and locations propagate to the same point; there may also be “shadow regions” that are not covered by any rays. As a result of the focusing of rays, the amplitude of the wave is larger at a caustic than elsewhere. This makes caustics in light waves easily visible in a coffee cup. An important feature of caustics is that they lead to a phase shift in the wave as it passes through a caustic.

When many caustics are present, the global pattern of rays becomes very complicated. This complexity is a major difficulty in the practical implementation of ray-tracing methods.

Remark 2.8 It is possible to define the notion of single-valued weak solution of a Hamilton-Jacobi equation called a *viscosity solution*. In making the viscosity solution single-valued, one has to give up its smoothness (it may have corners or other singularities). Although viscosity solutions are not the relevant ones for the phase of a linear wave train, a number of attempts have been made to use them in the context of ray tracing because they are easier to compute by finite difference methods than the multi-valued solutions.

2.3 The transport equation and wave action

In the previous section, we discussed the rays associated with a wave train solution (2.10) whose frequency and wavenumber (2.11) satisfy the dispersion relation (2.12). The variation in the amplitude A of the wave train is governed by the dynamics of the wave motion. This typically leads to a *transport equation* for A . The transport equation implies, in particular, the conservation of *wave action*. For a linear wave equation with a Hamiltonian or variational structure, the *wave action density* is $|A|^2$, in suitable canonical coordinates, and the wave-action flux is $\mathbf{C}|A|^2$, where \mathbf{C} is the group velocity.

The variation of A along rays is given by the *transport equation*,

$$A_t + \mathbf{C} \cdot \nabla A + \frac{1}{2} \nabla \cdot \mathbf{C} A = 0. \quad (2.15)$$

Conservation of wave action is the equation

$$\partial_t |A|^2 + \nabla \cdot (\mathbf{C} |A|^2) = 0. \quad (2.16)$$

It follows that

$$\frac{d}{dt} |A|^2 + (\nabla \cdot \mathbf{C}) |A|^2 = 0,$$

where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{C} \cdot \nabla.$$

Thus, the wave action propagates along rays. A useful physical interpretation of the wave action is as the number density of “quanta” of the wave-field. Slow changes in the medium do not create or destroy quanta.

The energy density of a wave is typically given by $E = \omega |A|^2$, so that action is energy divided by frequency. In a stationary medium, the frequency is constant, and conservation of wave action is equivalent to conservation of wave energy. In a non-stationary medium, the wave may exchange energy with the medium, so that wave-energy is not conserved because the energy of each quantum may change, although the number remains the same. The energy is associated with time-translation invariance; the wave action with phase translation invariance.

An alternative approach to wave action via ensemble averages (Hayes, Andrews and MacIntyre..see Section...).

The presence of dissipation leads to a decrease in wave action. Nonlinear effects, such as three wave resonant interactions, do not preserve the number of “quanta” and therefore they do not conserve wave action. Four wave resonant interactions may, however, conserve wave action (see Section ..).

A quantity, such as the wave action, that does not change under slow variations of external parameters (in this case, the properties of the medium), is called an *adiabatic invariant*. Wave action is a generalization to infinite-dimensional Hamiltonian wave equations of the action in finite-dimensional Hamiltonian systems that is an adiabatic invariant. (Unfortunately, the term “action” is used in several different, but related, ways.)

2.4 Adiabatic invariants

A basic example illustrating the notion of an adiabatic invariant is the harmonic oscillator with slowly-varying frequency,

$$\ddot{x} + \omega_0^2(\varepsilon t)x = 0. \quad (2.17)$$

When $\varepsilon \ll 1$, this ODE describes small-amplitude oscillations of a pendulum whose length is changing slowly relative to its period. For another simple example of an adiabatic invariant, a ball bouncing between slowly moving walls, see Exercice 2.8.

The energy of an oscillator of mass m is

$$E = \frac{1}{2m} (\dot{x}^2 + \omega_0^2 x^2). \quad (2.18)$$

We look for a solution of (2.17) the form

$$x(t; \varepsilon) = X \left(\frac{\varphi(\varepsilon t)}{\varepsilon}, \varepsilon t; \varepsilon \right), \quad (2.19)$$

where the function $\varphi(\tau)$ is to be determined. In order to obtain an asymptotic solution that is valid on time-scales $t = O(1/\varepsilon)$, we require that $X(\theta, \tau; \varepsilon)$ is a periodic function of θ ; for definiteness, we suppose that the period is 2π . Using the method of multiple scales, we find that $X(\theta, \tau; \varepsilon)$ satisfies the PDE

$$\omega^2 X_{\theta\theta} + \omega_0^2 X - \varepsilon \{2\omega X_{\theta\tau} + \omega_\tau X_\theta\} + \varepsilon^2 X_{\tau\tau} = 0, \quad (2.20)$$

where

$$\omega = -\varphi_\tau. \quad (2.21)$$

We look for an asymptotic expansion of X of the form

$$X(\theta, \tau; \varepsilon) \sim \sum_{n=0}^{\infty} \varepsilon^n X^{(n)}(\theta, \tau) \quad \text{as } \varepsilon \rightarrow 0. \quad (2.22)$$

Using this expansion in (2.20), and equating coefficients of ε^n to zero, we find that

$$\omega^2 X_{\theta\theta}^{(0)} + \omega_0^2 X^{(0)} = 0, \quad (2.23)$$

$$\omega^2 X_{\theta\theta}^{(1)} + \omega_0^2 X^{(1)} = 2\omega X_{\theta\tau}^{(0)} + \omega_\tau X_\theta^{(0)}, \quad (2.24)$$

$$\omega^2 X_{\theta\theta}^{(n)} + \omega_0^2 X^{(n)} = 2\omega X_{\theta\tau}^{(n-1)} + \omega_\tau X_\theta^{(n-1)} - X_{\tau\tau}^{(n-2)}, \quad n \geq 2. \quad (2.25)$$

The condition that equation (2.23) has a 2π -periodic solution for $X^{(0)}$ implies that $\omega^2 = \omega_0^2$. Without loss of generality, we suppose that

$$\omega = \omega_0. \quad (2.26)$$

Then integration of (2.21) gives

$$\varphi(\tau) = \varphi_0 - \int_0^\tau \omega_0(\tau') d\tau'.$$

The solution of (2.23) is

$$X^{(0)}(\theta, \tau) = B(\tau)e^{i\theta} + \text{c.c.}, \quad (2.27)$$

where B is a function of integration. The use of (2.26) and (2.27) in (2.24) implies that

$$X_{\theta\theta}^{(1)} + X^{(1)} = \frac{i}{\omega_0^2} (2\omega_0 B_\tau + \omega_{0\tau} B) e^{i\theta} + \text{c.c.}$$

This equation has a 2π -periodic solution for $X^{(1)}$ is that

$$2\omega_0 B_\tau + \omega_{0\tau} B = 0,$$

which implies that

$$\frac{d}{d\tau} (\omega_0 |B|^2) = 0.$$

From (2.18), (2.22), and (2.27), the energy of the oscillator is given asymptotically by

$$E \sim \frac{\omega_0^2 |B|^2}{m}.$$

It follows that

$$\frac{d}{d\tau} \left(\frac{E}{\omega_0} \right) = 0,$$

corresponding to conservation of wave action. The quantum-mechanical interpretation is that the energy of the oscillator changes because its energy levels change as the frequency changes, but for very slow changes, the number of quanta occupying each energy level remains the same. This explains the origin of the term “adiabatic” (due originally to Eherenfest), which in thermodynamics refers to isentropic changes, because the entropy depends only on the distribution of energy levels...

The Hamiltonian form of the harmonic oscillator equations are

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}$$

where $q = x$, $p = m\dot{x}$, and

$$H(p, q; \omega_0) = \frac{1}{2m} p^2 + \frac{1}{2} \omega_0^2 q^2.$$

Action-angle variables for the system with constant ω_0 are

$$I =$$

The adiabatic invariant is

$$I = \oint p dq,$$

which is the area enclosed by the periodic orbit. Thus, in the adiabatic limit, as the orbits deform slowly, the area they enclose remains constant.

More generally, consider a completely integrable finite-dimensional Hamiltonian system, with action-angle coordinates (φ, \mathbf{I}) and Hamiltonian $H = H(\mathbf{I}; \lambda)$, depending on a parameter λ . Suppose that λ varies slowly in time.

2.5 References

The general theory of the kinematics of dispersive waves was developed by Lighthill and Whitham. We have followed their descriptions in [31] and [52].

2.6 Exercises

Exercise 2.1 Find the dispersion relations of:

- (a) the linearized KdV (Korteweg-de Vries) equation

$$u_t + u_{xxx} = 0;$$

- (b) the linearized BBM (Benjamin-Bona-Mahony) equation

$$(-\partial_x^2 + 1) u_t + u_x = 0;$$

- (c) the linearized BO (Benjamin-Ono) equation

$$u_t + H[u_x] = 0,$$

where H denotes the Hilbert transform;

- (d) the Klein-Gordon equation

$$u_{tt} - \Delta u + u = 0.$$

Exercise 2.2 Let $\Omega' \subset \mathbb{R}^d$, and $\Omega = \mathbb{R} \times \Omega'$. We write $\mathbf{x} = (x, \mathbf{x}')$, where $x \in \mathbb{R}$ and $\mathbf{x}' \in \Omega'$. If Δ is the Laplacian with respect to \mathbf{x} , and Δ' is the Laplacian with respect to \mathbf{x}' , then

$$\Delta = \partial_x^2 + \Delta'.$$

Look for solutions of the wave-guide problem

$$\begin{aligned} u_{tt} &= c_0^2 \Delta u & \mathbf{x} &\in \mathbb{R} \times \Omega', \\ u &= 0 & \mathbf{x} &\in \mathbb{R} \times \partial\Omega', \end{aligned}$$

of the form

$$u = e^{i(kx - \omega t)} \varphi(\mathbf{x}').$$

Show that the dispersion relation of this problem has infinitely many modes,

$$\omega^2 = k^2 + \omega_n^2,$$

where $\omega_n = c_0 \lambda_n$, and $\lambda = \lambda_n$, with $n \in \mathbb{N}$ is an eigenvalue of the Dirichlet problem

$$\begin{aligned} -\Delta' \varphi &= \lambda_n \varphi, \\ \varphi &= 0 & \text{in } \Omega'. \end{aligned}$$

Exercise 2.3 Consider a dispersion relation $\omega = W(\mathbf{k})$, where $W : \mathbb{R}^d \rightarrow \mathbb{R}$ is homogeneous of degree one, meaning that

$$W(\lambda \mathbf{k}) = \lambda W(\mathbf{k}) \quad \text{for } \lambda > 0.$$

Show that the wave is nondispersive.

