

JWKB APPROXIMATION

Contributions to the Theory

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1965

NORTH-HOLLAND PUBLISHING COMPANY
AMSTERDAM

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PRINTED IN BELGIUM

P R E F A C E

Our interest in the problems treated in the present book arose in connection with a special quantal problem for which a precise knowledge of the properties of the JWKB-approximation, especially the connection formulae, was needed. Since the existing literature — in spite of its abundance — did not provide what we were looking for, we were actually compelled to try to find our own way out of the impasse. To begin with our intention was to publish our achievements in the usual way in some scientific journal. However, the material soon grew too large to be published as one article. Furthermore, since the JWKB-approximation is of interest to a wide circle of scientists working in several different branches of physics, we decided to publish our work as a book. Thus, apart from the formal derivation of the JWKB-solutions in chapter 2, we present a new investigation of the JWKB-approximation.

The book contains a rigorous treatment of the one-dimensional JWKB-approximation. Using the ideas introduced by Zwaan and Kemble as a starting point we develop a method for examining the properties of the JWKB-approximation which is powerful also in intricate and complicated applications. In the first place we have had quantal problems in mind and hence, in the main part of the book, we assume the coefficients of the differential equation considered to be real on the real axis. This assumption simplifies the treatment. There are, however, important applications, for instance in the theory of electromagnetic waves, where the reality condition is not fulfilled. It should therefore be pointed out that the general theory in chapters 3, 4, and 7, is not subject to the above mentioned restriction and that the method can be worked out also when the coefficients are complex.

It is hoped that this book will be enlightening to all who wish to master the JWKB-approximation, and that the method developed will prove to be useful in justifying further applications of the JWKB-method.

We are much indebted to Professor Anders Reiz, Dr. Hans Ryde, Dr. Alf Sjölander, and Professor Ulf Uhlhorn who kindly read the manuscript and made valuable comments. We also wish to thank Mr. Mattias Soop who checked the formulae, suggested some formal improvements in the presentation, and was helpful in reading the proofs. We are grateful to Mr. Gyula Jakab who drew the figures, and to Mrs. Ingrid Blidholm, Mrs. Ingrid Fåhraeus, and Mrs. Britt Egerland whose secreterial assistance was most valuable. Finally, it is a pleasure to thank Mrs. Karin Ryde who, in spite of many other duties, spared no effort in correcting the language.

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Uppsala, July 1964

CONTENTS

CHAPTER 1. INTRODUCTION	1
CHAPTER 2. FORMAL DERIVATION OF THE JWKB-APPROXIMATION . .	10
CHAPTER 3. DERIVATION OF AN EXACT FORMULA FOR THE GENERAL SOLUTION OF THE SCHRÖDINGER EQUATION	13
CHAPTER 4. BASIC ESTIMATES AND LIMITING PROPERTIES OF THE F -MATRIX	26
CHAPTER 5. SYMMETRY PROPERTIES OF THE F -MATRIX CONNECTING TWO POINTS ON THE REAL AXIS	30
CHAPTER 6. ESTIMATES OF THE F -MATRIX CONNECTING TWO POINTS ON THE REAL AXIS	34
6.1. Estimates of the F -matrix connecting two points in the same classically allowed region	34
6.2. Estimates of the F -matrix connecting two points in the same classically forbidden region.	35
6.3. Estimates of the F -matrix connecting two points on opposite sides of a classical turning point	36
6.4. Estimates of the F -matrix connecting two points on opposite sides of an overdense potential barrier	43
6.5. Estimates of the F -matrix connecting two points on opposite sides of an underdense potential barrier	51
CHAPTER 7. PROPERTIES OF THE F -MATRIX IN THE REGION AROUND A WELL ISOLATED ZERO OR POLE OF $Q^2(z)$	60
7.1. Auxiliary formulae	61
7.2. Properties of the F -matrix in the region around a well isolated zero of the first order for $Q^2(z)$	65
7.3. Properties of the F -matrix in the region around a well isolated zero of the order n for $Q^2(z)$	69
7.4. Properties of the F -matrix in the region around a well isolated pole of the first or second order for $Q^2(z)$	74

CHAPTER 8. THE WAVE FUNCTION IN A REGION OF THE REAL AXIS WHERE THERE IS AT THE MOST ONE CLASSICAL TURNING POINT	80
8.1. Estimate of the accuracy of the JWKB-approximation in a classically allowed region	80
8.2. Estimate of the accuracy of the JWKB-approximation in a classically forbidden region.	81
8.3. The connection formulae for the JWKB-approximations of the same wave function on opposite sides of a classical turning point.	83
CHAPTER 9. BARRIER TRANSMISSION	90
9.1. Barrier penetration when the kinetic energy of the incident particle lies below the energy corresponding to the top of the barrier.	92
9.2. Super-barrier transmission when the kinetic energy of the incident particle lies slightly above the energy corresponding to the top of the barrier	97
CHAPTER 10. BOUND STATES	102
CHAPTER 11. THE RADIAL EQUATION OF MOTION FOR A PARTICLE IN A CENTRAL FIELD OF FORCE	110
11.1. The modification corresponding to the replacement of $l(l+1)$ by $(l+\frac{1}{2})^2$ in the JWKB-formulae	112
11.1.1. Application to the radial wave equation for hydrogen-like ions	117
11.1.2. Application to the three-dimensional harmonic oscillator.	120
11.1.3. Application to the determination of the asymptotic phases in scattering problems	125
11.2. The modification corresponding to the omission of the centrifugal barrier in the JWKB-formulae	131
REFERENCES	135
INDEX	136

INTRODUCTION

The mathematical approximation method, in this work called the JWKB-approximation, which gives the connection between classical mechanics and quantum mechanics, has been known for a long time. In fact it may be traced back to papers by Carlini, 1817, Liouville, 1837, and Green, 1837. After that the method has been developed by many people, and today there exists an extensive literature on the subject. We shall not, however, try to give any historical review here, nor any extensive list of references. These can be found in a recent monograph on the subject by HEADING [1962] and also in some of our other references. We want only to make a few remarks in connection with the name given to the method. Important results in the development of the theory, namely the so called connection formulae, seem to have been derived for the first time by Gans, 1915, but were rediscovered independently by Jeffreys, 1923, and Kramers, 1926. Brillouin, Wentzel, and Kramers in 1926 introduced the method in quantum mechanics applying it to Schrödinger's wave equation. Since then the method has been called the WKB-method by most writers in theoretical physics, though this is not a very appropriate name as should be obvious even from the few words said above on the development of the theory. There are also writers who have tried to introduce other names, e.g. the Liouville-Green approximation or the phase-integral method. In a recent review article by B.S. JEFFREYS [1961] it is suggested that the method should be called the asymptotic approximation method. As long as one uses asymptotic expansions to derive the formulae, as has in fact been done in most investigations hitherto, this name might be considered convenient. We have found it inadequate, however, to use this name in the present work, since we have avoided the use of asymptotic series and have based our investigation on a convergent series expansion, being an exact solution of the differential equation. Since the concept "WKB" is so frequent among theoretical physicists, we use it without trying to find the most appropriate order of the letters. To do justice to Jeffreys we follow some authors and add the

letter J, which for chronological reasons we place first, thus speaking of the JWKB-approximation.

The JWKB-method is of wide application not only in quantum mechanics but also in many other branches of theoretical physics, e.g. in the theory of electromagnetic waves. It has been used for many years with great success, and it is well known that in several common applications the method gives very accurate results. One is apt to believe that such an old method, having been thoroughly studied from purely mathematical points of view and tested numerically by comparison with known exact results, should be freed of obscurities and that contradictory opinions among specialists as to its properties should have been ruled out long ago. Actually this is not the case. On the contrary, there has been very much criticism and dispute especially concerning the connection formulae. When one studies the existing literature carefully enough, one finds surprisingly many unsatisfactory features. Thus in many of the best text-books on quantum mechanics the treatment of the JWKB-method and its applications is unclear. Especially the comments on the connection formulae and their one-directional nature, which is even quite disregarded by some authors, contain ambiguities and misconceptions. In fact, most authors use the connection formulae in both directions, for instance when treating barrier penetration problems. Usually in such problems the derivations only become unnecessarily complicated and insignificant terms appear in the result, but sometimes more serious difficulties may appear. There is already an extensive literature available, establishing conditions for the existence of approximate solutions of the JWKB-type in well defined regions of the complex plane. To obtain these conditions the authors almost exclusively use asymptotic expansions, the leading terms of which give the JWKB-formulae. Thus the errors are expressed in terms of O -symbols, which is necessarily somewhat vague. Another disadvantage is the fact that asymptotic expansions of given solutions have different forms in different regions of the complex plane, and the problem of tracing a solution with known asymptotic behaviour in one region of the complex plane to regions where other forms of the asymptotic expansion have to be used, is not very simple. The above mentioned disputes as regards the connection formulae illustrate this fact. The problem has been treated with more or less rigour by many people. In the first place we mention Jeffreys and Langer, to whom reference is frequently made. Less known among theoretical physicists is a work by SEIFERT [1942-43], who gives a clear and mathematically satisfactory treatment based on the use

