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Asymptotic Solutions of the One-Dimensional Schrödinger Equation

S. Yu. Slavyanov

American Mathematical Society

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Asymptotic Solutions of the One-Dimensional Schrödinger Equation

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АСИМПТОТИКА РЕШЕНИЙ ОДНОМЕРНОГО УРАВНЕНИЯ ШРЕДИНГЕРА

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ABSTRACT. The book is devoted to asymptotic analysis of solutions of second order ordinary differential equations with a small parameter. The main emphasis is on various constructive schemes of obtaining asymptotic solutions, their advantages and drawbacks, and specific computations. The author gives a complete overview of the state of the theory and also concentrates on some lesser known aspects and problems, in particular the problems in which exponentially small terms should be taken into account or the analysis of equations with close transition points. Such applications as the derivation of the formulas for the quasiclassical quantization, spectrum splitting in a symmetrical potential, etc. are considered. The book can be used by researchers and graduate students working in ordinary differential equations and mathematical problems of quantum mechanics.

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Preface to the English Edition

This book was written in 1985–1988. It reflectes the experience and the views of the author at that time, and was intended for readers interested in applications rather than in rigorous theory. After that the author almost stopped doing research in the area (a few exceptions are papers [**1*–3***][1]). Meanwhile the new revolutionary period of much deeper understanding of asymptotics started. Therefore, when the American Mathematical Society kindly suggested publishing the English translation of the book, the author was at a loss. Should he make changes in the structure and the text of the book, or it should be left unmodified? The author has chosen the second possibility taking into account that:

(i) for the above-mentioned readers the changes were not so vital;

(ii) the author himself could not be regarded as a real expert in the new trends.

Still the author feels it is his duty at least to mention the major recent achievements and to give a short list of references.

Even in the book itself asymptotic solutions of the Schrödinger equation are exposed beyond the scope of the Poincaré definition of asymptotics. Although the author has nothing to change in formulas, the argumentation is essentially heuristic rather than rigorous. The really mathematical presentation of what is called "exponential asymptotics," when exponentially small terms (which should be neglected in the Poincaré sense) are dealt with, is based on the use of Borel transform. The example of the approach to asymptotics on the basis of Borel summability was given by Silverstone et al. [**4***]. A much more general formulation arranged as the "resurgence theory" has been presented by Écalle [**5***]. Rather abstract ideas of Écalle were later developed and modified by Pham [**6***], Voros [**7***], and others. Mathematical treatment of exponential asymptotics more adequate to numerical mathematics and closer to heuristic argumentation was proposed by Kruskal and Costin [**8***].

Another crucial idea (which is not presented in the book)—the method of smoothing the asymptotic expansions near the Stokes line—was suggested by Berry [**9***]. Berry's smoothing process appeared to be very general and valid beyond the scope of Stokes' phenomena. More rigorous treatment of the process was given by McLeod [**10***].

Behavior of asymptotic expansions in the vicinity of coalescing turning points, which is studied in the book, received better justification in papers by Dunster [**11***].

It is also necessary to mention the notion of hyperasymptotics proposed by Berry and Howls [**12***] and extended to solutions of differential equations by Olde Daalhuis and Olver [**13***]. This notion is remarkable since it goes beyond the

[1]The numbers in this preface refer to additional references at the end of the reference list.

scope of formal asymptotics taken as the basis of the ansatz. On the other hand, hyperasymptotics gives the tool for much better numerical estimates than any other form of asymptotics.

Finally, it is author's pleasure and duty to thank the American Mathematical Society for choosing to publish this book, which is rather far from conventional mathematics; senior editor of the AMS, Sergei Gelfand, for patience in negotiations with the author; and the translator of the book, Vadim Khidekel, for carefully searching for misprints in the Russian edition.

Saying it frankly, the author is very enthusiastic about the research process but cares much less about final checking. Therefore, the reader should be aware of still existing misprints in the text.