Exercise 2.4 Establish (2.8). (See Section 7.7 of [20] for a detailed proof.)

Exercise 2.5 Show that the stationary phase approximation is a wave train.

Exercise 2.6 Show that the gravity water waves, with dispersion relation (2.9), generated by a ship moving at a constant speed through deep water form an angle of $\tan^{-1} 1/(2\sqrt{2})$, or approximately 19.5° , to the direction of motion of the ship. (For further discussion of the generation of dispersive wave patterns by sources with constant velocity, see [32].)

Exercise 2.7 Show that the angle of waves generated by a stationary source of internal waves whose frequency is ω is $\sin^{-1}(\omega/\omega_0)$, where ω_0 is the Brunt-Väisälä frequency.

Exercise 2.8 Ball bouncing between slowly varying walls.

Chapter 3

Linear Hyperbolic Waves

In this chapter, we study the geometrical optics, or high-frequency, limit of solutions of linear hyperbolic PDEs.

3.1 The wave equation

The most fundamental example of a hyperbolic PDE is the wave equation for $u(\mathbf{x}, t) \in \mathbb{R}$,

$$u_{tt} - \Delta u = 0. \quad (3.1)$$

We look for an asymptotic solution as $\varepsilon \rightarrow 0$ of the form

$$u(\mathbf{x}, t; \varepsilon) = u\left(\frac{\varphi(\mathbf{x}, t)}{\varepsilon}, \mathbf{x}, t; \varepsilon\right),$$

Using the chain rule, we find that $u(\theta, \mathbf{x}, t; \varepsilon)$ satisfies

$$(\varphi_t^2 - |\nabla \varphi|^2) u_{\theta\theta} + \varepsilon \{2(\varphi_t u_{\theta t} - \nabla \varphi \cdot \nabla u_\theta) + (\varphi_{tt} - \Delta \varphi) u_\theta\} = O(\varepsilon^2),$$

Expanding u in a power series expansion with respect to ε ,

$$u = u^{(0)} + \varepsilon u^{(1)} + O(\varepsilon^2),$$

and equating coefficients of ε^0 and ε to zero, we find that

$$(\varphi_t^2 - |\nabla \varphi|^2) u_{\theta\theta}^{(0)} = 0, \quad (3.2)$$

$$(\varphi_t^2 - |\nabla \varphi|^2) u_{\theta\theta}^{(1)} + 2(\varphi_t u_{\theta t}^{(0)} - \nabla \varphi \cdot \nabla u_\theta^{(0)}) + (\varphi_{tt} - \Delta \varphi) u_\theta^{(0)} = 0. \quad (3.3)$$

Equation (3.2) has a nontrivial solution for $u^{(0)}$ if and only

$$\varphi_t^2 - |\nabla \varphi|^2 = 0.$$

This equation is the eikonal equation for the wave equation. Equivalently, the local frequency $\omega = -\varphi_\tau$ and local wavenumber $\mathbf{k} = \nabla \varphi$ must satisfy the dispersion

relation of (3.1),

$$\omega^2 = |\mathbf{k}|^2.$$

One class of solutions of (3.2) is then

$$u^{(0)}(\theta, \mathbf{x}, t) = a(\mathbf{x}, t)f(\theta),$$

where a is an arbitrary real-valued wave amplitude, and f is an arbitrary real-valued function.

Equation (3.3) then implies that

$$2(\varphi_t a_t - \nabla \varphi \cdot \nabla a) + (\varphi_{tt} - \Delta \varphi) a = 0.$$

This equation is called the *transport equation* for a . We can also write it as

$$a_t + \mathbf{C} \cdot \nabla a + \frac{1}{2}(\nabla \cdot \mathbf{C}) a = 0,$$

where

$$\mathbf{C} = -\frac{\nabla \varphi}{\varphi_t}$$

is the group velocity of the wave. Note that the wave equation is nondispersive, and the phase and group velocities coincide.

Continuing this expansion to higher orders, we obtain an asymptotic solution of the form

$$u(\mathbf{x}, t; \varepsilon) \sim \sum_{n=0}^{\infty} \varepsilon^n a^{(n)}(\mathbf{x}, t) f^{(n)}\left(\frac{\varphi(\mathbf{x}, t)}{\varepsilon}\right),$$

where

$$\frac{d^n f^{(n)}}{d\theta^n} = f.$$

Different choices of the function f describe different waveforms. For example, if $f(\theta) = e^{i\theta} + \text{c.c.}$, then we get the harmonic solution

$$u \sim \sum_{n=0}^{\infty} i^{-n} \varepsilon^n a^{(n)} e^{i\varphi/\varepsilon} + \text{c.c.},$$

while if

$$f(\theta) = \begin{cases} \theta^r / r! & \text{if } \theta > 0, \\ 0 & \text{if } \theta < 0, \end{cases}$$

we get (after a rescaling by ε^{-r}) the wavefront expansion

$$u \sim \begin{cases} \sum_{n=0}^{\infty} a^{(n)} \varphi^{n+r} / (n+r)! & \text{if } \varphi > 0, \\ 0 & \text{if } \varphi < 0. \end{cases}$$

Thus, the propagation of both high-frequency waves and singularities are described by this geometrical optics solution. For linear equations, these two features are intimately related through the Fourier transform, but the connection is less direct for nonlinear waves.

A fundamental difference between linear dispersive waves and nondispersive hyperbolic waves is that the wave profile of a dispersive wave must be harmonic, whereas the wave profile of a hyperbolic wave may be arbitrary.

3.2 First order hyperbolic systems

We consider an $m \times m$ linear first order system of PDEs in d space-dimensions,

$$\mathbf{u}_t + \sum_{\alpha=1}^d A^\alpha(\mathbf{x}) \mathbf{u}_{x_\alpha} = 0, \quad (3.4)$$

where $\mathbf{x} = (x_1, \dots, x_d) \in \mathbb{R}^d$, $\mathbf{u}(\mathbf{x}, t) \in \mathbb{R}^m$, and the $A^\alpha(\mathbf{x})$ are $m \times m$ coefficient matrices.

For $\mathbf{k} = (k_1, \dots, k_d) \in \mathbb{R}^d$, we denote the eigenvalues of the matrix

$$\sum_{\alpha=1}^d k_\alpha A^\alpha(\mathbf{x})$$

by $\lambda_i(\mathbf{k}, \mathbf{x})$, where $1 \leq i \leq m$, and we denote corresponding left and right eigenvectors by $\mathbf{l}_i(\mathbf{x}, \mathbf{k})$ and $\mathbf{r}_i(\mathbf{x}, \mathbf{k})$, respectively, so that

$$\sum_{\alpha=1}^d k_\alpha A^\alpha \mathbf{r}_i = \lambda_i \mathbf{r}_i, \quad \mathbf{l}_i^T \sum_{\alpha=1}^d k_\alpha A^\alpha = \lambda_i \mathbf{l}_i^T.$$

Definition 3.1 The first order system (3.4) is *hyperbolic* at $\mathbf{x} \in \mathbb{R}^d$, with t as a time-like direction, if the eigenvalues $\{\lambda_1(\mathbf{k}, \mathbf{x}), \dots, \lambda_m(\mathbf{k}, \mathbf{x})\}$ are real for every $\mathbf{k} \in \mathbb{R}^d$, and the eigenvectors $\{\mathbf{r}_1(\mathbf{k}, \mathbf{x}), \dots, \mathbf{r}_m(\mathbf{k}, \mathbf{x})\}$ form a basis of \mathbb{R}^m . If, in addition, the eigenvalues $\{\lambda_1(\mathbf{k}, \mathbf{x}), \dots, \lambda_m(\mathbf{k}, \mathbf{x})\}$ are distinct for every $\mathbf{k} \in \mathbb{R}^d \setminus \{0\}$, then (3.4) is *strictly hyperbolic*.

When convenient, we normalize the eigenvectors so that

$$\mathbf{l}_i^T \mathbf{r}_j = \delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

The characteristic variety is the surface in (\mathbf{k}, λ) space such that

$$\det \left[\sum_{\alpha=1}^d k_\alpha A^\alpha - \lambda I \right] = 0.$$

The slowness surface has equation

$$\det \left[\sum_{\alpha=1}^d \xi_{\alpha} A^{\alpha} - I \right] = 0.$$

The slowness surface is...

Example 3.2 The wave and Dirac equations.

Example 3.3 Light, and other electromagnetic waves, consist of oscillating electric and magnetic fields, \mathbf{E} and \mathbf{B} , respectively. In a vacuum, these fields satisfy the Maxwell equations

$$\begin{aligned} \mathbf{B}_t + \nabla \times \mathbf{E} &= 0, \\ \mathbf{E}_t - c_0^2 \nabla \times \mathbf{B} &= 0, \\ \nabla \cdot \mathbf{B} &= 0, \\ \nabla \cdot \mathbf{E} &= 0, \end{aligned}$$

where c_0 is the speed of light ($c_0 \approx 3 \times 10^9 \text{ ms}^{-1}$).

We will discuss further examples of first-order hyperbolic systems (such as the acoustic equations) in Chapter 6.