of asymptotic series. OLVER [1961] has in a recent work obtained limits of error for special solutions from convergent series. His results are valid, however, only within regions of the complex plane, where one and the same form of an asymptotic expansion could be used. What he achieves, compared to those who use asymptotic expansions, is thus a definite upper bound instead of an O-symbol, but he has left untouched the important problem of obtaining more general limits of error, valid over several such regions as mentioned above. ZWAAN [1929] and KEMBLE [1935] have used a different approach to which we shall return below. In spite of the abundant literature there is still lacking a convenient method for obtaining definite limits of error in more general cases, and even quite recently HEADING [1962] (cf. his p. 59) has expressed the opinion that "this vagueness must be accepted as one of the inherent weaknesses of the phase-integral method". The problem of obtaining such limits of error is not only of academic or mathematical interest but is especially important in some physical applications, since the JWKB-method is sometimes used with so little rigour that one cannot have confidence in the results.

The present work originated in connection with a special physical problem adapted to be treated by means of the JWKB-method. As regards this method the lack of a satisfactory and rigorous treatment allowing for the physical aspects then grew more and more embarrassing. On examining the literature we found a convenient starting point for such a treatment in the above mentioned papers by Zwaan and by Kemble. Zwaan's idea was to allow the independent variable in the differential equation to take complex values and to derive a connection formula by tracing the solution in the complex plane around the critical point. To quote Birkhoff's judgement (BIRKHOFF [1933]) : "Zwaan's treatment is extremely suggestive, although lacking in essential respects". An attempt to put Zwaan's method on a rigorous basis was made by Kemble in a well-known paper (KEMBLE [1935]). Kemble transformed in a convenient way the original linear differential equation of the second order to a system of two linear differential equations of the first order. However, he obviously did not realize that these equations have exact solutions in terms of fairly simple convergent series, and therefore he integrated them in an approximate way, which is both complicated and difficult to follow. It is our intention in the present work to develop a theory of the JWKB-method in a rigorous and systematic way on the basis of Zwaan's idea and the first order differential equations in Kemble's paper.

We derive the exact solution of these differential equations and express

it in terms of a z -dependent matrix, which then becomes our main tool for discussing the properties of the JWKB-solutions. The theory developed provides a sound basis for handling the JWKB-method. It leads to satisfactory estimates of the accuracy of the JWKB-approximation, and it is also powerful in proving exact relations in connection with the use of the JWKB-formulae. In some cases these exact results are already well known from comparisons with results obtained by other methods, e.g. as concerning the energy levels of the harmonic oscillator and the hydrogen atom. (In this connection we refer to a paper by BIRKHOFF [1933], where the semi-classical quantization condition is treated rigorously for a special class of potentials.) In some other cases the exact relations have not been revealed before, and it may be that they are not easily proved by methods based on asymptotic expansions. We are thinking of certain exact relations, derived in chapter 7, between the elements of the above mentioned matrix. The approximate form of the elements themselves can be found in Heading's book (HEADING [1962]), where they are called Stokes' constants. We consider it an advantage of our approach to the JWKB-method that one is able to work with an exact solution and to make all approximations in the final formulae, yet having a close contact with the JWKB-formulae in all steps of the calculations. As concerns the physical applications treated in the present work, several of them are discussed rigorously for the first time and satisfactory estimates of the errors involved are obtained. The whole systematic treatment of the theory of the JWKB-method, built on our exact solution of Kemble's differential equations, is also new.

In the rest of this introductory chapter we shall give a survey of the contents of this book. At the same time we shall also make some remarks about the treatments of the JWKB-method given by other authors.

In chapter 2 the JWKB-formulae are derived in a well-known way, and conditions for their validity as they appear by the derivation are given. The conditions are given more carefully than is usual in textbooks in theoretical physics. We have included this chapter in order to be able to make a comparison with our later treatment.

Chapter 3 forms the basis of all subsequent chapters. We first transform the one-dimensional Schrödinger equation $d^2\psi/dz^2 + Q^2(z)\psi = 0$ into a system of two differential equations of the first order in the way devised by Kemble. Our treatment is only somewhat more general, since from the start it allows for the possibility of modifying the JWKB-method by replacing the function $Q(z)$ in the usual JWKB-formulae by another

function $q(z)$, which can be chosen conveniently. Using an iteration procedure, we then obtain the general solution of Kemble's system of differential equations in terms of convergent series. We have gained considerably in simplicity and clarity by introducing a matrix formalism. Thus we write the solution in terms of a second order matrix $F(z, z_0)$ depending on a fixed point z_0 and a variable point z . The elements of $F(z, z_0)$ are given by convergent series expansions. The general solution $\psi(z)$ of the original differential equation can be expressed exactly in terms of the elements of the matrix $F(z, z_0)$ and the JWKB-functions at the point z .

In chapter 4 we obtain basic estimates for the elements of the matrix $F(z, z_0)$ on the assumption that the points z_0 and z can be joined by a path along which the absolute values of the exponential functions in the JWKB-formulae vary monotonically. This is an important assumption, which seems to be essential for obtaining adequate estimates. To estimate the matrix $F(z, z_0)$ in other cases we divide a conveniently chosen path from z_0 to z into parts fulfilling the above mentioned assumption and then use matrix multiplication. The estimates obtained reflect characteristic properties of the matrix $F(z, z_0)$ connected with Stokes' phenomenon, which plays an important role in dealing with the JWKB-method. Besides deriving the basic estimates for the matrix $F(z, z_0)$, we also consider in chapter 4 certain limiting values for the elements of this matrix.

In chapter 5 we introduce the assumption that the function $Q^2(z)$ is real on the real axis, and we derive certain relations between the elements of the F -matrix connecting any two points on the real x -axis. These relations, which we call symmetry relations, arise because of the fact that the Schrödinger equation contains only real quantities on the real axis. Thus, if the function $\psi(x)$ is a solution, so is also the complex conjugate function $\psi^*(x)$ if the independent variable x is real. The symmetry relations play an important role in the following chapters.

Using the basic estimates and the symmetry relations, we obtain in chapter 6 estimates for the F -matrix connecting two points on the real axis. First we treat the most simple cases that the two points lie either in the same classically allowed region or in the same classically forbidden region. Then we consider the cases that the two points lie on opposite sides of a classical turning point, on opposite sides of an overdense potential barrier, or on opposite sides of an underdense potential barrier, respectively. The resulting estimates form important corner-stones in our treatment of the JWKB-method. Further corner-stones of this kind can be derived from the results

of chapter 7. Thus, an approximate formula for the F -matrix connecting two points on opposite sides of a well isolated zero of an arbitrary even order can immediately be obtained by multiplying together such matrices as given in our formulae (7.13a) and (7.13b).

In chapter 7, where the function $Q^2(z)$ is in general not restricted to be real on the real axis, we choose $q^2(z)$ conveniently and derive approximate formulae for the F -matrix connecting two points on different anti-Stokes' lines emerging either from a well isolated zero of an arbitrary order for $q^2(z)$ or from a pole of the first or second order for $q^2(z)$. These formulae, which replace commonly used qualitative arguments connected with Stokes' phenomenon, give a good insight into the mechanism of the JWKB-method.