S. Yu. Slavyanov
St. Petersburg, February 1996

Preface

This book grew out of the graduate-level course "Asymptotic Methods in the Theory of Ordinary Differential Equations," given by the author at the Department of Physics of St. Petersburg University. The reader is supposed to be familiar with basic notions of the theory of ordinary differential equations and the complex analysis.

Asymptotic methods are important in modern mathematical physics. They allow the qualitative and quantitative tracing of the limit passages from one physical theory to another, for example, from quantum to classical mechanics, or from wave to geometrical optics. They can also clarify many important physical phenomena such as the long-range propagation of radio waves in the atmosphere and acoustical waves in the ocean, the binding of atoms in molecules, radioactive decay, and many others.

This book is devoted to a specific problem in the theory of asymptotic methods, to asymptotic expansions of the solutions of second-order linear homogeneous ordinary differential equations with a small coefficient of the higher derivative. This equation can be written in a standard form as

$$y''(x) + p^2\big(\lambda - q(x)\big)y(x) = 0. \tag{1}$$

Equation (1) is often referred to as the one-dimensional Schrödinger equation with the potential $q(x)$ and the energy λ. Quantum terminology is used throughout the book, although equation (1) can also arise in other fields of physics. The coefficient p is assumed to be "large." Its meaning from the mathematical point of view is explained by the definitions of asymptotic expansions. In practical applications of asymptotic formulas it is sufficient that the parameter p take the values of at least tens.

This book emphasizes the presentation of various algorithms for constructing asymptotic expansions of the solutions of equation (1), discussion of their advantages and disadvantages, and the computational details, which are important for the readers—physicists and engineers. The proofs are given with less detail; sometimes they are omitted completely.

All the methods of deriving asymptotic solutions of equation (1) are based on a simple idea that "similar" equations have "similar" solutions. In the simplest case, an equation with constant coefficients is chosen as a *comparison equation* to (1). However, such an approach fails in a vicinity of what is known as *transition points*, that is, the points where $\lambda - q(x)$ has either zeros or simple poles. Obtaining uniform asymptotics of the solutions of equation (1) in a vicinity of transition points and matching asymptotic expansions are the main goals of the theory presented. Two methods are commonly used: introducing a comparison equation in a more general form, and bypassing transition points using the complex argument. The choice of method is determined by the requirements for the result and by the properties of the potential $q(x)$. Usually, the "better" the potential, the more complete and precise the results.

In Chapter I the properties of comparison functions—the Airy functions, the parabolic cylinder functions, the Bessel functions, etc.—are presented. These functions are used to derive asymptotic solutions of equation (1) near transition points. They also help us to illustrate the important general definitions of Stokes lines and Stokes phenomena. The asymptotics of comparison functions for large values of the argument are derived in a universal way: by calculating the asymptotics of the Laplace contour integrals that represent these functions. If the argument of a complex variable is changed, the integration contour has to be deformed. Such a deformation may be discontinuous at some values of the argument; this results in abrupt changes in the form of the asymptotics. These changes are called the Stokes phenomenon.

Contrary to the conventional Poincaré definition of an asymptotic expansion, in this book the exponentially decreasing terms are carefully kept in the background of the dominant asymptotic series. First, this enables us to improve the accuracy that can be achieved by asymptotic formulas (this was first pointed out by F. Olver). Second, this helps us to formalize the algorithms for calculating exponentially small corrections to eigenvalues in various applications. As a result, asymptotic formulas for comparison functions derived in this book often differ from what most handbooks on special functions present. Also, the Stokes phenomenon is interpreted from a different point of view.

Chapter II is concerned with the methods of constructing the asymptotic expansions for solutions of equation (1) with an arbitrary potential $q(x)$. The first two sections deal with well-known subjects: writing asymptotic solutions in intervals of the complex plane in the absence of transition points. Only the main ideas are discussed. For more information on the subject the reader is referred to the book of Fedoryuk (1983). More attention is paid to studies of asymptotics near transition points, especially to nontraditional issues such as various simplifications of general uniform formulas, regularization of integrals, passage to the limit when the transition points approach one another, the role of a second-order pole singularity in the coefficients of equation (1), and so forth.