3.3 Geometrical optics

We look for a solution of (3.4), depending on a small parameter $\varepsilon > 0$, of the form

$$\mathbf{u}^{\varepsilon}(\mathbf{x}, t) = \mathbf{U}^{\varepsilon} \left(\mathbf{x}, t, \frac{\varphi(\mathbf{x}, t)}{\varepsilon} \right), \quad (3.5)$$

where $\varphi : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R}$. The function $\mathbf{u}^{\varepsilon}(\mathbf{x}, t)$ in (3.5) satisfies (3.4) if and only if $\mathbf{U}^{\varepsilon}(\mathbf{x}, t, \theta)$ satisfies

$$\left(\varphi_t I + \sum_{\alpha=1}^d \varphi_{x_{\alpha}} A^{\alpha} \right) \mathbf{U}_{\theta}^{\varepsilon} + \mathbf{U}_t^{\varepsilon} + \sum_{\alpha=1}^d A^{\alpha} \mathbf{U}_{x_{\alpha}}^{\varepsilon} = 0 \quad (3.6)$$

on $\theta = \varphi(\mathbf{x}, t)/\varepsilon$. We will look for a function $\mathbf{U}^{\varepsilon}(\mathbf{x}, t, \theta)$ that satisfies (3.6) for all $(\mathbf{x}, t, \theta) \in \mathbb{R}^d \times \mathbb{R} \times \mathbb{R}$. Thus, we have replaced the PDE (3.4) in $(d+1)$ variables by the PDE (3.6) in $(d+2)$ variables. This replacement may not appear to be an improvement at first sight, but we can construct an asymptotic solution of (3.6) by the use of a regular perturbation expansion, whereas the solution (3.5) of (3.4) depends in a singular way on ε .

We look for an asymptotic solution of (3.6) of the form

$$\mathbf{U}^{\varepsilon}(\mathbf{x}, t, \theta) = \mathbf{U}^{(0)}(\mathbf{x}, t, \theta) + \varepsilon \mathbf{U}^{(1)}(\mathbf{x}, t, \theta) + \varepsilon^2 \mathbf{U}^{(2)}(\mathbf{x}, t, \theta) + O(\varepsilon^3).$$

3.4 References

3.5 Exercises

Exercise 3.1 Obtain the geometrical optic approximation of the wave equation

$$u_{tt} = c^2(x, t)\Delta u. \quad (3.7)$$

Chapter 4

Nonlinear Dispersive Waves

4.1 Introduction

A translation-invariant, nonlinear, dispersive wave equation typically has a one-parameter family of periodic travelling wave solutions of the form

$$u(\mathbf{x}, t) = U(\mathbf{k} \cdot \mathbf{x} - \omega t; a), \quad (4.1)$$

where $U(\theta + 2\pi; a) = U(\theta; a)$, the parameter a measures the amplitude of the wave, and frequency ω satisfies a *nonlinear dispersion relation*

$$\omega = W(\mathbf{k}; a^2). \quad (4.2)$$

The dependence of the frequency of a nonlinear oscillator on its amplitude is well-known in classical mechanics (see Exercise 4.1).

The travelling wave solutions (4.1) typically bifurcate off the linear harmonic waves, and as $a \rightarrow 0$,

$$U(\theta; a) = Ae^{i\theta} + \text{c.c.} + O(a^2) \quad \text{where } |A| = a. \quad (4.3)$$

We consider a wave train

$$u(\mathbf{x}, t) \sim A(\mathbf{x}, t)e^{i(\mathbf{k}_0 \cdot \mathbf{x} - \omega_0 t)} + \text{c.c.},$$

where the “carrier” wavenumber \mathbf{k}_0 and frequency ω_0 satisfy the linearized dispersion relation,

$$\omega_0 = W(\mathbf{k}_0; 0),$$

and the amplitude A is small and slowly varying. The Fourier transform of the wave train with respect to \mathbf{x} is then centered near $\mathbf{k} = \mathbf{k}_0$, so we may approximate the nonlinear dispersion relation by its Taylor expansion about $\mathbf{k} = \mathbf{k}_0$ and $a = 0$:

$$W(\mathbf{k}; |A|^2) \sim \omega_0 + \mathbf{C} \cdot (\mathbf{k} - \mathbf{k}_0) + \frac{1}{2} (\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{D} (\mathbf{k} - \mathbf{k}_0) + \gamma |A|^2. \quad (4.4)$$

Here,

$$\mathbf{C} = \frac{\partial W}{\partial \mathbf{k}}(\mathbf{k}_0; 0)$$

is the linearized group velocity at $\mathbf{k} = \mathbf{k}_0$,

$$D = \frac{\partial^2 W}{\partial \mathbf{k}^2}(\mathbf{k}_0; 0)$$

is the linearized dispersion tensor at $\mathbf{k} = \mathbf{k}_0$, and

$$\gamma = \frac{\partial W}{\partial(a^2)}(\mathbf{k}_0; 0),$$

measures the change in frequency with amplitude. The invariance of (4.3) under the phase change $\theta \mapsto \theta + \pi$ implies that

$$\frac{\partial W}{\partial a}(\mathbf{k}_0; 0) = 0,$$

so there is no linear term in a in the Taylor expansion.

The PDE for A with the dispersion relation (4.4) is

$$i(A_t + \mathbf{C} \cdot \nabla A) = \frac{1}{2} \nabla \cdot (D \nabla A) + \gamma |A|^2 A. \quad (4.5)$$

If the wave motion is isotropic, then

$$D = \beta I,$$

and, in a reference frame moving with the group velocity in which $\mathbf{x} \mapsto \mathbf{x} - \mathbf{C}t$, equation (4.5) becomes the *nonlinear Schrödinger equation* (NLS equation),

$$iA_t = \frac{1}{2} \beta \Delta A + \gamma |A|^2 A.$$

If β, γ are nonzero, then we may normalize this equation to get

$$iA_t = -\Delta A + \sigma |A|^2 A. \quad (4.6)$$

where $\sigma = -\text{sgn } \beta\gamma$.

The sign σ in (4.6) is essential, and cannot be removed by a further normalization of variables. If $\sigma = 1$, then (4.6) is the *focusing NLS equation*, while if $\sigma = -1$, then (4.6) is the *defocusing NLS equation*. The Hamiltonian form of (4.6) is

$$iA_t = \frac{\delta \mathcal{H}}{\delta A^*},$$

where the Hamiltonian \mathcal{H} is defined by

$$\mathcal{H} = \int \nabla A \cdot \nabla A^* + \frac{1}{2} A^2 (A^*)^2 \, d\mathbf{x}.$$

The Hamiltonian is conserved, as follows from the conservation law

$$\left(\nabla A \cdot \nabla A^* + \frac{1}{2} \sigma A^2 (A^*)^2 \right)_t + \dots = 0.$$

Hence, for the defocusing Schrödinger equation ($\sigma = 1$), an energy estimate implies that $A(\cdot, t)$ is bounded in $L^4(\mathbb{R}^d) \cap H^1(\mathbb{R}^d)$. For the focusing Schrödinger equation, however, the L^4 and H^1 norms of A may blow up simultaneously while conserving energy.

A useful quantum mechanical interpretation of (4.6) is as a Schrödinger equation for a particle moving in a potential $V = \sigma|A|^2$. In the case of the focusing NLS equation, a local concentration in $|A|$ creates a potential well, thus tending to further concentrate $|A|$. In one space-dimension, the balance between the linear dispersion and nonlinear self-attraction of a wave packet leads to localized travelling wave solutions, called *solitons*,

$$A = \dots$$

The self-focusing of a wave packet in two, or more, space-dimensions, may lead to the formation of singularities in finite time.

Benjamin-Fier (modulational) instability... Dark solitons... IST...

4.2 Nonlinear Klein-Gordon equation

We consider a nondimensionalized, nonlinear Klein-Gordon equation for $u(\mathbf{x}, t) \in \mathbb{R}$,

$$u_{tt} - \Delta u + f(u) = 0, \quad (4.7)$$

where $f : \mathbb{R} \rightarrow \mathbb{R}$. We assume that $f(0) = 0$, so that $u = 0$ is a solution of (4.7), and that f has the Taylor expansion at $u = 0$,

$$f(u) = u + \alpha u^2 + \beta u^3 + O(u^4). \quad (4.8)$$

We look for a multiple-scale solution

$$u = u(\theta, \eta, \xi, \tau; \varepsilon^{1/2}),$$

where $\varepsilon > 0$ is a small parameter, and

$$\theta = \frac{\varphi(\varepsilon \mathbf{x}, \varepsilon t)}{\varepsilon}, \quad \eta = \frac{\psi(\varepsilon \mathbf{x}, \varepsilon t)}{\varepsilon^{1/2}}, \quad \xi = \varepsilon \mathbf{x}, \quad \tau = \varepsilon t.$$

This ansatz corresponds to a wave train whose local frequency and wavenumber are $O(1)$ and vary over length and time scales of $O(1/\varepsilon)$.

Using the chain rule, we find that the partial derivative with respect to t has the expansion

$$\partial_t = \varphi_\tau \partial_\theta + \varepsilon^{1/2} \psi_\tau \partial_\eta + \varepsilon \partial_\tau,$$

with an analogous expansion for spatial derivatives. The PDE becomes

$$\begin{aligned} & (\varphi_\tau^2 - |\nabla\varphi|^2) u_{\theta\theta} + f(u) + 2\varepsilon^{1/2} (\varphi_\tau\psi_\tau - \nabla\varphi \cdot \nabla\psi) u_{\theta\eta} \\ & + \varepsilon \{2(\varphi_\tau u_{\theta\tau} - \nabla\varphi \cdot \nabla u_\theta) + (\varphi_{\tau\tau} - \Delta\varphi) u_\theta\} = O(\varepsilon^{3/2}), \end{aligned} \quad (4.9)$$

where ∇ denotes the gradient with respect to the “slow” space variable ξ . Expanding u in a power series expansion with respect to $\varepsilon^{1/2}$,

$$u = \varepsilon^{1/2} u^{(1)} + \varepsilon u^{(2)} + \varepsilon^{3/2} u^{(3)} + O(\varepsilon^2),$$

using this expansion in (4.9), Taylor expanding f , and equating coefficients of $\varepsilon^{1/2}$, ε , and $\varepsilon^{3/2}$ to zero, we find that

$$(\varphi_\tau^2 - |\nabla\varphi|^2) u_{\theta\theta}^{(1)} + u^{(1)} = 0, \quad (4.10)$$

$$\begin{aligned} & (\varphi_\tau^2 - |\nabla\varphi|^2) u_{\theta\theta}^{(2)} + u^{(2)} + 2(\varphi_\tau\psi_\tau - \nabla\varphi \cdot \nabla\psi) u_{\theta\eta}^{(1)} \\ & + \alpha \left(u^{(1)}\right)^2 = 0, \end{aligned} \quad (4.11)$$

$$\begin{aligned} & (\varphi_\tau^2 - |\nabla\varphi|^2) u_{\theta\theta}^{(3)} + u^{(3)} + 2(\varphi_\tau\psi_\tau - \nabla\varphi \cdot \nabla\psi) u_{\theta\eta}^{(2)} \\ & + 2\alpha u^{(1)} u^{(2)} + \beta \left(u^{(1)}\right)^3 + 2(\varphi_\tau u_{\theta\tau}^{(1)} - \nabla\varphi \cdot \nabla u_\theta^{(1)}) \\ & + (\varphi_{\tau\tau} - \Delta\varphi) u_\theta^{(1)} + (\psi_\tau^2 - |\nabla\psi|^2) u_{\eta\eta}^{(1)} = 0. \end{aligned} \quad (4.12)$$

We will look for solutions that are periodic in the phase variable θ . In order to obtain an asymptotic solution which does not contain secular terms that grow in θ , it is crucial to require that the period of u in θ is independent of (ξ, τ) . By rescaling the phase function φ , we may choose this period to be 2π without any loss of generality, so that

$$u(\theta + 2\pi, \eta, \xi, \tau; \varepsilon^{1/2}) = u(\theta, \eta, \xi, \tau; \varepsilon^{1/2}),$$

Each $u^{(n)}$ is then also 2π -periodic in θ .

