FROM THE ATOMIC HYPOTHESIS TO MICROLOCAL ANALYSIS

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Summary

Many physical and geometrical phenomena, although global, are determined by their local or instantaneous properties and governed by systems of differential or partial

differential equations. Differential systems often give very short and striking laws governing physical or mathematical phenomena, e.g. Newton's laws for gravitation and the movement of planets, Maxwell's equations for the electromagnetic field. But they are often very hard to solve, sometimes impossible, and it was important to build methods to construct approximate or asymptotic solutions.

In this chapter we describe two important examples some general methods of developing asymptotic solutions and theories: the WKB method applied to the Schrödinger equation (section 2), and microlocal analysis, applied to high frequency Asymptotics for the wave equation (section 3). In the WKB method for Schrödinger's equation the small parameter is the Planck constant, or more accurately (since the Planck constant is an absolute constant) the ration between Planck's constant and the size of actions at the scale of the phenomena under scrutiny, which is usually very small. In microanalysis, applied to the wave equation, the large parameter is the size of frequency, which is indeed very large in light phenomena at our scale (so that we can observe sharp shades) - much less when one tries to describe sound propagation.

Since a long time two points of view have prevailed in physics: the corpuscular point of view, which is the point of view adopted by Newton to describe light, and the wave point of view adopted by Huygens. Both account for large parts of the observations but they are rather incompatible or even contradictory (a more unifying point of view emerged with quantum physics). It is remarkable that the apparent contradiction between the particle and wave point of views is attenuated by these asymptotic theories; in many cases particles and the Hamiltonian mechanics which govern their movements appear as an asymptotic limit of the wave theory.

1 Introduction

The question of using waves or particles to describe physical phenomena like the propagation of fluids, gas, electricity and light has been a central issue of science since the beginning of scientific times. Descartes developed geometric optics, which is best explained by a corpuscular vision of light; Huygens developed wave analysis and was already quite aware of the particle/wave duality. Ideas became more precise in the 19th century; Boltzmann favored atoms while Mach, slightly earlier, was the leader of the vigorous school which used what we call at present waves. Both points of view become eventually totally entangled in the 20th century with the advent of quantum physics.

A fundamental idea of quantum physics is that small objects behave both as waves and particles, and that physical observables do not commute and cannot be measured simultaneously (Heisenberg). In Schrödinger’s approach, an elementary particle is described by its wave amplitude $\varphi(x,t)$, which is a complex valued function of a space variable $x \in \mathbb{R}^3$ (depending on time t). Equivalently this is represented by the Fourier transform:

$$\hat{\varphi}(\xi) = \int_{\mathbb{R}^n} e^{-ix\cdot\xi} \varphi(x)\, d^n x, \tag{1.1}$$

a function of an momentum variable $\xi \in \mathbb{R}^3$ (still depending on time).

The original function is given back by the Fourier reciprocity formula (inverse Fourier transform):

$$\varphi(x) = (2\pi)^{-n} \int_{\mathbb{R}^n} e^{ix\cdot\xi} \hat{\varphi}(\xi)\, d^n\xi\,. \tag{1.2}$$

In this description, "particles" - corresponding to the case where $\varphi(x)$ vanishes outside a small set, well localized in space, can sometimes be viewed as limits of waves, or conversely, but Heisenberg's incertitude principle, which says that one cannot have at the same time access to the position and the velocity of small objects as elementary particle is "obvious": φ and $\hat{\varphi}$ cannot both have a 1-point support - in fact if one vanishes outside of a bounded set, the other is analytic and cannot vanish outside of a bounded set. A more precise yet elementary formulation, for functions f of one variable, is given by the inequality:

$$\int_{\mathbb{R}} |xf(x)|^2\, dx \int_{\mathbb{R}} |\xi \hat{f}(\xi)|^2\, d\xi \geq 2\pi \left(\int_{\mathbb{R}} |f(x)|^2\, dx\right)^2 , \tag{1.3}$$

which is true for any square integrable function $\varphi \in L^2(\mathbb{R})$ (Equality is reached with the Gaussian function: $\varphi(x) = e^{-\frac{1}{2}x^2}$). Observe that the first integral in the left hand side of (1.3) measures by its smallness the fact that f "is localized" near zero, and the second does the same for $\hat{f}$. This is an elementary quadratic inequality: integrating by parts one gets, for any real α: $\int (xf)^2 - \alpha f^2 + \alpha^2 f'^2 = \int (xf + \alpha f')^2 \geq 0$ hence $\int (xf)^2 \int f'^2 \geq \int f^2$, which is equivalent to (1.3).