In chapter 8 we consider the wave function $\psi(x)$ on the real axis. First we discuss the accuracy of the JWKB-approximation in a classically allowed as well as in a classically forbidden region. In the latter case the error of the dominating term is in general larger than the other term, and therefore there arises the question of finding a criterion for whether both terms of the JWKB-approximation are significant or not. We give a sufficient criterion of this kind. The important problem of finding the JWKB-approximations of the same wave function on opposite sides of a classical turning point is then treated in detail, and we obtain connection formulae containing estimates of the error involved. The commonly used connection formulae are given in (8.20) and (8.21). In textbooks on quantum mechanics the first one is often given only for the special case that $\gamma = \frac{1}{2}\pi$. This is regrettable since the more general form gives a much better insight into the way the connection formulae work. Besides these connection formulae we have also derived the connection formula (8.19). Although this formula can be obtained from (8.20), we have considered it convenient to give it separately. The formula is for instance well adapted for treating the problem of penetration through a potential barrier. The inherent one-directional nature of the connection formulae has led to many controversial discussions and misconceptions. Langer, who has made important contributions to the theory and has strongly emphasized the one-sided nature of the connection formulae, has pronounced the opinion that the difficulty with these formulae seems to be "circumventable only by *picking* special solutions in a suitable way, and holding fast to them, throughout the discussion" (LANGER [1934]). We find, however, that there remains no difficulty with the connection formulae, if they are treated and formulated in a convenient way and due

regard is taken of the conditions for their validity. The one-sided nature of the connection formulae is deeply rooted in the theory of the JWKB-method and cannot be circumvented in any way. This should be quite obvious from our derivation. As an example of applying the connection formula (8.21) we treat in a simple and straightforward way a boundary value problem, which has previously been treated by H. JEFFREYS [1956] in order to reject a criticism put forward by Langer. We believe that Jeffreys' treatment is perfectly right although unnecessarily complicated, since he seems to be of the opinion that such boundary value problems cannot be handled by using the usual one-directional connection formulae. Our treatment shows clearly that applications of this kind lie wholly within the scope of these formulae. Once they are conveniently formulated and the conditions for their validity stated, they can be applied directly in simple and straightforward ways for solving physical problems.

As we have already mentioned, the treatments of the connection formulae in most textbooks and even in some of the best ones are not satisfactory. For instance in those by BOHM [1961] and by MERZBACHER [1961], as well as in the treatise by MORSE and FESHBACH [1953], this subject is presented in unclear and more or less misleading ways. The same can be said of the treatment of the connection formulae in Pauli's article on quantum mechanics in *Handbuch der Physik* (PAULI [1958]). Pauli uses the careful term "richtige Zuordnung" but does not mention the one-sided nature of the connection formulae. He gives formulae, which exactly preserve the current density through the classical turning point, since he includes in the classically forbidden region a small term of the JWKB-type that is in general negligible compared to the error of the larger term. Pauli points out the insignificance of this term, but nevertheless he adds the comment: "Bei allen Fragen jedoch, wo nicht nur der Betrag von $u(x)$, sondern auch die Phase von $u(x)$ eine Rolle spielt, ist es berechtigt, ihn beizubehalten", which is quite ununderstandable. In Heading's recent book on phase-integral methods (HEADING [1962]) the connection formulae are discussed in several places. Heading seems to consider that the connection formula (8.21) can be applied in both directions [cf. his equation (4.11)]. When discussing the connection formula (8.20) with $\gamma = \frac{1}{2}\pi$ he makes several remarks as to the conservation of current density and the use of this formula in the forbidden sense (cf. his pp. 87, 89, and 97). Actually we do not exactly understand what Heading aims at in this discussion, but we think that the simple answer to the question, why inconsistencies have not appeared on using the connection

formulae in the wrong directions, is that the contributions obtained by doing so have been insignificant in the cases treated.

Utilizing the investigation of the F -matrix given in chapter 6, we study in chapter 9 the problem of transmission of particles through a potential barrier. The energy of the particles may be either smaller or larger than the energy corresponding to the top of the barrier, the discussion being quite analogous in both cases. We express the reflection and transmission coefficients in terms of the F -matrix and obtain simple approximate formulae by means of the estimates derived in chapter 6. For the case that the potential barrier is overdense and the classical turning points are well separated the problem can also be solved in a very simple and straightforward way by means of the connection formulae (8.19) and (8.21). However, we have given the treatment based directly on the F -matrix formalism because we wanted to further elucidate this problem in order to rule out the element of controversy, which has been attached to the application of the JWKB-method to this problem.

In chapter 10 we consider the stationary states of a particle in a potential well. To put the treatment on a rigorous basis it is important to know the properties of certain limiting values of the elements of the F -matrix and of the coefficients of the JWKB-functions. These limiting values are here discussed rigorously for the first time. On the basis of the results obtained we derive an exact quantization condition, which is very convenient for estimating the accuracy of the semi-classical quantization condition, since the correction term appears in closed form simply as the argument of the quotient of two elements of the F -matrix. As an application we consider the linear harmonic oscillator and prove in a simple way that the correction term is exactly equal to zero in this case. Thus we obtain a new proof of the well-known fact that the semi-classical quantization condition is exactly valid in the special case of the harmonic oscillator.

The treatment of the radial wave equation for a particle in a spherically symmetric field of force involves special problems which are discussed in chapter 11. In many important cases the JWKB-formulae are improved if $l(l+1)$ is replaced by $(l+\frac{1}{2})^2$. A fertile idea for justifying this modification was used by Kemble in his well-known book on quantum mechanics (KEMBLE [1937]). On developing in chapter 3 the basis of our treatment we have already allowed for the possibility of modifying the JWKB-functions in an arbitrary way by introducing the unspecified function $q(z)$. The modification of replacing $l(l+1)$ by $(l+\frac{1}{2})^2$ can therefore be discussed merely

by choosing the function $q(r)$ conveniently. Similarly we also discuss another but less known modification of the JWKB-formulae for the solution of the radial wave equation. This modification, which corresponds to leaving out the centrifugal barrier entirely, can be used in some cases where neither the unmodified JWKB-method nor the modification of this method corresponding to the replacement of $l(l+1)$ by $(l+\frac{1}{2})^2$ can be expected to give satisfactory results.

The theory developed in chapter 11 is also applied to some special problems. Thus we prove that if $l(l+1)$ is replaced by $(l+\frac{1}{2})^2$ the semi-classical quantization condition is exact for the hydrogen atom and for the three-dimensional harmonic oscillator. We also treat the problem of determining the asymptotic phases in scattering problems and derive an exact formula, which is the same as the usual formula obtained according to the JWKB-method with $l(l+1)$ replaced by $(l+\frac{1}{2})^2$ except for a correction term, which appears as half the argument of the quotient of two elements of the F -matrix. For the special potential given by (11.41) the correction term is proved to be zero and consequently the asymptotic phases obtained according to the JWKB-approximation with $l(l+1)$ replaced by $(l+\frac{1}{2})^2$ are exact.

FORMAL DERIVATION OF THE JWKB-APPROXIMATION

In this chapter we shall derive the well-known formulae for the JWKB-approximation by means of the expansions generally used in this connection. We shall, however, be more careful than authors in general are with the conditions for its validity.

The differential equation

$$\frac{d^2 \psi}{dx^2} + \left(\frac{Q(x)}{\lambda} \right)^2 \psi = 0 \quad (2.1)$$

where λ is a "small" parameter, can formally be solved by expanding ψ as follows

$$\psi(x) = \exp \left\{ \frac{1}{\lambda} \int_{x_0}^x dx \sum_{\nu=0}^{\infty} y_{\nu}(x) \lambda^{\nu} \right\}$$

where x_0 is a constant, which can be chosen conveniently. Inserting this expansion into the differential equation (2.1) and putting the coefficients of the successive powers of λ equal to zero, we obtain the following set of equations

$$y_0 = \pm i Q$$

$$\frac{dy_{\nu-1}}{dx} = - \sum_{\mu=0}^{\nu} y_{\mu} y_{\nu-\mu} \quad \nu = 1, 2, 3, \dots$$

from which the series $\sum_{\nu=0}^{\infty} y_{\nu}(x) \lambda^{\nu}$ can be determined. It is well known that this series is in general not convergent but only asymptotic. Retaining in the expression for ψ only the first three terms in the exponent and using a convenient normalization, we get the second order JWKB-approximation

$$\psi(x) = \left(\frac{Q}{\lambda} \right)^{-\frac{1}{2}} \exp \left\{ \pm i \int_{x_0}^x (1 + \frac{1}{2} \varepsilon_0) \frac{Q}{\lambda} dx \right\} \quad (2.2)$$

where ε_0 is a function defined by

$$\varepsilon_0 = \left(\frac{Q}{\lambda} \right)^{-\frac{3}{2}} \frac{d^2}{dx^2} \left(\frac{Q}{\lambda} \right)^{-\frac{1}{2}}. \quad (2.3)$$

One may expect the derivation of (2.2) to be justified if

$$|y_2 \lambda^2| \ll |y_1 \lambda| \ll |y_0|$$

i.e. if

$$\frac{1}{2} |\varepsilon_0| \ll \frac{1}{2} \left| \frac{d}{dx} \left(\frac{\lambda}{Q} \right) \right| \ll 1. \quad (2.4)$$

If the further condition

$$\frac{1}{2} \left| \int_{x_0}^x \varepsilon_0 \frac{Q}{\lambda} dx \right| \ll 1 \quad (2.5)$$

is fulfilled, one can instead of (2.2) use the well-known first order JWKB-approximation

$$\psi = \left(\frac{Q}{\lambda} \right)^{-\frac{1}{2}} \exp \left\{ \pm i \int_{x_0}^x \frac{Q}{\lambda} dx \right\}. \quad (2.6)$$

Similar derivations of the formulae for the JWKB-approximation are given in many textbooks on quantum mechanics, but with few exceptions it is said that the condition for their validity is only the last inequality in (2.4). Therefore we want to emphasize that the magnitude of the function ε_0 , which appears to the left in the chain of inequalities (2.4) as well as in the condition (2.5) is very important. This fact will be further elucidated in the following chapters.