Equation (4.10) has a nontrivial 2π -periodic solution for $u^{(1)}$ if and only

$$\varphi_\tau^2 - |\nabla\varphi|^2 = 1.$$

Equivalently, the local frequency $\omega = -\varphi_\tau$ and local wavenumber $\mathbf{k} = \nabla\varphi$ must satisfy the linearized dispersion relation of (4.7),

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

The solution of (4.10) is then

$$u^{(1)}(\theta, \eta, \xi, \tau) = A(\eta, \xi, \tau) e^{i\theta} + \text{c.c.}, \quad (4.13)$$

where $A(\eta, \xi, \tau) \in \mathbb{C}$ is an arbitrary complex-valued wave amplitude, and c.c. denotes the complex conjugate of the preceding term.

Equation (4.11) becomes

$$u_{\theta\theta}^{(2)} + u^{(2)} + 2(\varphi_\tau \psi_\tau - \nabla \varphi \cdot \nabla \psi) u_{\theta\eta}^{(1)} + \alpha \left(u^{(1)} \right)^2 = 0. \quad (4.14)$$

Using (4.13) in (4.14), we get

$$u_{\theta\theta}^{(2)} + u^{(2)} = -2i(\varphi_\tau \psi_\tau - \nabla \varphi \cdot \nabla \psi) A_\eta e^{i\theta} + \alpha (A^2 e^{2i\theta} + |A|^2)^2 + \text{c.c.} = 0. \quad (4.15)$$

Proposition 4.1 The ODE

$$u_{\theta\theta} + u = f(\theta),$$

where $f : \mathbb{T} \rightarrow \mathbb{R}$, has a 2π -periodic solution for u if and only if

$$\int_{\mathbb{T}} f(\theta) e^{-i\theta} d\theta = 0.$$

Proof. Take the L^2 -inner product with $e^{i\theta}$. □

The application of this solvability condition to (4.15) implies that

$$\varphi_\tau \psi_\tau - \nabla \varphi \cdot \nabla \psi = 0.$$

This equation may also be written as

$$\psi_\tau + \mathbf{C} \cdot \nabla \psi = 0,$$

where

$$\mathbf{C} = -\frac{\nabla \varphi}{\varphi_\tau} = \frac{\mathbf{k}}{\omega}$$

is the linearized group velocity associated with the phase φ . Thus, ψ must be constant along the rays associated with φ .

The corresponding solution for $u^{(2)}$ is then

$$u^{(2)}(\theta, \eta, \xi, \tau) = B(\eta, \xi, \tau) e^{2i\theta} + M(\eta, \xi, \tau) + \text{c.c.},$$

where

$$B = \frac{1}{3} \alpha A^2, \quad M = -\alpha |A|^2.$$

Here, we omit from $u^{(2)}$ for simplicity a solution of the homogeneous equation, proportional to $e^{\pm\theta}$, which does not affect the final result. (This component could also be absorbed into A .) The important components of $u^{(2)}$ are the mean component M and the second-harmonic component $B e^{2i\theta}$ that are driven by the quadratically nonlinear self-interaction of the fundamental harmonic.

Imposing the solvability condition on (4.12) in a similar way, and using the solution for $u^{(2)}$ in the result, we obtain an NLS equation for the amplitude A of the wavetrain:

$$i \left\{ \varphi_\tau A_\tau - \nabla \varphi \cdot \nabla A + \frac{1}{2} (\varphi_{\tau\tau} - \Delta \varphi) A \right\} \\ + \frac{1}{2} (\psi_\tau^2 - |\nabla \psi|^2) A_{\eta\eta} + \frac{3\beta}{2} - \frac{5\alpha^2}{4} |A|^2 A = 0.$$

The nonlinear term has two components, one proportional to β from direct cubically nonlinear interactions (e.g. $\omega + \omega - \omega \rightarrow \omega$), and one proportional to α^2 from successive quadratically nonlinear self-interactions (e.g. $\omega + \omega \rightarrow 2\omega$, followed by $2\omega - \omega \rightarrow \omega$, or $\omega - \omega \rightarrow 0$ followed by $0 + \omega \rightarrow \omega$).

We may also write this equation as

$$i \left\{ A_\tau + \mathbf{C} \cdot \nabla A + \frac{1}{2} (\operatorname{div} \mathbf{C}) A \right\} + \beta A_{\eta\eta} + \gamma |A|^2 A = 0,$$

where

$$\beta = \frac{\psi_\tau^2 - |\nabla \psi|^2}{2\varphi_\tau}, \quad \gamma = \frac{6\beta - 5\alpha^2}{4\varphi_\tau}.$$

4.3 Mean-field interactions

4.4 Modulation of large amplitude dispersive waves

We again use the nonlinear Klein-Gordon equation to illustrate the basic ideas of modulation theory for large amplitude dispersive waves (*cf.* [53]).

We look for a solution of (4.7) of the form

$$u(\mathbf{x}, t; \varepsilon) = u \left(\frac{\varphi(\varepsilon \mathbf{x}, \varepsilon t)}{\varepsilon}, \varepsilon \mathbf{x}, \varepsilon t; \varepsilon \right).$$

Here, we abuse notation slightly by using the same symbol u on either side of this equation. We will require that

$$u(\theta + 2\pi, \xi, \tau; \varepsilon) = u(\theta, \xi, \tau; \varepsilon).$$

The function $u(\mathbf{x}, t; \varepsilon)$ is a solution of (4.7) if $u(\theta, \xi, \tau; \varepsilon)$ satisfies

$$(\varphi_\tau^2 - |\nabla \varphi|^2) u_{\theta\theta} + f(u) \\ + \varepsilon \{ 2(\varphi_\tau u_{\theta\tau} - \nabla \varphi \cdot \nabla u_\theta) + (\varphi_{\tau\tau} - \Delta \varphi) u_\theta \} = O(\varepsilon^2),$$

where ∇ denotes the gradient with respect to ξ .

We look for a large-amplitude asymptotic solution,

$$u = u^{(0)} + \varepsilon u^{(1)} + O(\varepsilon^2).$$

We find that

$$\begin{aligned} (\varphi_\tau^2 - |\nabla\varphi|^2) u_{\theta\theta}^{(0)} + f(u^{(0)}) &= 0, \\ (\varphi_\tau^2 - |\nabla\varphi|^2) u_{\theta\theta}^{(1)} + f'(u^{(0)}) u^{(1)} + 2(\varphi_\tau u_{\theta\tau}^{(0)} - \nabla\varphi \cdot \nabla u_\theta^{(0)}) + (\varphi_{\tau\tau} - \Delta\varphi) u_\theta^{(0)} &= 0. \end{aligned}$$

4.5 Reaction-diffusion equations

We consider a system of reaction-diffusion equations,

$$\mathbf{u}_t = \Delta \mathbf{u} + \mathbf{f}(\mathbf{u}),$$

where $\mathbf{u}(\mathbf{x}, t) \in \mathbb{R}^m$, and $\mathbf{f} : \mathbb{R}^m \rightarrow \mathbb{R}^m$. We assume that the reaction ODE $\mathbf{u}_t = \mathbf{f}(\mathbf{u})$ has an isolated limit cycle solution with period T ,

$$\mathbf{u} = \mathbf{U}(t), \quad \mathbf{U}(t+T) = \mathbf{U}(t).$$

We look for a solution that consists of coupled limit cycle oscillations with a slowly varying phase:

$$\mathbf{u}(\mathbf{x}, t; \varepsilon) = \mathbf{u}(t + \varphi(\varepsilon\mathbf{x}, \varepsilon^2 t), \varepsilon\mathbf{x}, \varepsilon^2 t; \varepsilon).$$

Writing

$$\theta = t + \varphi(\varepsilon\mathbf{x}, \varepsilon^2 t), \quad \xi = \varepsilon\mathbf{x}, \quad \tau = \varepsilon^2 t,$$

we find by expanding derivatives that $\mathbf{u}(\theta, \xi, \tau; \varepsilon)$ satisfies

$$\mathbf{u}_\theta + \varepsilon\varphi_\tau \mathbf{u}_\theta$$

Amplitude “slaved” to frequency. Kuramoto-Shivashinsky equation for phase dynamics.

4.6 References

For a recent account of the Nonlinear Schrödinger equation, see [51].

4.7 Exercises

Exercise 4.1 Frequency dependence of a nonlinear oscillator

$$\ddot{x} + V'(x) = 0.$$

Chapter 5

The Hamiltonian description of waves

5.1 Poisson brackets

One of the most direct ways to describe the Hamiltonian structure of a wave equation is in terms of Poisson brackets. Let

$$\mathcal{F} : C_c^\infty(\mathbb{R}^d) \rightarrow \mathbb{R}$$

be a functional defined on the space of test functions. We say that \mathcal{F} is differentiable if for each $u \in C_c^\infty(\mathbb{R}^d)$ there exists a function $v \in C_c^\infty(\mathbb{R}^d)$ such that

$$\left. \frac{d}{d\varepsilon} \mathcal{F}(u + \varepsilon \varphi) \right|_{\varepsilon=0} = \int_{\mathbb{R}^d} v \varphi \, dx.$$

We write

$$v = \frac{\delta \mathcal{F}}{\delta u}.$$

If $\mathcal{D} : C_c^\infty(\mathbb{R}^d) \rightarrow C_c^\infty(\mathbb{R}^d)$ is a skew-symmetric operator, then we define the Poisson bracket

$$\{\mathcal{F}, \mathcal{G}\} = \int \frac{\delta \mathcal{F}}{\delta u} \mathcal{D} \frac{\delta \mathcal{G}}{\delta u} \, d\mathbf{x}.$$

We require that $\{\cdot, \cdot\}$ satisfies the Jacobi identity

$$\{\mathcal{F}, \{\mathcal{G}, \mathcal{H}\}\} + \{\mathcal{G}, \{\mathcal{H}, \mathcal{F}\}\} + \{\mathcal{H}, \{\mathcal{F}, \mathcal{G}\}\} = 0$$

for all functionals $\mathcal{F}, \mathcal{G}, \mathcal{H}$.