Mathematical tools dealing with these difficulties and with asymptotic calculus generally were developed systematically; they can be considered as the starting point of *microlocal analysis*. Two basic examples have motivated this theory: the Schrödinger equation and the theory of the wave equation. Asymptotic analysis with respect to the parameter $\hbar$ is quite natural for the Schrödinger equation; it leads to the notion of pseudo-differential calculus with a parameter, or semi-classical calculus. Expansions in terms of high frequencies are even older and also quite natural in the description of light waves; they lead to the calculus of pseudo-differential operators, developed by L. Nirenberg, J.J. Kohn, L. Hörmander etc. in the late sixties.

Microlocal analysis develops a very geometrical manner of dealing with this asymptotic calculus, reconciling asymptotically in a remarkable manner the techniques of wave analysis (Fresnel's description of light) and of particle analysis (geometrical optics). The name was pinpointed in 1970 when were announced in the Nice international congress the definition of the wavefront set (L. Hörmander, M. Sato), the possibility of using canonical transformations (J.V. Egorov), and the description of remarkably simple microlocal models for complicated systems of differential equations (M. Sato).

This program has several outgrowths, such as:

- The construction of high frequency approximations of the solutions of the Maxwell and wave equations, including significant qualitative and quantitative information. This is used e.g. in the design of antennas and in the evaluation of the radar stealthiness of a plane or a missile. Much work was devoted to this analysis, both in the U.S.A. and in the Soviet Union, e.g. in the work of J. Keller, V. Babich and their collaborators. An important point was evaluating what part of the wave is diffracted by the obstacle. Later work in this direction used in a significant manner propagation of "Gevrey regularity" (in fact Gevrey $_3$) and "Gevrey microanalysis", see Section 3.9.4.

- A precise analysis of the distribution of eigenvalues of the Laplace operator in a bounded domain (see Section 3.8) begins with H. Weyl's remarkable asymptotic estimate of the eigenvalues. The error term in this evaluation turned out to be very difficult to control, and the best result was given by L. Hörmander, who used for this Fourier integral operators for the first time, in his paper on the spectral function of elliptic operators. Many other beautiful results relating the spectrum of the Laplace operator on a domain and the geometry, of the domain or relations between the spectrum and the configuration of closed geodesics are made possible and precise using microlocal analysis, see Section 3.8; significantly a founding paper by M. Kac on this subject is titled "can you hear the shape of a drum".

- Analysis of the scattering of quantum particles by a localized potential, or of a wave by an obstacle, in particular with the description of the scattering frequencies.

The tools introduced are general enough to produce results for many problems related to those above: Dirac equation, Maxwell equations, equations of elasticity with no stress on the boundary etc.

Microlocal analysis is also used for more theoretical results, e.g. in the proof of sophisticated variants of Holmgren's uniqueness theorem.

In this chapter we have concentrated on the Schrödinger and the wave equations, which illustrate particularly well the motivations and methods of microlocal analysis, and for which results are quite striking.

We have mostly followed the presentation of L. Hörmander, which remains close to our usual insight in analysis or geometry.

A more algebraic approach, based on the fact that distributions are superpositions of boundary (edge) values of holomorphic functions defined in angular complex sectors, and using deeply and systematically the theory of holomorphic functions of several variables, was developed by the Japanese mathematicians (M. Sato, T. Kawai, M. Kashiwara).