We remark that if ε_0 is identically equal to zero, the third and all subsequent terms in the expansion used in the above derivation are equal to zero, which means that the JWKB-formulae (2.6) give exact solutions of the differential equation (2.1). From (2.3) it follows that the condition for ε_0 to be identically equal to zero is

$$\left(\frac{Q(x)}{\lambda} \right)^2 = (Cx + D)^{-4} \quad (2.7)$$

where C and D are arbitrary constants. If the function $[Q(x)/\lambda]^2$ is of this form, the JWKB-formulae (2.6) provide two linearly independent exact solutions of the differential equation (2.1).

The formula (2.6) indicates that the general solution of the differential equation (2.1) is given by the approximate formula

$$\psi = A \left(\frac{Q}{\lambda} \right)^{-\frac{1}{2}} \exp \left\{ i \int_{x_0}^x \frac{Q}{\lambda} dx \right\} + B \left(\frac{Q}{\lambda} \right)^{-\frac{1}{2}} \exp \left\{ -i \int_{x_0}^x \frac{Q}{\lambda} dx \right\} \quad (2.8)$$

where A and B are arbitrary constants. It is very natural that the validity of this approximate solution should depend on an integral such as the one in the condition (2.5). In fact, at any point, let us say x_0 , one can choose the constants A and B in (2.8) such that the approximate solution (2.8) and its first derivative coincide exactly with the corresponding quantities for a given solution of the differential equation (2.1). The question is then how far one can move away from the point x_0 before the approximate solution becomes bad. According to the elementary treatment in this chapter the answer is that one must not move so far that the condition (2.5) is violated. In the rigorous treatment which will be given in the following chapters we shall see that the conditions which we have now obtained for the validity of the approximate solution (2.8) are not quite satisfactory. The reason for this is that there is an interference between the two terms in (2.8) which cannot be neglected in a rigorous treatment of the problem. As we shall see later on, this interference is connected with Stokes' phenomenon in the theory of asymptotic expansions. The question of the accuracy of (2.8) and the question whether in a classically forbidden region it is meaningful to keep both terms in (2.8) cannot be answered in a satisfactory way by using only the elementary derivation of this chapter.

The parameter λ was introduced only as a formal mathematical tool for obtaining the desired expansion of ψ . In the given differential equation for ψ and in the final JWKB-formulae for its solution the parameter λ and the function Q appear only in the combination Q/λ , and we can therefore delete λ simply by writing Q instead of Q/λ .

DERIVATION OF AN EXACT FORMULA FOR THE GENERAL SOLUTION OF THE SCHRÖDINGER EQUATION

We consider the one-dimensional time-independent Schrödinger equation

$$\frac{d^2\psi}{dz^2} + Q^2(z)\psi = 0 \quad (3.1)$$

where z is a complex variable, and $Q^2(z)$ is a function which is analytic and single-valued in a certain region of the complex z -plane. Guided by the result of the formal derivation of the JWKB-approximation, we introduce instead of z and ψ new variables w and φ which we define by

$$\psi = [q(z)]^{-\frac{1}{2}} \varphi(z) \quad (3.2)$$

$$w(z) = \int^z q(\zeta) d\zeta \quad (3.3)$$

where $q(z)$ is a so far unspecified function of z . As long as $q(z)$ is allowed to be an arbitrary function, this is the most general transformation of the differential equation (3.1), which preserves its reduced form, i.e. the form in which no term containing the first derivative of the dependent variable is present. The differential equation (3.1) thus transforms to

$$\frac{d^2\varphi}{dw^2} + (1 + \varepsilon)\varphi = 0 \quad (3.4)$$

where ε is a function defined by

$$\varepsilon = \frac{Q^2 - q^2}{q^2} - q^{-\frac{1}{2}} \frac{d^2}{dw^2} (q^{\frac{1}{2}}) = \frac{Q^2 - q^2}{q^2} + q^{-\frac{3}{2}} \frac{d^2}{dz^2} (q^{-\frac{1}{2}}). \quad (3.5a)$$

The following alternative ways of writing this formula are also useful

$$\varepsilon = \frac{Q^2 - q^2}{q^2} + \frac{1}{q^2} \left\{ \frac{3}{4} \left(\frac{1}{q} \frac{dq}{dz} \right)^2 - \frac{1}{2} \frac{1}{q} \frac{d^2q}{dz^2} \right\} \quad (3.5b)$$

$$\varepsilon = \frac{Q^2 - q^2}{q^2} + \frac{1}{2} \left\{ \frac{1}{q} \frac{d^2}{dz^2} \left(\frac{1}{q} \right) - \frac{1}{2} \left[\frac{d}{dz} \left(\frac{1}{q} \right) \right]^2 \right\} \quad (3.5c)$$

$$\varepsilon = \frac{Q^2 - q^2}{q^2} + \frac{1}{16q^6} \left\{ 5 \left[\frac{d}{dz} (q^2) \right]^2 - 4q^2 \frac{d^2}{dz^2} (q^2) \right\}. \quad (3.5d)$$

The functions $\exp\{iw\}$ and $\exp\{-iw\}$ are exact solutions of the differential equation (3.4) if $\varepsilon \equiv 0$, i.e. if $q(z)$ satisfies the differential equation

$$q^2 - q^{\dagger} \frac{d^2}{dz^2} (q^{\dagger}) = Q^2. \quad (3.6)$$

Knowing any solution $q(z)$ of this differential equation, one has the following two linearly independent, exact solutions of the differential equation (3.1) :

$$\psi = q^{\dagger} \exp \left\{ \pm i \int^z q(\zeta) d\zeta \right\}. \quad (3.7)$$

It is interesting to note that, if $Q^2(z)$ is real on the real axis, every solution of (3.1), which has not a constant phase on this axis, i.e. which is not equal to a real function times a complex constant, can (except for a constant factor) be represented in the form (3.7) with $q(z)$ real on the real axis. This connection between amplitude and phase on the real axis for such a solution is easily obtained by substituting for ψ in (3.1) a product of a real amplitude function and a variable phase factor of the absolute value 1, and then separating the resulting equation into real and imaginary parts.

By choosing $q^2(z)$ equal to $Q^2(z)$ one obtains in many important cases a function $\varepsilon(z)$ which is not equal to zero but is "small". One may then expect the formula (3.7) to give approximate solutions of the differential equation (3.1), and thus one obtains the usual JWKB-approximation. A generalized JWKB-approximation based on another choice of $q^2(z)$ is useful when $Q^2(z)$ has a certain kind of singularity, in the neighbourhood of which the usual JWKB-approximation breaks down. The requirement that ε shall be "small" also in the neighbourhood of the singularity then leads to the use of a function $q^2(z)$ which differs essentially from $Q^2(z)$ in the neighbourhood of the singularity but is elsewhere approximately the same as $Q^2(z)$. A general improvement of the JWKB-approximation can obviously be obtained by finding a function $q^2(z)$ which makes ε very small everywhere in the region considered, i.e. which is there an approximate solution of (3.6). HECHT and MAYER [1957] have used the Schwarzian derivative formalism, the convenience of which has been pointed out by Löwdin (quoted in HECHT and MAYER [1957]), and have evolved an iteration scheme for solving the equation (3.6). Under special conditions they are thus able to compute generalized JWKB-functions (3.7) that satisfy the differential equation (3.1) to any desired degree of accuracy.