5.2 Interaction of dispersive wave trains

We consider the resonant interaction of four weakly nonlinear dispersive waves. The frequencies ω_j and wavenumbers k_j satisfy the four wave resonance condition

$$\omega_1 + \omega_2 + \omega_3 + \omega_4 = 0,$$

$$k_1 + k_2 + k_3 + k_4 = 0.$$

When the interacting waves are not spatially modulated, the wave field $u(x, t)$ has the form

$$u \sim \sum_{j=1}^4 A_j(t) e^{i(k_j x - \omega_j t)} + \text{c.c.}, \quad (5.1)$$

where A_j is the complex amplitude of the j th wave. To simplify the discussion, we suppose there is a single space dimension, so $x \in \mathbb{R}$. The amplitudes $A_j(t)$ satisfy a system of nonlinear ordinary differential equations, the four wave resonant interaction equations [7],

$$iA_{jt} + \sum_{k=1}^4 \Lambda_{jk} |A_k|^2 A_j + \Gamma_j A_p^* A_q^* A_r^* = 0. \quad (5.2)$$

In (5.2), the indices (j, p, q, r) run over cyclic permutations of $(1, 2, 3, 4)$, and the real numbers Λ_{jk} and Γ_j are interaction coefficients.

For a single spatially modulated wavepacket, the complex amplitude $A(x - Ct, t)$ is a function of time t and a spatial variable $x - Ct$ in a reference frame moving with the group velocity C of the wave. In a suitable limit in which cubically nonlinear and dispersive effects are of the same order of magnitude, the amplitude $A(\xi, t)$ satisfies a nonlinear Schrödinger (NLS) equation,

$$iA_t + \mu A_{\xi\xi} + \lambda |A|^2 A = 0. \quad (5.3)$$

For the four wave resonant interaction of spatially nonuniform waves, the wave field $u(x, t)$ is given by

$$u \sim \sum_{j=1}^4 A_j(x - C_j t, t) e^{i(k_j x - \omega_j t)} + \text{c.c.} \quad (5.4)$$

A common practice in the study of the resonant interaction of spatially nonuniform waves is to add the spatial derivative terms from the NLS equation (5.3) directly into the four wave interaction equations (5.2). Knobloch and DeLuca [28] pointed out that this result does not follow from a systematic asymptotic expansion unless the group velocities of the different waves are almost identical. When the group velocities are significantly different, as is usually the case, the nonlinear terms appearing in the equation for A_j must be averaged in a reference frame moving with the group velocity C_j of the j th wave. Thus, the complex wave amplitudes $A_j(\xi, t)$ satisfy the following system of nonlocally coupled NLS equations,

$$iA_{jt} + \mu_j A_{j\xi\xi} + \lambda_j |A_j|^2 A_j + \sum_{k \neq j} \Lambda_{jk} \overline{|A_k|^2} A_j + \Gamma_j \langle A_p^* A_q^* A_r^* \rangle^{(j)} = 0, \quad (5.5)$$

where

$$\overline{|A_n|^2}(t) = \lim_{T \rightarrow \infty} \int_0^T |A_n|^2(s, t) ds, \quad (5.6)$$

$$\begin{aligned} \langle A_p^* A_q^* A_r^* \rangle^{(j)}(\xi, t) &= \lim_{T \rightarrow \infty} \int_0^T A_p^*(\xi + (C_j - C_p)s, t) \\ &\quad A_q^*(\xi + (C_j - C_q)s, t) A_r^*(\xi + (C_j - C_r)s, t) ds. \end{aligned} \quad (5.7)$$

An interesting feature of these equations, which does not occur in the case of two nonlocally coupled NLS equations studied in [28], is that the coupling is not only through terms which are completely spatially averaged. The coupling terms which involve four different wave amplitudes are themselves spatially dependent. These terms are similar to the ones which occur in the three-wave resonant interaction equations for weakly nonlinear hyperbolic waves [35].

There are analogous nonlocal equations for n -wave interactions. For example, the nonlocal three wave resonant interaction equations are

$$i A_{jt} + \mu_j A_{j\xi\xi} + \Gamma_j \langle A_p^* A_q^* \rangle^{(j)} = 0,$$

where (j, p, q) is a cyclic permutation of $(1, 2, 3)$, and

$$\langle A_p^* A_q^* \rangle^{(j)}(\xi, t) = \lim_{T \rightarrow \infty} \int_0^T A_p^*(\xi + (C_j - C_p)s, t) A_q^*(\xi + (C_j - C_q)s, t) ds.$$

As an example, we derive the nonlocal four wave resonant interaction equations for a simple model problem, the KdV equation

$$u_t + \left(\frac{1}{2} u^2 \right)_x + u_{xxx} = 0. \quad (5.8)$$

The linearized dispersion relation of (5.8) is

$$\omega = -k^3. \quad (5.9)$$

The associated group velocity is

$$C = -3k^2.$$

The dispersion relation (5.9) does not allow three wave interactions. One simplifying feature of (5.8) is that the interaction coefficients for mean-field interactions vanish, because it is in conservative form.

The KdV equation gives an asymptotic description of the resonant interaction of weakly dispersive shallow water waves when the phase velocities of the interacting waves are nearly equal.

We look for an expansion of (5.8) of the form

$$\begin{aligned} u &= \varepsilon u_1(x, t, X, T, \tau) + \varepsilon^2 u_2(x, t, X, T, \tau) \\ &\quad + \varepsilon^3 u_3(x, t, X, T, \tau) + O(\varepsilon^4), \end{aligned} \quad (5.10)$$

where the multiple scale variables are evaluated at

$$X = \varepsilon x, \quad T = \varepsilon t, \quad \tau = \varepsilon^2 t. \quad (5.11)$$

Using (5.10) and (5.11) in (5.8), and equating coefficients of ε , ε^2 , and ε^3 to zero leads to the following perturbation equations:

$$\mathcal{L}u_1 = 0, \quad (5.12)$$

$$\mathcal{L}u_2 + \mathcal{M}u_1 + \left(\frac{1}{2}u_1^2\right)_x = 0, \quad (5.13)$$

$$\mathcal{L}u_3 + \mathcal{M}u_2 + \mathcal{N}u_1 + (u_1 u_2)_x + \left(\frac{1}{2}u_1^2\right)_X = 0. \quad (5.14)$$

Here, the linear operators \mathcal{L} , \mathcal{M} , and \mathcal{N} are defined by

$$\begin{aligned} \mathcal{L}u &= u_t + u_{xxx}, \\ \mathcal{M}u &= u_T + 3u_{xxX}, \\ \mathcal{N}u &= u_\tau + 3u_{XX}. \end{aligned} \quad (5.15)$$

A solution of (5.12) is

$$u_1 = \sum_{j=-J}^J A_j(X, T, \tau) e^{i\theta_j}, \quad (5.16)$$

where A_j ($j = 1, \dots, J$) are arbitrary complex-valued wave amplitudes, and

$$\begin{aligned} \theta_j &= k_j x - \omega_j t, \\ \omega_j &= -k_j^3, \\ \theta_{-j} &= -\theta_j, \\ A_{-j} &= A_j^*, \\ A_0 &= 0. \end{aligned}$$

Equation (5.13) can be solved for u_2 provided that the coefficients of $\exp(i\theta_j)$ in the terms involving u_1 are zero. This solvability condition implies that

$$A_{jT} + C_j A_{jX} = 0, \quad (5.17)$$

where $C_j = -3k_j^2$ is the group velocity of the j^{th} wave. The solution of (5.17) is

$$A_j = A_j(\xi_j, \tau), \quad \xi_j = X - C_j T.$$

A solution of (5.13) for u_2 is then

$$u_2 = \sum_j D_j(X, T, \tau) e^{i\theta_j} + \sum_{q,r} B_{qr}(X, T, \tau) e^{i(\theta_q + \theta_r)}, \quad (5.18)$$

where the D_j are arbitrary complex-valued functions and

$$\begin{aligned} B_{qr} &= \alpha_{qr} A_q A_r, \\ \alpha_{qr} &= \frac{1}{6k_q k_r} \quad \text{if } k_q + k_r \neq 0, \\ \alpha_{qr} &= 0 \quad \text{if } k_q + k_r = 0. \end{aligned} \tag{5.19}$$

Equation (5.14) can be solved for u_3 provided that

$$D_j T + C_j D_j X + A_{j\tau} + 3ik_j A_{j\xi\xi} + ik_j \sum_{p,q,r}^{(j)} A_p B_{qr} = 0, \tag{5.20}$$

where

$$\sum_{p,q,r}^{(j)}$$

denotes the sum over p, q, r such that

$$\begin{aligned} \omega_p + \omega_q + \omega_r &= \omega_j, \\ k_p + k_q + k_r &= k_j. \end{aligned}$$

To avoid secular terms in D_j on the intermediate time scale T , the average of (5.20) with respect to T keeping $X - C_j T = \xi$ fixed must be zero. Using (5.19), this solvability condition implies that $A_j(\xi, \tau)$ satisfies

$$A_{j\tau} + 3ik_j A_{j\xi\xi} + ik_j \sum_{p,q,r}^{(j)} \alpha_{qr} \langle A_p A_q A_r \rangle^{(j)} = 0. \tag{5.21}$$

The explicit expression for the j -average is

$$\begin{aligned} \langle A_p A_q A_r \rangle^{(j)}(\xi, \tau) &= \\ \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T &A_p(\xi + (c_j - c_p)s, \tau) A_q(\xi + (c_j - c_q)s, \tau) A_r(\xi + (c_j - c_r)s, \tau) ds \end{aligned}$$

Now consider the simplest case of a single resonant quartet ($J = 4$), such that

$$\begin{aligned} \omega_1 + \omega_2 + \omega_3 + \omega_4 &= 0, \\ k_1 + k_2 + k_3 + k_4 &= 0. \end{aligned}$$

There are three types of terms which contribute to the sum

$$\sum_{p,q,r}^{(j)} \alpha_{qr} \langle A_p A_q A_r \rangle^{(j)}$$

The first type of term is the one wave, self-interaction:

$$\omega_j + \omega_j - \omega_j - \omega_j = 0.$$

This has the coefficient

$$\alpha_{j,j} + \alpha_{-j,j} + \alpha_{j,-j} = \alpha_{j,j} = \frac{1}{6k_j^2},$$

since $\alpha_{j,-j} = \alpha_{-j,j} = 0$. In this case, the average does not alter the corresponding term,

$$|A_j|^2 A_j,$$

since A_j depends only on ξ , which is held constant when taking the average.