2. The Schrödinger Equation and Semiclassical Analysis

2.1 Schrödinger equation

This is the equation

$$\frac{\hbar}{i}\partial_t\phi - \frac{\hbar^2}{2}\Delta\phi + V\phi = 0 \quad , \tag{2.1}$$

where $V(x)$, the potential, is a real valued function. We will not go into the explanation of the role of the Schrödinger equation in modern physics; it is however important to recall the following facts.

1. The solution of the equation with prescribed initial data $\phi(x,0) = \phi_0$, is given by a unitary group of operators in the Hilbert space $L^2(\mathbb{R}^n)$:

$\phi(x,t) = \phi_t = e^{\frac{t}{i\hbar}H}\phi_0$.

The generator H is a selfadjoint operator extending the differential operator $\frac{1}{2}\hbar^2\Delta_x - V$ (differential operators are not bounded operators, and there may be several "natural" selfadjoint extensions, in particular on bounded domains, and it is not always easy to prove that there is one if V is unbounded and not positive; but here we will usually write $H = \frac{1}{2}\hbar^2\Delta_x - V$ and ignore this difficulty. Since e^{itH} is unitary, the L^2-norm $\|\phi_t\|$ is invariant:

$$\|\phi_t\|^2 = \int_{\mathbb{R}^n} |\phi(x,t)|^2\, dx = \|\phi_0\|^2 . \tag{2.2}$$

In quantum physics this is normalized to 1 and $|\phi(x,t|^2$ is then interpreted as the probability density, at time t, of the presence of a particle at a point x.

2. The Planck constant $\hbar$ is a physical constant determined by experiment. What is not constant is the scale at which one makes measures or observations. At the atomic scale (very small lengths and short times) $\hbar$ is not at all negligible and one must deal with the complete Schrödinger equation above (this accounts very accurately for what is observed experimentally). On our macroscopic scale however, $\hbar$ is comparatively very small and is treated as a vanishing quantity ($\hbar \to 0$). This does not mean that one can replace $\hbar$ by 0 in the equation, because we are typically dealing with a "singular perturbation", i.e. the terms which vanish involve higher order derivatives than those which remain. What one is really interested in is the asymptotic behavior of solutions for $\hbar \to 0$, hoping that this will turn out to be simpler than the global behavior of complete solutions, realize a connection between quantum and classical mechanic and eventually produce new tools to analyze the original equation.

More generally semi-classical analysis studies asymptotic solutions of differential equations $Pf \simeq 0$, or $Pf \simeq g$, for $\hbar \to 0$, where P is an asymptotic differential operator of the form:

$$P(x,\hbar D_x,\hbar) \sim \sum \hbar^k P_k(x,\hbar D), \tag{2.3}$$

associated to a function (symbol) $p(x,\xi,\hbar)$, and $f \sim \sum \hbar^k f_k$ is an asymptotic function or distribution, so as g. Here and in the entire sequel, we have set:

$$D = \frac{1}{i}\partial = \frac{1}{i}(\partial_{x_1},\ldots,\partial_{x_n}).$$

A remarkable feature of semi-classical analysis is that it relates the study of asymptotic solutions to classical mechanics, using what is now called "micro-local analysis". The Schrödinger equation is its first and most important motivation and application.

2.2 WKB Asymptotics

It is customary to look for oscillating asymptotic solutions of the Schrödinger Eq.(2.1) in the form:

$$\phi_\hbar(x,t) \simeq e^{\frac{i}{\hbar}S(x,t)}(a(x,t)+O(\hbar)). \tag{2.4}$$

The exponent $S(x,t)$ is called *phase* and $a(x,t)$ *amplitude*. The W.K.B. method is the method for producing such asymptotic solutions (W.K.B. stands for Wentzel-Kramer-Brillouin): note that we have the operator relation