After these introductory considerations we shall now assume that the function $q^2(z)$ has been chosen in a convenient way, and we shall derive an exact formula for the general solution of the differential equation (3.4). For this purpose we first transform (3.4) into a system of two linear differential equations of the first order, using a familiar technique similar to Lagrange's method for determining the general solution of an inhomogeneous differential equation of the second order in terms of the general solution of the corresponding homogeneous differential equation. We assume the complex w -plane to be cut such that the functions appearing are all single-valued and express φ in the form

$$\varphi = a_1(w) \exp\{i w\} + a_2(w) \exp\{-i w\} \quad (3.8)$$

where $a_1(w)$ and $a_2(w)$ are functions of w which are to be determined in a convenient way. From (3.8) we get

$$\frac{d\varphi}{dw} = i a_1 \exp\{i w\} - i a_2 \exp\{-i w\} \quad (3.9)$$

if we impose on $a_1(w)$ and $a_2(w)$ the condition

$$\frac{da_1}{dw} \exp\{i w\} + \frac{da_2}{dw} \exp\{-i w\} = 0. \quad (3.10)$$

The reason for imposing this condition is that the expression (3.9) for $d\varphi/dw$ is then exactly the same as if the quantities $a_1(w)$ and $a_2(w)$ were constants. Using (3.8), (3.9), and (3.10), we can replace the second order differential equation (3.4) by the following system of two first order differential equations

$$\begin{aligned} \frac{da_1}{dw} &= \frac{1}{2} i \varepsilon \{a_1 + a_2 \exp\{-2i w\}\} \\ \frac{da_2}{dw} &= -\frac{1}{2} i \varepsilon \{a_2 + a_1 \exp\{2i w\}\}. \end{aligned} \quad (3.11)$$

For the case that $q(z)$ is chosen to be equal to $Q(z)$ the differential equations (3.11) have been given by KEMBLE [1935] who has used them for estimating in a very approximate way how a_1 and a_2 change with w . Kemble's treatment is rather complicated and not sufficiently rigorous to form a satisfactory basis for the theory of the JWKB-approximation, but it has been of great value to us as a starting point for the present work. Avoiding a transformation suggested by Feenberg and used by KEMBLE [1935, 1937], which is not only unnecessary but also inconvenient, we shall by a straight-forward

procedure derive an exact formula for the general solution of the differential equations (3.11).

By introducing the column vector

$$\mathbf{a}(w) = \begin{pmatrix} a_1(w) \\ a_2(w) \end{pmatrix} \quad (3.12)$$

and the matrix

$$\mathbf{M}(w) = \frac{1}{2}i\varepsilon \begin{pmatrix} 1 & \exp\{-2iw\} \\ -\exp\{2iw\} & -1 \end{pmatrix} \quad (3.13)$$

with the properties $\det \mathbf{M}(w) = 0$ and $\text{Tr} \mathbf{M}(w) = 0$, we can write the system of differential equations (3.11) in matrix form as follows

$$\frac{d\mathbf{a}}{dw} = \mathbf{M}(w) \mathbf{a}. \quad (3.14)$$

This differential equation can be replaced by the integral equation

$$\mathbf{a}(w) = \mathbf{a}(w_0) + \int_{w_0}^w dw_1 \mathbf{M}(w_1) \mathbf{a}(w_1) \quad (3.15)$$

the solution of which can be obtained by an iteration procedure and is

$$\mathbf{a}(w) = \mathbf{F}(w, w_0) \mathbf{a}(w_0) \quad (3.16)$$

where

$$\begin{aligned} \mathbf{F}(w, w_0) = & 1 + \int_{w_0}^w dw_1 \mathbf{M}(w_1) + \int_{w_0}^w dw_1 \mathbf{M}(w_1) \int_{w_0}^{w_1} dw_2 \mathbf{M}(w_2) + \\ & + \int_{w_0}^w dw_1 \mathbf{M}(w_1) \int_{w_0}^{w_1} dw_2 \mathbf{M}(w_2) \int_{w_0}^{w_2} dw_3 \mathbf{M}(w_3) + \dots \end{aligned} \quad (3.17)$$

The formulae (3.16) and (3.17) give the general solution of the differential equation (3.14) in any region where $\mathbf{M}(w)$ is analytic. To show the convergence of the series (3.17) and the validity of the solution (3.16) we assume that

$$\sum_j |M_{ij}(w)| \leq m(w)$$

where $m(w)$ is a non-negative quantity which is independent of the index i and shall fulfill a further condition mentioned below. Using one and the

same conveniently chosen path for all the integrations in the general term on the right-hand side of (3.17), we get for the matrix elements of this general term the inequality

$$\begin{aligned} \sum_j \left| \left\{ \int_{w_0}^w dw_1 M(w_1) \int_{w_0}^{w_1} dw_2 M(w_2) \dots \int_{w_0}^{w_{n-1}} dw_n M(w_n) \right\}_{ij} \right| &\leq \\ &\leq \int_{w_0}^w |dw_1| m(w_1) \int_{w_0}^{w_1} |dw_2| m(w_2) \dots \int_{w_0}^{w_{n-1}} |dw_n| m(w_n) = \\ &= \frac{1}{n!} \left\{ \int_{w_0}^w m(w_1) |dw_1| \right\}^n \end{aligned}$$

from which it follows that in any region of the complex w -plane, where the integral $\int_{w_0}^w |m(w_1) dw_1|$ along a conveniently chosen path from w_0 to w

is bounded, the series on the right-hand side of (3.17) is absolutely and uniformly convergent. As long as w is finite we can then multiply (3.17) by $M(w)$ and integrate term-by-term, obtaining

$$F(w, w_0) = 1 + \int_{w_0}^w dw_1 M(w_1) F(w_1, w_0)$$

from which it follows that the column vector $\mathbf{a}(w)$, which is given by (3.16), actually satisfies the integral equation (3.15) and that

$$\frac{\partial F(w, w_0)}{\partial w} = M(w) F(w, w_0). \quad (3.18)$$

The above considerations prove the convergence of the series (3.17) defining the F -matrix and the validity of the solution (3.16) except for those points in the complex z -plane where the functions ε or w are infinite, which can happen only when $q^2(z)$ has zeros or singularities.

The derivative with respect to w of any element or the matrix $F(w, w_0)$ is obtained from (3.18) and (3.13). By a simple direct calculation one finds that

$$\frac{\partial}{\partial w} \det F(w, w_0) = 0$$

which implies that the determinant of the matrix $F(w, w_0)$ is independent

of w . Since, furthermore, $F(w, w_0)$ is a unit matrix for $w = w_0$, we get

$$\det F(w, w_0) = 1. \quad (3.19)$$

The formula (3.16) shows that

$$F(w_0, w) = \{F(w, w_0)\}^{-1}.$$

Performing explicitly the matrix inversion on the right-hand side of this formula, and remembering (3.19), we get

$$\begin{pmatrix} F_{11}(w_0, w) & F_{12}(w_0, w) \\ F_{21}(w_0, w) & F_{22}(w_0, w) \end{pmatrix} = \begin{pmatrix} F_{22}(w, w_0) & -F_{12}(w, w_0) \\ -F_{21}(w, w_0) & F_{11}(w, w_0) \end{pmatrix}. \quad (3.20)$$

This formula for expressing the elements of the matrix $F(w_0, w)$ in terms of the elements of the inverse matrix $F(w, w_0)$ will be frequently used in the following.

The formula (3.17) would be of limited value for our purposes if it were not so that the elements of the product matrix $M(w_1)M(w_2)\dots M(w_n)$, appearing in the general term on the right-hand side of (3.17), can be factorized very nicely as follows

$$\begin{aligned} & M(w_1)M(w_2)\dots M(w_n) = \\ & = (\frac{1}{2}i)^n \varepsilon(w_1)\varepsilon(w_2)\dots\varepsilon(w_n) [1 - \exp\{-2i(w_1 - w_2)\}][1 - \exp\{-2i(w_2 - w_3)\}] \\ & \dots [1 - \exp\{-2i(w_{n-1} - w_n)\}] \begin{pmatrix} 1 & \exp\{-2iw_n\} \\ -\exp\{2iw_1\} & -\exp\{2i(w_1 - w_n)\} \end{pmatrix}. \quad (3.21) \end{aligned}$$