The second type of term is the two-wave interaction:

$$\omega_j + \omega_s - \omega_j - \omega_s = 0,$$

where $1 \leq s \leq 4$ and $s \neq j$. This has the coefficient

$$2\alpha_{j,s} + 2\alpha_{j,-s} + 2\alpha_{s,-s} = 0,$$

since $\alpha_{j,-s} = -\alpha_{j,s}$ and $\alpha_{s,-s} = 0$. Thus, in this example, interaction terms of the form

$$\langle |A_s|^2 \rangle A_j$$

do not appear; presumably this is because there are no mean-field interactions for (5.8).

The third type of term is the four-wave interaction:

$$\omega_j + \omega_p + \omega_q + \omega_r = 0,$$

where (j, p, q, r) is a fixed cyclic permutation of $(1, 2, 3, 4)$. The corresponding coefficient in the sum is

$$2(\alpha_{-q,-r} + \alpha_{-r,-p} + \alpha_{-p,-r}) = -\frac{1}{3} \frac{k_j}{k_p k_q k_r}.$$

Using these expressions in (5.21), and multiplying the result by i , gives the final amplitude equations,

$$iA_{j\tau} - 3k_j A_{j\xi\xi} - \frac{1}{6k_j} |A_j|^2 A_j + \frac{k_j^2}{3k_p k_q k_r} \langle A_p^* A_q^* A_r^* \rangle^{(j)} = 0, \quad (5.22)$$

where (j, p, q, r) runs through cyclic permutations of $(1, 2, 3, 4)$.

Chapter 6

Hyperbolic conservation laws

6.1 Conservation laws

We consider a first order system of conservation laws

$$\mathbf{u}_t + \sum_{\alpha=1}^d \mathbf{f}^\alpha(\mathbf{u})_{x_\alpha} = 0. \quad (6.1)$$

Here, $\mathbf{u}(\mathbf{x}, t) \in \mathbb{R}^m$ is a vector of conserved quantities, and $\mathbf{f}^\alpha: \mathbb{R}^m \rightarrow \mathbb{R}^m$ is the flux vector in the α^{th} direction.

We say that \mathbf{u} is a *weak solution* of (6.1) if

$$\int_{\mathbb{R}^{d+1}} \left\{ \varphi_t \mathbf{u} + \sum_{\alpha=1}^d \varphi_{x_\alpha} \mathbf{f}^\alpha(\mathbf{u}) \right\} d\mathbf{x} dt = 0$$

for every test function $\varphi \in C_c(\mathbb{R}^{d+1})$.

6.2 The compressible Euler equations

A fundamental example of a hyperbolic system of conservation laws is the compressible Euler, or gas dynamics, equations that describe the flow of a simple compressible fluid. We denote the density of the fluid by ρ , the pressure by p , the specific internal energy by e , and the velocity by \mathbf{u} . Conservation of mass, momentum, and energy imply that ([19], [53])

$$\begin{aligned} \rho_t + \nabla \cdot (\rho \mathbf{u}) &= 0, \\ (\rho \mathbf{u})_t + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} - \mathbf{T}) &= 0, \\ \left[\rho \left(e + \frac{1}{2} \mathbf{u} \cdot \mathbf{u} \right) \right]_t + \nabla \cdot \left[\rho \left(e + \frac{1}{2} \mathbf{u} \cdot \mathbf{u} \right) \mathbf{u} - \mathbf{T} \mathbf{u} + \mathbf{q} \right] &= 0. \end{aligned} \quad (6.2)$$

Here, \mathbf{T} is the Cauchy stress tensor, \mathbf{q} is the heat flux vector, and \otimes denotes the tensor product,

$$[\mathbf{u} \otimes \mathbf{v}]_{ij} = u_i v_j.$$

For an inviscid gas with no thermal conductivity, the constitutive relations for the stress and heat flux are

$$\mathbf{T} = -p\mathbf{I}, \quad \mathbf{q} = 0. \quad (6.3)$$

The internal energy e is given in terms of the density ρ and the pressure p by an equation of state, $e = e(\rho, p)$. The specific entropy $s(\rho, p)$ and the temperature $T(\rho, p)$ satisfy the thermodynamic identity

$$Tds = de + p d\left(\frac{1}{\rho}\right).$$

The sound speed $c(\rho, p)$ is defined by

$$c^2 = \left. \frac{\partial p}{\partial \rho} \right|_s. \quad (6.4)$$

For an ideal gas with constant specific heats, we have

$$e = \frac{1}{(\gamma - 1)} \frac{p}{\rho}, \quad p = \kappa \exp(s/c_v) \rho^\gamma, \quad c^2 = \frac{\gamma p}{\rho},$$

where the constant $\gamma > 1$ is the ratio of specific heats, c_v is the specific heat at constant volume, and κ is a constant. A detailed discussion of equations of state for real gases is given in [37].

For smooth solutions, the non-dissipative gas dynamics equations (6.2), (6.3) are equivalent to the equations in non-conservative form,

$$\begin{aligned} \rho_t + \mathbf{u} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{u} &= 0, \\ \mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{\rho} \nabla p &= 0, \\ s_t + \mathbf{u} \cdot \nabla s &= 0. \end{aligned} \quad (6.5)$$

In (6.5), we use $(\rho, \mathbf{u}, s)^T$ as the vector of dependent variables, and $p = p(\rho, s)$ is a given function. If shocks are present, then one must use the weak form of the conservative equations (6.2) rather than (6.5). Alternatively, for piecewise smooth solutions, one can use (6.5) in the regions where the solution is smooth, supplemented by the jump conditions across shocks derived from the weak form of (6.2).

Other important equations are the incompressible Euler equations, and the compressible and incompressible Navier-Stokes equations.

6.3 Acoustics

Linearizing (6.5) about a constant background state, $\mathbf{u} = 0$, $\rho = \rho_0$, and $s = s_0$, we get the acoustics equations,

$$\begin{aligned}\rho'_t + \rho_0 \nabla \cdot \mathbf{u}' &= 0, \\ \rho_0 \mathbf{u}'_t + c_0^2 \nabla \rho' + d_0 \nabla s' &= 0, \\ s'_t &= 0.\end{aligned}\tag{6.6}$$

In (6.6), ρ' stands for the perturbation in the density from ρ_0 , so that $\rho = \rho_0 + \rho'$, with \mathbf{u}' and s' defined similarly, $c_0 = c(\rho_0, s_0)$ is the sound speed in the unperturbed state, and

$$d_0 = \left. \frac{\partial p}{\partial s} \right|_{\rho} (\rho_0, s_0).\tag{6.7}$$

In d space-dimensions, the plane-wave solutions

$$\begin{bmatrix} \rho' \\ \mathbf{u}' \\ s' \end{bmatrix} = a (\mathbf{k} \cdot \mathbf{x} - \lambda(\mathbf{k})t) \begin{bmatrix} \hat{\rho} \\ \hat{\mathbf{u}} \\ \hat{s} \end{bmatrix}$$

satisfy (6.6) if λ satisfies

$$\lambda^d [\lambda^2 - c_0^2 |\mathbf{k}|^2] = 0.\tag{6.8}$$

The root

$$\lambda^2 = c_0^2 |\mathbf{k}|^2.$$

corresponds to sound waves, whose phase velocity $\mathbf{c} = c_0 \mathbf{k}/|\mathbf{k}|$ is normal to the surfaces of constant phase, and has magnitude equal to the sound speed c_0 . The associated right eigenspace is one dimensional, and is spanned by

$$\begin{bmatrix} \hat{\rho} \\ \hat{\mathbf{u}} \\ \hat{s} \end{bmatrix} = \begin{bmatrix} \rho_0 \\ c_0^2 \mathbf{k}/\lambda \\ 0 \end{bmatrix}.$$

Thus, sound waves carry longitudinal velocity perturbations ($\hat{\mathbf{u}}$ is parallel to \mathbf{k}), and density and pressure perturbations at constant entropy.

The root $\lambda = 0$ is a multiple eigenvalue for $d > 1$. The d -dimensional eigenspace is spanned by the vectors

$$\begin{bmatrix} \hat{\rho} \\ \hat{\mathbf{u}} \\ \hat{s} \end{bmatrix} = \begin{bmatrix} -d_0 \\ 0 \\ c_0^2 \end{bmatrix}, \quad \text{and} \quad \begin{bmatrix} \hat{\rho} \\ \hat{\mathbf{u}} \\ \hat{s} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{k}^\perp \\ 0 \end{bmatrix},$$

where \mathbf{k}^\perp runs over $(d-1)$ linearly independent vectors such that $\mathbf{k}^\perp \cdot \mathbf{k} = 0$. These eigenvectors correspond to entropy waves at constant pressure, and vorticity waves, respectively.

6.4 References

See Dafermos [9] and Serre [46].

Chapter 7

Variational Equations

7.1 Classical fields

An important class of hyperbolic partial differential equations consists of the the variational hyperbolic equations that arise in classical field theory [27]. These include the equations for scalar, tensor, or spinor fields on a Lorentzian space time, the Einstein field equations in general relativity, and the wave map equations [50].