In Chapter III we study some applied problems. They are not always closely connected with real physical problems. Both models and specific problems arising in various fields of physics are considered. In the first section we derive the formulas for a semiclassical quantization. In Section 2 the contribution of boundary conditions at finite points to semiclassical quantization is studied on a model problem of submarine acoustics. In the next two sections we present the algorithms to distinguish exponentially small terms in power expansions. Then we pass to the scattering problem and the problem of a periodic potential. Throughout the book the case when the spectral parameter is proportional to some power of the large parameter (which leads to close turning points) is analyzed separately and the physical meaning of this assumption is discussed.

In Chapter IV several technical questions are discussed. They are mostly related to the numerical realization of asymptotic methods such as computing phase integrals and the correspondence between exact solutions and asymptotics. In Section 3 we concentrate on applying the main notions of Stokes lines and Stokes constants to the equations with polynomial coefficients that are more complicated than the equations for special functions. This section was written by M. A. Kovalevskiĭ at the author's request.

Much less analytical results exist here and we have to turn more to numerical methods. On the other hand, the problems under consideration become more and more complicated, and this will necessarily result in using these equations as the comparison equations. The author is very grateful to M. A. Kovalevskiĭ for writing this section.

Many physicists and mathematicians developed and used in their work asymptotic methods for equation (1). Sometimes it is very difficult to establish the authorship of an idea, method, or formula. We will name the scientists that made the most important contributions to this theory. Among foreign scientists we should mention H. Poincaré, G. Stokes, G. Green, J. Liouville, A. Zwaan, and H. Jeffreys, who put forth the main ideas; G. Wentzel, H. Kramers, and L. Brillouin who were the first to apply asymptotic methods to the quantum mechanical problems (WKB method). We also mention the monographs and papers of R. Langer, G. Birkhoff, E. Kemble, T. Cherry, V. Torson, K. Budden, A. Erdélyi, F. Olver, J. Heading, N. Fröman, and P. O. Fröman, which summed up various aspects of the theory. The contribution of Soviet scientists to the development of asymptotic methods is also very important. V. A. Fock and his student M. I. Petrashen′ succeeded in deriving asymptotic solutions of classical problems of quantum mechanics. The paper of A. A. Dorodnytsyn was an important milestone in the theory. M. V. Fedoryuk gave rigorous justification of Zwaan's methods. V. P. Maslov proposed a new method for obtaining asymptotic expansions. E. E. Dubrovskaya, E. E. Nikitin, N. I. Zhirnov, and R. Ya. Damburg applied asymptotic methods to solve many particular quantum mechanical problems. The problems of the diffraction and propagation of waves were studied using asymptotic methods by V. S. Buldyrev, L. M. Brekhovskikh, G. I. Makarov, and V. V. Novikov. The lectures of L. I. Ponomarev, V. S. Buldyrev, V. M. Babich, and I. A. Molotkov provide a good study of asymptotic methods.

The book of M. V. Fedoryuk, in which a complete picture of the latest progress in the asymptotic theory of ordinary differential equations is presented on a very high scientific level, was published in 1983. The present monograph complements that book and aims to help the reader develop skills of working with asymptotic expansions (with many details).

The author attempted to present a sufficiently full picture of the whole theory and at the same time pay more attention to nontrivial aspects, which are less studied in principal monographs. The problems to whose solution the author contributed are also discussed (the problems of the subordinate exponential function in the background of the dominant one, problems with close transition points, algorithms for calculating phase integrals, etc.).

We want to point out some technical details of the book's structure. The formulas are numbered independently in each chapter. Within a chapter, the first digit of the equation number indicates the number of the section. For references within a chapter, its number is not given. References to scientific publications are mostly concentrated in the "Comments" sections. The author and the year of publication are indicated. The bibliography at the end of the book includes not only the entries cited in the text but also additional papers and monographs that the author believes to contain important results concerning the asymptotic solutions of the one-dimensional Schrödinger equation. The author is very grateful

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