This is an important fact which makes it possible for us to obtain the explicit expressions for the elements of the F -matrix as fairly simple series. Substituting (3.21) into (3.17), we thus obtain

$$\begin{aligned} F_{11}(w, w_0) &= 1 + \int_{w_0}^w dw_1 \frac{1}{2}i \varepsilon(w_1) + \\ &+ \int_{w_0}^w dw_1 \frac{1}{2}i \varepsilon(w_1) \int_{w_0}^{w_1} dw_2 \frac{1}{2}i \varepsilon(w_2) [1 - \exp\{-2i(w_1 - w_2)\}] + \\ &+ \int_{w_0}^w dw_1 \frac{1}{2}i \varepsilon(w_1) \int_{w_0}^{w_1} dw_2 \frac{1}{2}i \varepsilon(w_2) [1 - \exp\{-2i(w_1 - w_2)\}] \times \\ &\times \int_{w_0}^{w_2} dw_3 \frac{1}{2}i \varepsilon(w_3) [1 - \exp\{-2i(w_2 - w_3)\}] + \dots \quad (3.22a) \end{aligned}$$

$$\begin{aligned}
F_{12}(w, w_0) &= \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) \exp\{-2i w_1\} + \\
&+ \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) \int_{w_0}^{w_1} dw_2 \frac{1}{2} i \varepsilon(w_2) \times \\
&\quad \times [1 - \exp\{-2i(w_1 - w_2)\}] \exp\{-2i w_2\} + \\
&+ \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) \int_{w_0}^{w_1} dw_2 \frac{1}{2} i \varepsilon(w_2) [1 - \exp\{-2i(w_1 - w_2)\}] \times \\
&\quad \times \int_{w_0}^{w_2} dw_3 \frac{1}{2} i \varepsilon(w_3) [1 - \exp\{-2i(w_2 - w_3)\}] \exp\{-2i w_3\} + \dots
\end{aligned} \tag{3.22b}$$

$$\begin{aligned}
F_{21}(w, w_0) &= - \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) \exp\{2i w_1\} + \\
&- \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) \exp\{2i w_1\} \times \\
&\quad \times \int_{w_0}^{w_1} dw_2 \frac{1}{2} i \varepsilon(w_2) [1 - \exp\{-2i(w_1 - w_2)\}] + \\
&- \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) \exp\{2i w_1\} \times \\
&\quad \times \int_{w_0}^{w_1} dw_2 \frac{1}{2} i \varepsilon(w_2) [1 - \exp\{-2i(w_1 - w_2)\}] \times \\
&\quad \times \int_{w_0}^{w_2} dw_3 \frac{1}{2} i \varepsilon(w_3) [1 - \exp\{-2i(w_2 - w_3)\}] - \dots
\end{aligned} \tag{3.22c}$$

$$\begin{aligned}
F_{22}(w, w_0) &= 1 - \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) + \\
&- \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) \int_{w_0}^{w_1} dw_2 \frac{1}{2} i \varepsilon(w_2) \times \\
&\quad \times [1 - \exp\{-2i(w_1 - w_2)\}] \exp\{2i(w_1 - w_2)\} +
\end{aligned}$$

$$\begin{aligned}
& - \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) \int_{w_0}^{w_1} dw_2 \frac{1}{2} i \varepsilon(w_2) [1 - \exp\{-2i(w_1 - w_2)\}] \times \\
& \quad \times \int_{w_0}^{w_2} dw_3 \frac{1}{2} i \varepsilon(w_3) [1 - \exp\{-2i(w_2 - w_3)\}] \times \\
& \quad \times \exp\{2i(w_1 - w_3)\} - \dots \quad (3.22d)
\end{aligned}$$

Examining the structure of these formulae, one finds that the expressions for $F_{22}(w, w_0)$ and $F_{21}(w, w_0)$ are obtained from those for $F_{11}(w, w_0)$ and $F_{12}(w, w_0)$, respectively, simply by replacing i by $-i$. We may also mention that the factors in the general term on the right-hand side of (3.22d) can be arranged in such a way that the formula looks more simple, but as it is written above, it is more convenient for deriving the estimates to be given in the next chapter.

Having derived in exact form the general solution of the differential equation (3.4), we can easily obtain the corresponding expression for the general solution of the original differential equation (3.1). Let us, however, first say a few words about the notations.

It is convenient to introduce the row vector

$$f(z) = (f_1(z) \quad f_2(z)) \quad (3.23)$$

where $f_1(z)$ and $f_2(z)$ are the JWKB-functions defined by

$$f_1(z) = q(z)^{-\frac{1}{2}} \exp\{i w(z)\} \quad (3.24a)$$

$$f_2(z) = q(z)^{-\frac{1}{2}} \exp\{-i w(z)\}. \quad (3.24b)$$

As regards the a -coefficients and the F -matrix we shall in the following write $\mathbf{a}(z)$ instead of $\mathbf{a}[w(z)]$ and $\mathbf{F}(z, z_0)$ instead of $\mathbf{F}[w(z), w(z_0)]$, if there is no risk for misunderstandings. Derivatives with respect to z will be indicated by primes.

Using (3.2), (3.8), (3.9), (3.12), (3.23), and (3.24a, b), we can write the general solution of (3.1) and its derivative as follows

$$\psi(z) = a_1(z) f_1(z) + a_2(z) f_2(z) = f(z) \mathbf{a}(z) \quad (3.25a)$$

$$\psi'(z) = a_1(z) f_1'(z) + a_2(z) f_2'(z) = f'(z) \mathbf{a}(z) \quad (3.25b)$$

where according to (3.16)

$$\mathbf{a}(z) = \mathbf{F}(z, z_0) \mathbf{a}(z_0). \quad (3.26)$$

The formulae (3.25a, b) and (3.26) together with the explicit expressions (3.22a, b, c, d) for the elements of the matrix $F(z, z_0)$ constitute the exact solution of the Schrödinger equation (3.1), on which all of our considerations of approximate JWKB-solutions in the following will be based.

Repeated use of (3.26) immediately gives the following multiplication rule for the F -matrix

$$F(z_2, z_0) = F(z_2, z_1) F(z_1, z_0). \quad (3.27)$$

It is often important to know how the elements of the matrix $F(z, z_0)$ depend on the lower limit in the integral (3.3) defining $w(z)$. This can easily be found by noting that according to (3.22a, b, c, d) the quantities $F_{11}(z, z_0)$, $F_{22}(z, z_0)$, $F_{12}(z, z_0) \exp\{2i w\}$, and $F_{21}(z, z_0) \exp\{-2i w\}$, where w stands for either $w(z)$ or $w(z_0)$, are all independent of the lower limit in the integral (3.3).

At this point we shall give certain relations which allow $a(z)$ and $F(z, z_0)$ to be obtained from two linearly independent solutions of the differential equation (3.1). These relations can easily be derived by purely algebraic manipulations, but they are nevertheless convenient to have explicitly at hand and will be referred to later.

We consider two solutions $\psi(z)$ and $\bar{\psi}(z)$ of the differential equation (3.1) and denote the corresponding a -vectors by $a(z)$ and $\bar{a}(z)$, respectively. It is convenient to introduce the following matrices

$$W_\psi(z) = \begin{pmatrix} \psi(z) & \bar{\psi}(z) \\ \psi'(z) & \bar{\psi}'(z) \end{pmatrix} \quad (3.28)$$

$$W_f(z) = \begin{pmatrix} f_1(z) & f_2(z) \\ f_1'(z) & f_2'(z) \end{pmatrix} \quad (3.29)$$

$$A(z) = \begin{pmatrix} a_1(z) & \bar{a}_1(z) \\ a_2(z) & \bar{a}_2(z) \end{pmatrix} \quad (3.30)$$

in terms of which the formulae (3.25a, b) for the wave functions $\psi(z)$ and $\bar{\psi}(z)$ can be written as follows

$$W_\psi(z) = W_f(z) A(z). \quad (3.31)$$

This matrix equation gives

$$A(z) = W_f^{-1}(z) W_\psi(z) \quad (3.32)$$

since the matrix $W_f(z)$ has an inverse matrix $W_f^{-1}(z)$. Noting that

$$\det W_f(z) = -2i \quad (3.33)$$

one sees immediately that

$$W_f^{-1}(z) = \frac{1}{2}i \begin{pmatrix} f_2'(z) & -f_2(z) \\ -f_1'(z) & f_1(z) \end{pmatrix}. \quad (3.34)$$

Looking at the 11- and 21-elements of the matrix equation (3.32), we therefore find that the a -coefficients $a_1(z)$ and $a_2(z)$ corresponding to any given solution $\psi(z)$ of the differential equation (3.1) can be expressed as follows

$$a_1(z) = -\frac{1}{2}i \{f_2(z) \psi'(z) - f_2'(z) \psi(z)\} \quad (3.35a)$$

$$a_2(z) = \frac{1}{2}i \{f_1(z) \psi'(z) - f_1'(z) \psi(z)\}. \quad (3.35b)$$

From (3.32) and (3.33) we get

$$\det A(z) = \frac{1}{2}i \det W_\psi(z). \quad (3.36)$$

Since in the differential equation (3.1) there is no term containing the first derivative $d\psi/dz$, the Wronskian $\det W_\psi(z)$ is independent of z . As is well known this Wronskian is different from zero if, and only if, the solutions $\psi(z)$ and $\bar{\psi}(z)$ are linearly independent.