7.2 A nonlinear wave equation

7.3 Wave maps

Wave maps are the Lorentzian analog of harmonic maps on a Riemannian manifold, and are stationary points of a natural action functional. In this paper, we derive a nonlinear geometrical optics solution for large amplitude wave maps. We show that, in an appropriate limit, a general wave map equation reduces to a wave map equation on $(1 + 1)$ -dimensional Minkowski space, with an additional lower order term that describes the effect of focusing or defocusing on the wave. Null coordinates on this space are a phase variable and an arc-length parameter along the rays associated with the phase. The asymptotic equation has a variational formulation. The additional lower order term in the asymptotic equation arises from a factor in its Lagrangian that is proportional to the cross-sectional area of ray tubes. This factor relates volumes in the $(1 + 1)$ -dimensional Minkowski space to volumes in the original Lorentzian space.

Apart from their intrinsic geometrical significance, wave maps are of interest because they provide a simple model for some nonlinear features of general relativity [38].

We will consider geometrical optics expansion for wave maps. A more complicated analog of the wave map expansion derived here applies to large-amplitude, high-frequency solutions of the Einstein field equations in general relativity, and

leads to the equations for colliding plane gravitational waves.

Let \mathcal{M} be a Lorentzian manifold with metric g of signature $(-, +, \dots, +)$, and \mathcal{N} a Riemannian manifold with metric h . A map $u : \mathcal{M} \rightarrow \mathcal{N}$ is called a wave map if it is a stationary point of the action functional

$$\mathcal{S}[u] = \frac{1}{2} \int_{\mathcal{M}} \langle du, du \rangle d\mu, \quad (7.1)$$

where $\langle \cdot, \cdot \rangle$ denotes the natural inner product associated with g and h , and $d\mu$ is the natural volume form on \mathcal{M} . In local coordinates x^α on \mathcal{M} and u^a on \mathcal{N} , the wave map action functional is given by

$$\mathcal{S}[u] = \frac{1}{2} \int_{\mathcal{M}} h_{ab}(u) \frac{\partial u^a}{\partial x^\alpha} \frac{\partial u^b}{\partial x^\beta} g^{\alpha\beta}(x) \sqrt{-g(x)} dx, \quad (7.2)$$

where we use the summation convention, and

$$g = \det [g_{\alpha\beta}].$$

The Euler-Lagrange equation associated with \mathcal{S} is

$$\square_g u^a + \Gamma_{bc}^a(u) g^{\alpha\beta}(x) \frac{\partial u^b}{\partial x^\alpha} \frac{\partial u^c}{\partial x^\beta} = 0, \quad (7.3)$$

where \square_g is the d'Alembertian operator on \mathcal{M} ,

$$\square_g u = \frac{1}{\sqrt{-g}} \frac{\partial}{\partial x^\alpha} \left(g^{\alpha\beta} \sqrt{-g} \frac{\partial u}{\partial x^\beta} \right), \quad (7.4)$$

and Γ_{bc}^a are the connection coefficients on \mathcal{N} ,

$$\Gamma_{bc}^a = \frac{1}{2} h^{ae} \left(\frac{\partial h_{ce}}{\partial u^b} + \frac{\partial h_{be}}{\partial u^c} - \frac{\partial h_{bc}}{\partial u^e} \right). \quad (7.5)$$

We look for a multiple-scale, nonlinear geometrical optics solution of (7.3) of the form

$$u^a = u^a \left(x, \frac{\varphi(x)}{\varepsilon}; \varepsilon \right), \quad (7.6)$$

where $\varphi : \mathcal{M} \rightarrow \mathbb{R}$ is a phase function, and $u^a(x, \theta; \varepsilon)$ is a function of $x = (x^\alpha)$ and the “fast” phase variable,

$$\theta = \frac{\varphi}{\varepsilon}. \quad (7.7)$$

We define a wave-vector one-form k , with covariant components k_α and contravariant components k^α , by

$$k = d\varphi, \quad k_\alpha = \frac{\partial \varphi}{\partial x^\alpha}, \quad k^\alpha = g^{\alpha\beta} k_\beta. \quad (7.8)$$

From (7.6) and (7.8), we have

$$\frac{\partial u^a}{\partial x^\alpha} = \frac{1}{\varepsilon} k_\alpha u_\theta^a + \partial_\alpha u^a, \quad (7.9)$$

where the subscript θ denotes the partial derivative with respect to θ at constant x , and ∂_α denotes the partial derivative with respect to x^α at constant θ .

Use of (7.6) in the wave map equation (7.3), and expansion of derivatives as in (7.9), implies that $u^a(x, \theta; \varepsilon)$ satisfies

$$\begin{aligned} & \frac{1}{\varepsilon^2} (k_\alpha k^\alpha) \{ u_{\theta\theta}^a + \Gamma_{bc}^a(u) u_\theta^b u_\theta^c \} \\ & + \frac{1}{\varepsilon} \{ 2k^\alpha \partial_\alpha u_\theta^a + 2\Gamma_{bc}^a(u) k^\alpha \partial_\alpha u^b u_\theta^c + (\square_g \varphi) u_\theta^a \} \\ & + \square_g u^a + \Gamma_{bc}^a(u) g^{\alpha\beta} \partial_\alpha u^b \partial_\beta u^c = 0. \end{aligned} \quad (7.10)$$

We look for a power series expansion of u^a as $\varepsilon \rightarrow 0$ of the form

$$u^a(x, \theta; \varepsilon) = u_0^a(x, \theta) + \varepsilon u_1^a(x, \theta) + O(\varepsilon^2). \quad (7.11)$$

We use (7.11) in (7.10), Taylor expand the result with respect to ε , and equate coefficients of ε^{-2} and ε^{-1} to zero. This gives the equations

$$(k_\alpha k^\alpha) \{ u_{0\theta\theta}^a + \Gamma_{bc}^a(u_0) u_{0\theta}^b u_{0\theta}^c \} = 0, \quad (7.12)$$

$$\begin{aligned} & (k_\alpha k^\alpha) \left\{ u_{1\theta\theta}^a + 2\Gamma_{bc}^a(u_0) u_{1\theta}^b u_{0\theta}^c + \frac{\partial \Gamma_{bc}^a}{\partial u^e}(u_0) u_1^e u_{0\theta}^b u_{0\theta}^c \right\} \\ & + 2k^\alpha \partial_\alpha u_{0\theta}^a + 2\Gamma_{bc}^a(u_0) k^\alpha \partial_\alpha u_0^b u_{0\theta}^c + (\square_g \varphi) u_{0\theta}^a = 0. \end{aligned} \quad (7.13)$$

The leading order perturbation equation (7.12) is satisfied provided that

$$k_\alpha k^\alpha = 0. \quad (7.14)$$

From (7.8) and (7.14), it follows that the phase $\varphi(x)$ satisfies the eikonal equation,

$$g^{\alpha\beta} \frac{\partial \varphi}{\partial x^\alpha} \frac{\partial \varphi}{\partial x^\beta} = 0. \quad (7.15)$$

A global solution of (7.15) may not exist because of the formation of caustics. The asymptotic expansion breaks down when this occurs, and we consider the solution only in regions of \mathcal{M} where φ is a well-defined, smooth function.

The use of (7.14) in (7.13) implies that $u_0^a(x, \theta)$ satisfies the equation

$$k^\alpha \partial_\alpha u_{0\theta}^a + \Gamma_{bc}^a(u_0) k^\alpha \partial_\alpha u_0^b u_{0\theta}^c + \frac{1}{2} (\square_g \varphi) u_{0\theta}^a = 0. \quad (7.16)$$

An asymptotic solution of (7.3) is therefore given by (7.6) and (7.11), where the phase φ satisfies the eikonal equation (7.15), and the leading order approximation u_0^a satisfies (7.16).

We define a partial derivative ∂_s along the rays associated with φ by

$$\partial_s = k^\alpha \partial_\alpha, \quad (7.17)$$

and define J by

$$k^\alpha \partial_\alpha J = (\square_g) \varphi J \quad (7.18)$$

Then, using a subscript s to denote the partial derivative ∂_s , and dropping the zero subscript on u_0^a to simplify the notation, we may write (7.16) as

$$u_{s\theta}^a + \Gamma_{bc}^a(u) u_s^b u_\theta^c + \frac{J_S}{2J} u_\theta^a = 0. \quad (7.19)$$

This equation has the same form as a wave map equation on $(1+1)$ -dimensional Minkowski space, where (s, θ) are null-coordinates, with an additional lower order term proportional to u_θ^a , whose coefficient is a function of s on a given ray. The lower order term describes the effect of focusing or defocusing of the wavefronts on the wave.

Equation (7.19) is the Euler-Lagrange equation of the functional

$$\mathcal{S}_0[u] = \int h_{ab}(u) u_s^a u_\theta^b J(s) ds d\theta. \quad (7.20)$$

As in linear geometrical optics (see §22.5 of [39], for example), that the function J is proportional to the cross-sectional area of the ray tubes associated with φ .

The action functional in (7.20) differs from the wave map action functional in (7.2) on $(1+1)$ -dimensional Minkowski space, because the volume form $J(s) ds d\theta$ differs from the natural volume form $ds d\theta$. The origin of the volume form in the asymptotic action functional may be understood in a heuristic way as follows. The wave map action functional \mathcal{S} in (7.2) is given by

$$\mathcal{S}[u] = \int_{\mathcal{M}} L d\mu, \quad (7.21)$$

where $d\mu = \sqrt{-g} dx$ is the natural volume form on \mathcal{M} , and the action density L is given by

$$L = \frac{1}{2} h_{ab}(u) \frac{\partial u^a}{\partial x^\alpha} \frac{\partial u^b}{\partial x^\beta} g^{\alpha\beta}(x). \quad (7.22)$$

Using the derivative expansion (7.9) in (7.22), and simplifying the result with the help of (7.14) and (7.17), we find that L has the expansion

$$L = \frac{1}{\varepsilon} h_{ab}(u_0) u_{0s}^a u_{0\theta}^b + O(1). \quad (7.23)$$

If we consider an infinitesimal tube of rays on a wavefront $\varphi = \text{constant}$, with $(m-2)$ -dimensional cross-sectional area σ , where $m = \dim \mathcal{M}$, then the corresponding volume element in \mathcal{M} is given by $d\mu = \sigma ds d\varphi$, or from (7.7),

$$d\mu = \varepsilon \sigma ds d\theta. \quad (7.24)$$

The use of (7.23) and (7.24) in (7.21) gives

$$\mathcal{S}[u] = \mathcal{S}_0[u_0] + O(\varepsilon),$$

where \mathcal{S}_0 is the action functional defined in (7.20).