$$\begin{aligned} e^{-\frac{i}{\hbar}S}\left(\frac{\hbar}{i}\partial_t - \frac{\hbar^2}{2}\Delta + V\right)e^{\frac{i}{\hbar}S} \quad &= \\ &(S_t + \frac{1}{2}|S_x|^2 + V)a \\ &\quad + \frac{\hbar}{i}(a_t + S_x.a_x + \frac{1}{2}\Delta_x S\ a)) \\ &\quad\quad - \frac{1}{2}\hbar^2\Delta_x a \end{aligned} \tag{2.5}$$

which follows from the elementary relations $e^{-\frac{i}{\hbar}S}(\frac{\hbar}{i}\partial_k)e^{\frac{i}{\hbar}S} = \frac{\hbar}{i}\partial_k + \partial_k S$. Inserting this in (2.4), we get for 0-order terms the *"eiconal equation"*:

$$\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla_x S)^2 + V(x) = 0 \tag{2.6}$$

and for 1st order terms the *"transport equation"*:

$$\partial_t a + \frac{1}{2}\nabla_x S \cdot \nabla_x a + \frac{1}{2}(\Delta_x S)a = 0. \qquad (2.7)$$

The eiconal Eq.(2.6) is familiar in fluid mechanics and control theory, where it is called the *Hamilton-Jacobi equation*, and there are several ways of analyzing it. For our purpose the natural route is the connection with Hamiltonian systems. Let

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

be the Hamiltonian function associated with the operator $-\frac{1}{2}\hbar^2\Delta_x + V(x)$; the Hamiltonian vector field (see section 2.10) L_E is defined as

$$L_E = \sum \frac{\partial E}{\partial \xi_j}\partial_{x_j} - \frac{\partial E}{\partial x_j}\partial_{\xi_j} = \sum \xi_j \partial_{x_j} - \frac{\partial V}{\partial x_j}\partial_{\xi_j}.$$

Assuming that S is smooth (at least twice differentiable), we introduce the Lagrangian manifold $\Lambda_S \subset \mathbb{R}^{2n} \times \mathbb{R}$, set of all points (x,ξ,t) with $\xi = \nabla_x S(x,t)$. (Lagrangian means that the differential 2-form $\sum d\xi_j dx_j$ induces 0 on Λ_S, which follows from the Schwarz identities $\frac{\partial^2 S}{\partial x_i \partial x_j} = \frac{\partial^2 S}{\partial x_j \partial x_i}$. Lagrangian manifolds play a crucial role in microanalysis, as we will see further in Section 3).

Because Λ_S is Lagrangian, the Eiconal equation implies that the Lagrangian manifold is tangent to $\partial_t + L_a$, i.e. Λ_S is the union of integral curves of the system

$$\frac{dx}{dt} = \nabla_\xi H = \xi,$$

$$\frac{d\xi}{dt} = -\nabla_x H. \qquad (2.8)$$

with initial point (for $t = 0$) $x(0) = x_0 \in \mathbb{R}^n, \xi(0) = \nabla_x S(x_0)$.

For any $x_0 \in \mathbb{R}^n$ there exists a unique integral curve $x(t), \xi(t)$ with initial data $x(0) = x_0, \xi(0) = \xi_0 = \nabla_x S(x_0)$; the eiconal equation implies that along this curve we have $\frac{dS}{dt} = -E(x,\xi)$ i.e.

$$S(x(T)) - S(x(0)) = -\int_0^T \left(\frac{1}{2}\left(\frac{dx}{dt}\right)^2 + V(x)\right) dt. \qquad (2.9)$$

This determines the phase S completely, at least for small t, because the map

$(x,t) \mapsto (x(t),t)$ is one to one, at least for small t (this follows from the implicit function theorem).

Once S is known, the amplitude a is determined by integrating the transport equation along the integral curve above. This gives a solution mod. $\hbar^2$. One can improve and get an asymptotic solution mod. $\hbar^{-\infty}$, replacing a by an asymptotic sum $\sum \hbar^k a_k$: a_k is computed recursively as a solution of a transport equation $Ta_k = *$, where the transport operator T is the first order operator appearing in (2.7), and the right hand side is given in terms of the preceding a_j.

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Biographical Sketches

Boutet de Monvel Louis was born in 1941.
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