We next consider (3.26) and the corresponding equation for the bared column vector $\bar{a}(z)$. Utilizing the definition (3.30), we can write these equations as follows

$$A(z) = F(z, z_0) A(z_0). \quad (3.37)$$

Let us now assume that the two solutions $\psi(z)$ and $\bar{\psi}(z)$ are linearly independent, i.e. that $\det W_\psi(z) \neq 0$. Because of (3.36) we then have $\det A(z) \neq 0$, and hence the matrix $A(z)$ can be inverted. From (3.37) we therefore get

$$F(z, z_0) = A(z) A^{-1}(z_0). \quad (3.38)$$

Thus the matrix $F(z, z_0)$ can be written as the product of two matrices, one depending only on z and the other only on z_0 . Remembering (3.32), we can factorize the formula (3.38) for $F(z, z_0)$ further :

$$F(z, z_0) = W_f^{-1}(z) W_\psi(z) W_\psi^{-1}(z_0) W_f(z_0). \quad (3.39)$$

The convenience of using this formula in such cases where $W_\psi(z) = W_\psi(z_0)$, e.g. in the derivation of our formula (6.36), was pointed out to us by M. Soop.

We shall now say a few words about the rapidity with which the coefficients $a_1(z)$ and $a_2(z)$ change as z moves in the complex plane. The differential equations (3.11) rewritten as follows

$$\frac{1}{a_1} \frac{da_1}{dw} = \frac{1}{2} i \varepsilon \left\{ 1 + \frac{a_2 \exp\{-i w\}}{a_1 \exp\{i w\}} \right\}$$

$$\frac{1}{a_2} \frac{da_2}{dw} = -\frac{1}{2} i \varepsilon \left\{ 1 + \frac{a_1 \exp\{i w\}}{a_2 \exp\{-i w\}} \right\}$$

are convenient for a qualitative discussion of this question. A special consequence of these equations is the simple relation

$$\frac{da_1}{da_2} = -\exp\{-2i w\}.$$

Assuming the absolute value of ε to be "small", we can draw the following qualitative conclusions. In a region where the two terms on the right-hand side of (3.25a) are of the same order of magnitude, the coefficients $a_1(z)$ and $a_2(z)$ are both approximately constant. On the other hand, in a region where one of the two terms on the right-hand side of (3.25a) is much larger than the other term, the a -coefficient of the dominating term is approximately constant, whereas the a -coefficient of the other term may change considerably, but, as will be shown later on, the latter term is insignificant. These properties of the a -coefficients are closely related to Stokes' phenomenon in the theory of asymptotic expansions. In connection with the JWKB-approximation Stokes' phenomenon thus appears in the well-known fact that the same wave function $\psi(z)$ has sometimes to be approximated by different linear combinations of the functions $f_1(z)$ and $f_2(z)$ in different regions of the complex z -plane. In the literature on the JWKB-approximation one often uses rather loose arguments based on Stokes' phenomenon without formulating this phenomenon in a quantitative way. Such arguments are valuable for obtaining a first survey of a problem, but they lack in rigour and may be dangerous. We shall not use them in the following chapters but instead proceed by obtaining mathematically correct and satisfactory estimates for the elements of the F -matrix.

To conclude this chapter we shall make some remarks on the connection between our results and exact solutions given by OLVER [1961]. For this

purpose we introduce (3.16) into (3.8) and rearrange the terms appropriately, getting

$$\varphi(w) = a_1(w_0) [F_{11}(w, w_0) + \exp\{-2iw\} F_{21}(w, w_0)] \exp\{iw\} + \\ + a_2(w_0) [\exp\{2iw\} F_{12}(w, w_0) + F_{22}(w, w_0)] \exp\{-iw\}. \quad (3.40)$$

According to (3.25a) and (3.26) the corresponding formula for the solution $\varphi(z)$ is

$$\varphi(z) = a_1(z_0) [F_{11}(z, z_0) + \exp\{-2iw(z)\} F_{21}(z, z_0)] f_1(z) + \\ + a_2(z_0) [\exp\{2iw(z)\} F_{12}(z, z_0) + F_{22}(z, z_0)] f_2(z). \quad (3.41)$$

For the expressions in the square brackets in (3.40) and (3.41) we obtain from (3.22a-d) the following formulae

$$F_{11}(w, w_0) + \exp\{-2iw\} F_{21}(w, w_0) = \\ = 1 + \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) [1 - \exp\{-2i(w - w_1)\}] + \\ + \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) [1 - \exp\{-2i(w - w_1)\}] \times \\ \times \int_{w_0}^{w_1} dw_2 \frac{1}{2} i \varepsilon(w_2) [1 - \exp\{-2i(w_1 - w_2)\}] + \\ + \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) [1 - \exp\{-2i(w - w_1)\}] \times \\ \times \int_{w_0}^{w_1} dw_2 \frac{1}{2} i \varepsilon(w_2) [1 - \exp\{-2i(w_1 - w_2)\}] \times \\ \times \int_{w_0}^{w_2} dw_3 \frac{1}{2} i \varepsilon(w_3) [1 - \exp\{-2i(w_2 - w_3)\}] + \dots (3.42a)$$

$$\exp\{2iw\} F_{12}(w, w_0) + F_{22}(w, w_0) = \\ = 1 + \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) [1 - \exp\{-2i(w - w_1)\}] \exp\{2i(w - w_1)\} +$$

$$\begin{aligned}
& + \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) [1 - \exp\{-2i(w - w_1)\}] \times \\
& \quad \times \int_{w_0}^{w_1} dw_2 \frac{1}{2} i \varepsilon(w_2) [1 - \exp\{-2i(w_1 - w_2)\}] \exp\{2i(w - w_2)\} + \\
& + \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) [1 - \exp\{-2i(w - w_1)\}] \times \\
& \quad \times \int_{w_0}^{w_1} dw_2 \frac{1}{2} i \varepsilon(w_2) [1 - \exp\{-2i(w_1 - w_2)\}] \times \\
& \quad \times \int_{w_0}^{w_2} dw_3 \frac{1}{2} i \varepsilon(w_3) [1 - \exp\{-2i(w_2 - w_3)\}] \exp\{2i(w - w_3)\} + \dots
\end{aligned} \tag{3.42b}$$

If, in the expression on the right-hand side of (3.42a), the imaginary unit i is replaced by $-i$, one obtains the expression on the right-hand side of (3.42b). The series given by OLVER [1961] correspond to the right-hand sides of (3.42a) and (3.42b) and are thus simple combinations of our series for the elements of the F -matrix. Further we note that the two terms with arbitrary coefficients in the right member of (3.40) and (3.41), respectively, are linearly independent solutions of the corresponding differential equations (3.4) and (3.1). This is easily seen by noting that their Wronskian is different from zero (equal to $-2i$).

The difference between our results and Olver's is now clear: Olver has given two series, providing two linearly independent solutions of the differential equation, whereas we have derived four series (giving the elements of the F -matrix), in order to be able to follow at every step the changes in the JWKB-coefficients a_1 and a_2 . Olver has used his series to obtain limits of error for the JWKB-approximation under special conditions. His series, however, seem to be inconvenient for obtaining limits of error for the JWKB-approximation in more general cases. For this purpose it is essential not only to have an exact general solution in terms of convergent series but also to have the terms separated in such a way that the changes in the JWKB-coefficients a_1 and a_2 are revealed.

BASIC ESTIMATES AND LIMITING PROPERTIES OF THE F -MATRIX

The terms in the series defining the F -matrix have already been roughly estimated in the previous chapter. Our intention was then, however, only to prove the convergence of the series (3.17), and we did not get good estimates for the different elements of the F -matrix. It is our purpose in the present chapter to derive better estimates for these elements.

As has already been said in the previous chapter, the complex z - and w -planes are assumed to be cut such that all functions appearing in our formulae are single-valued. Since these functions are assumed to be analytic, the integrals in our formulae are independent of the path of integration in the z -plane or the w -plane. In the following we choose a convenient path Λ from z_0 to z (from w_0 to w) and assume all the integrals over w_1, w_2, w_3, \dots in our formulae to be performed along this same path of integration. Of course, the path Λ must never cross any cut in the complex plane.