The global existence of smooth solutions of (7.19), for smooth coefficient functions ρ and complete Riemannian target manifolds \mathcal{N} , follows from [14], [17]. Thus, there is no spontaneous development of singularities in a high frequency wave map when its rays do not focus at a caustic; such waves are locally approximated by $(1+1)$ -dimensional wave maps, which remain smooth. This behavior contrasts with the behavior of high frequency waves that satisfy hyperbolic conservation laws [4], [22], the Einstein field equations, or the hyperbolic variational equations studied in [15], [23], [24], where nonlinear effects can lead to the formation of singularities even in the absence of caustics.

If $\rho \neq 0$, we can normalize (7.19) by the introduction of a new ray parameter $t : \mathcal{M} \rightarrow \mathbb{R}$ that satisfies $t_s = \rho/2$, meaning that

$$k^\alpha \partial_\alpha t = \frac{1}{2} \square_g \varphi.$$

Changing variables from s to t , we find that (7.19) adopts the form

$$u_{t\theta}^a + \Gamma_{bc}^a(u) u_t^b u_\theta^c + u_\theta^a = 0. \quad (7.25)$$

The lower order term in (7.25) cannot be removed by a simple change of variables, unlike the corresponding lower order term in the inviscid Burgers equation that is obtained by the application of weakly nonlinear geometrical optics to hyperbolic systems of conservation laws [21].

7.3.1 Wave maps on Minkowski space

We suppose that the base space $\mathcal{M} = \mathbb{R}^{1+d}$ is Minkowski space with coordinates (t, \mathbf{x}) , where $\mathbf{x} = (x^1, \dots, x^d)$, and metric $g = \text{diag}(-1, 1, \dots, 1)$. The eikonal equation (7.15) is then

$$\varphi_t^2 = |\nabla \varphi|^2, \quad (7.26)$$

where ∇ denotes the gradient with respect to \mathbf{x} . As an explicit example of non-planar wave maps, we consider outgoing spherical waves, with phase

$$\varphi = r - t, \quad (7.27)$$

where $r = |\mathbf{x}|$. The phase (7.27) satisfies (7.26), and

$$\square_g \varphi = \frac{2c}{r}, \quad c = \frac{d-1}{2}.$$

Using the radial coordinate r as a parameter along the rays, we may write the asymptotic equation (7.19) as

$$u_{r\theta}^a + \Gamma_{bc}^a(u)u_r^b u_\theta^c + \frac{c}{r}u_\theta^a = 0. \quad (7.28)$$

In characteristic coordinates,

$$\varphi = r - t, \quad s = \frac{r + t}{2},$$

the exact equation for spherically symmetric wave maps is [5]

$$u_{s\varphi}^a + \Gamma_{bc}^a(u)u_s^b u_\varphi^c + \frac{c}{s + \varphi/2}u_\varphi^a = 0. \quad (7.29)$$

Thus, the asymptotic equation (7.28) is a simplification of the exact equation (7.29), in which the φ -dependence of the coefficient of the lower order coefficient is neglected.

A self-similar solution of (7.28) is given by

$$\begin{aligned} u^a &= v^a(\xi), \quad \xi = \frac{\theta}{r}, \\ \ddot{v}^a + \left(\frac{1-c}{\xi}\right)\dot{v}^a + \Gamma_{bc}^a(v)\dot{v}^b \dot{v}^c &= 0, \end{aligned} \quad (7.30)$$

where the dot denotes the derivative with respect to ξ . If the base Minkowski space has spatial dimension $d = 3$, then $c = 1$, and the self-similar solutions are geodesics in \mathcal{N} . Exact self-similar solutions for wave maps in $d = 3$ are constructed in [47].

An interesting special case of wave maps is that of wave maps from $(1 + d)$ -dimensional Minkowski space into an n -dimensional sphere \mathbb{S}^n . Embedding the sphere in Euclidean space, we write the map as

$$\mathbf{u} : \mathbb{R}^{1+d} \rightarrow \mathbb{S}^n \subset \mathbb{R}^{n+1},$$

where \mathbb{R}^{n+1} has coordinates u^a and is equipped with the Euclidean metric $h = \text{diag}(1, 1, \dots, 1)$. The wave map action functional is

$$\mathcal{S}[\mathbf{u}] = \int_{\mathbb{R}^{1+d}} \left\{ -\mathbf{u}_t^2 + |\nabla \mathbf{u}|^2 \right\} dt dx, \quad (7.31)$$

where

$$|\nabla \mathbf{u}|^2 = \sum_{\alpha=1}^d \sum_{a=1}^{n+1} \left(\frac{\partial u^a}{\partial x^\alpha} \right)^2,$$

and the wave map is subject to the constraint

$$\mathbf{u}^2 = 1.$$

The wave map equation is

$$-\mathbf{u}_{tt} + \Delta \mathbf{u} + \left(-\mathbf{u}_t^2 + |\nabla \mathbf{u}|^2 \right) \mathbf{u} = 0. \quad (7.32)$$

The use of the geometrical optics expansion (7.6) and (7.11) in (7.32) leads to an asymptotic solution of the form

$$\mathbf{u} = \mathbf{u}_0 \left(t, \mathbf{x}, \frac{\varphi(t, \mathbf{x})}{\varepsilon} \right) + O(\varepsilon), \quad (7.33)$$

where the phase φ satisfies the eikonal equation (7.26), and the leading order approximation $\mathbf{u}_0(t, \mathbf{x}, \theta)$ satisfies

$$\mathbf{u}_{0s\theta} + (\mathbf{u}_{0s} \cdot \mathbf{u}_{0\theta}) \mathbf{u}_0 + \frac{1}{2} \rho \mathbf{u}_{0\theta} = 0, \quad \mathbf{u}_0^2 = 1, \quad (7.34)$$

with

$$\partial_s = -\varphi_t \partial_t + \nabla \varphi \cdot \nabla, \quad \rho = -\varphi_{tt} + \Delta \varphi.$$

For planar phases, we have $\rho = 0$, and then (7.34) is just the wave map equation for maps from $(1+1)$ -dimensional Minkowski space into the sphere, which is completely integrable [41], [48]. For non-planar phases, we have $\rho \neq 0$, and the equation does not appear to be completely integrable in that case.

7.3.2 Diffraction

To account for the effect of diffraction on wave maps, we consider a solution of (7.3) of the form

$$u^a = u^a \left(x, \frac{\varphi(x)}{\varepsilon}, \frac{\psi(x)}{\varepsilon^{1/2}}; \varepsilon \right), \quad (7.35)$$

where ε is a small parameter, $\varphi, \psi : \mathcal{M} \rightarrow \mathbb{R}$ are functions, and $u^a(x, \theta, \eta; \varepsilon)$ is to be determined. We define k_α by (7.8), and let

$$\ell_\alpha = \frac{\partial \psi}{\partial x^\alpha}. \quad (7.36)$$

Use of (7.35) in (7.3) implies that

$$\begin{aligned} & \frac{1}{\varepsilon^2} (k_\alpha k^\alpha) \{ u_{\theta\theta}^a + \Gamma_{bc}^a(u) u_\theta^b u_\theta^c \} \\ & + \frac{1}{\varepsilon^{3/2}} (k_\alpha \ell^\alpha) \{ 2u_{\theta\eta}^a + 2\Gamma_{bc}^a(u) u_\theta^b u_\eta^c \} \\ & + \frac{1}{\varepsilon} \{ 2k^\alpha \partial_\alpha u_\theta^a + 2\Gamma_{bc}^a(u) k^\alpha \partial_\alpha u_\theta^b u_\theta^c + (\square_g \varphi) u_\theta^a \\ & + (\ell_\alpha \ell^\alpha) [u_{\eta\eta}^a + \Gamma_{bc}^a(u) u_\eta^b u_\eta^c] \} = O(\varepsilon^{-1/2}). \end{aligned} \quad (7.37)$$

Expanding u^a in (7.37) as

$$u^a(x, \theta; \varepsilon) = u_0^a(x, \theta, \eta) + \varepsilon^{1/2} u_1^a(x, \theta, \eta) + \varepsilon u_2^a(x, \theta, \eta) + O(\varepsilon^{3/2}), \quad (7.38)$$

and equating the coefficient of ε^{-2} to zero, we get (7.12) and (7.14), as before.

Equating the coefficient of $\varepsilon^{-3/2}$ to zero in (7.37), we obtain that

$$(k_\alpha \ell^\alpha) \{2u_{0\theta\eta}^a + 2\Gamma_{bc}^a(u_0)u_{0\theta}^b u_{0\eta}^c\} = 0. \quad (7.39)$$

This equation is satisfied provided that

$$k_\alpha \ell^\alpha = 0. \quad (7.40)$$

The use of (7.17) and (7.36) in (7.40) implies that $\partial_s \psi = 0$, meaning that ψ is constant along the rays associated with φ . Equating the coefficient of ε^{-1} to zero in (7.37), we obtain an equation for u_0^a ,

$$\begin{aligned} u_{0s\theta}^a + \frac{1}{2}(\ell_\alpha \ell^\alpha) u_{0\eta\eta}^a + \frac{1}{2}(\Box_g \varphi) u_{0\theta}^a \\ + \Gamma_{bc}^a(u_0) u_{0s}^b u_{0\theta}^c + \frac{1}{2}(\ell_\alpha \ell^\alpha) \Gamma_{bc}^a(u_0) u_{0\eta}^b u_{0\eta}^c = 0. \end{aligned} \quad (7.41)$$

This equation is a wave map equation on $(1+2)$ -dimensional Minkowski space time with an additional lower order term, proportional to $u_{0\theta}^a$. In (s, θ, η) -coordinates, the Minkowski metric components $g^{\alpha\beta}$ are given by

$$(g^{\alpha\beta}) = \frac{1}{2} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \ell_\alpha \ell^\alpha \end{pmatrix}.$$

The global existence of smooth solutions of the $(1+2)$ -dimensional wave map equations is an open question, so it is unclear whether or not the focusing of a smooth, high frequency wave map, as described by (7.41), can lead to the formation of singularities.

7.4 General relativity

7.5 Weakly nonlinear gravitational waves

7.6 Colliding plane waves

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