For the general term in the series (3.22a) we get the estimate

$$\left| \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) \int_{w_0}^{w_1} dw_2 \frac{1}{2} i \varepsilon(w_2) [1 - \exp\{-2i(w_1 - w_2)\}] \int_{w_0}^{w_2} \dots \right. \\ \left. \dots \int_{w_0}^{w_{n-1}} dw_n \frac{1}{2} i \varepsilon(w_n) [1 - \exp\{-2i(w_{n-1} - w_n)\}] \right| \leq \frac{1}{2M} \frac{(M\mu)^n}{n!}$$

where M is a number such that

$$\frac{1}{2} |1 - \exp\{-2i(w_{p-1} - w_p)\}| \leq M \quad (4.1)$$

for any possible division of the path of integration, and μ is defined by the formula

$$\mu = \int_{w_0}^w |\varepsilon(w_1) dw_1|. \quad (4.2)$$

Using the above estimate of the general term in the series (3.22a), we get

$$|F_{11}(w, w_0) - 1| \leq \frac{1}{2M} [\exp\{M\mu\} - 1]. \quad (4.3a)$$

Similar estimates are easily obtained for the other elements of the matrix $F(w, w_0)$. We shall give these estimates only for the important case that $|\exp\{iw\}|$ increases monotonically as one moves along the path \mathcal{A} from z_0 to z . Then we have

$$\begin{aligned} |\exp\{-2iw_p\}| &\leq |\exp\{-2iw_0\}| \\ |\exp\{2iw_1\}| &\leq |\exp\{2iw\}| \\ |\exp\{2i(w_1 - w_p)\}| &\leq |\exp\{2i(w - w_0)\}| \end{aligned}$$

and from (3.22b, c, d) we get

$$|F_{12}(w, w_0)| \leq \frac{1}{2M} [\exp\{M\mu\} - 1] |\exp\{-2iw_0\}| \quad (4.3b)$$

$$|F_{21}(w, w_0)| \leq \frac{1}{2M} [\exp\{M\mu\} - 1] |\exp\{2iw\}| \quad (4.3c)$$

$$|F_{22}(w, w_0) - 1| \leq \frac{1}{2} \mu + \frac{1}{2M} [\exp\{M\mu\} - 1 - M\mu] |\exp\{2i(w - w_0)\}|. \quad (4.3d)$$

Similarly we can estimate the quantities in (3.42a) and (3.42b), introduced in connection with our remarks concerning Olver's results, getting

$$|F_{11}(w, w_0) + \exp\{-2iw\} F_{21}(w, w_0) - 1| \leq \exp\{M\mu\} - 1 \quad (4.4a)$$

$$\begin{aligned} |\exp\{2iw\} F_{12}(w, w_0) + F_{22}(w, w_0) - 1| &\leq \\ &\leq [\exp\{M\mu\} - 1] |\exp\{2i(w - w_0)\}|. \end{aligned} \quad (4.4b)$$

Also (4.3a) will in the following treatment be used exclusively with the assumption that $|\exp\{iw\}|$ increases monotonically from z_0 to z along the path \mathcal{A} , and the estimates (4.3a-d) will then be called basic estimates. From (4.1) we see that, because of the assumption of monotonicity of $|\exp\{iw\}|$, we can always choose $M = 1$ in the basic estimates (4.3) and in (4.4). For the special case that $\text{Im}\{iw\}$ is constant along \mathcal{A} , which occurs for instance in a classically forbidden region, we can choose $M = \frac{1}{2}$.

We shall now turn our attention to the behaviour of the matrix $F(z, z_0)$ as z tends in a prescribed way towards a certain limiting point Z , lying either in the finite region of the complex z -plane or being the limiting value of a point moving towards infinity in a definite way. Let us assume that the points z_0 and Z can be joined by a path \mathcal{A} along which the absolute

value of $\exp\{iw(z)\}$ increases monotonically as z moves along A in the direction from z_0 towards Z . As z tends towards the limit Z along the path A , the μ -integral $\mu(z, z_0)$ defined by (4.2) is assumed to tend to a finite limiting value, whereas the absolute value of $\exp\{iw(z)\}$ is assumed to tend to infinity. Because of our assumption concerning $\mu(z, z_0)$ and our estimate of the general term in the series (3.22a) for $F_{11}(z, z_0)$, which was given previously in the present chapter, the series (3.22a) is uniformly convergent when z lies on A , and each term in this series tends to a finite limiting value as $z \rightarrow Z$ along A . Therefore

$$\lim_{\substack{z \rightarrow Z \\ \text{along } A}} F_{11}(z, z_0) \quad \text{exists and is finite.} \quad (4.5a)$$

From (3.22b) one similarly finds that

$$\lim_{\substack{z \rightarrow Z \\ \text{along } A}} F_{12}(z, z_0) \quad \text{exists and is finite.} \quad (4.5b)$$

In the same way one can from (3.22c) and (3.22d) prove the existence of finite limiting values for the functions $F_{21}(z, z_0) \exp\{-2iw(z)\}$ and $F_{22}(z, z_0) \exp\{-2iw(z)\}$ as $z \rightarrow Z$ along the path A . As we shall now show, these limiting values are actually equal to zero. For the general term in the series (3.22c) for $F_{21}(w(z), w(z_0))$ we use the estimate

$$\begin{aligned} & \left| \int_{w_0}^w dw_1 \frac{1}{2} i \varepsilon(w_1) \exp\{2iw_1\} \int_{w_0}^{w_1} dw_2 \frac{1}{2} i \varepsilon(w_2) [1 - \exp\{-2i(w_1 - w_2)\}] \int_{w_0}^{w_2} \dots \right. \\ & \quad \left. \dots \int_{w_0}^{w_{n-1}} dw_n \frac{1}{2} i \varepsilon(w_n) [1 - \exp\{-2i(w_{n-1} - w_n)\}] \right| \leq \\ & \leq \frac{1}{(n-1)!} [\mu(w, w_0)]^{n-1} \int_{w_0}^w |\exp\{2iw_1\} \varepsilon(w_1) dw_1| = \\ & = \frac{1}{(n-1)!} [\mu(w, w_0)]^{n-1} \left\{ \int_{w_0}^{\frac{1}{2}(w+w_0)} + \int_{\frac{1}{2}(w+w_0)}^w |\exp\{2iw_1\} \varepsilon(w_1) dw_1| \right\} \leq \\ & \leq \frac{1}{(n-1)!} [\mu(w, w_0)]^{n-1} \times \\ & \quad \times \left\{ \mu\left[\frac{1}{2}(w+w_0), w_0\right] |\exp\{i(w+w_0)\}| + \mu\left[w, \frac{1}{2}(w+w_0)\right] |\exp\{2iw\}| \right\} \end{aligned}$$

by means of which we find that

$$|F_{21}(w, w_0) \exp\{-2iw\}| \leq \\ \leq \frac{1}{2} \exp\{\mu(w, w_0)\} \left\{ \mu\left[\frac{1}{2}(w + w_0), w_0\right] |\exp\{-i(w - w_0)\}| + \mu\left[w, \frac{1}{2}(w + w_0)\right] \right\}.$$

Since the μ -integral along the whole path \mathcal{A} is assumed to have a finite value, and since the absolute value of $\exp\{iw(z)\}$ is assumed to tend to infinity as z approaches Z along \mathcal{A} , the last inequality shows that

$$\lim_{\substack{z \rightarrow Z \\ \text{along } \mathcal{A}}} F_{21}(z, z_0) \exp\{-2iw(z)\} = 0. \quad (4.5c)$$

From (3.22d) we similarly find that

$$\lim_{\substack{z \rightarrow Z \\ \text{along } \mathcal{A}}} F_{22}(z, z_0) \exp\{-2iw(z)\} = 0. \quad (4.5d)$$

As regards the a -coefficients, which are allowed to take any finite values at the point z_0 , we find from (3.26) and (4.5a-d) that

$$\lim_{\substack{z \rightarrow Z \\ \text{along } \mathcal{A}}} a_1(z) \quad \text{exists and is finite} \quad (4.6a)$$

$$\lim_{\substack{z \rightarrow Z \\ \text{along } \mathcal{A}}} a_2(z) \exp\{-2iw(z)\} = 0. \quad (4.6b)$$

The limiting properties for the elements of the matrix $F(z_0, z)$ are readily obtained from (4.5a-d) by using (3.20). Thus one finds that

$$\lim F_{22}(z_0, z) \quad \text{exists and is finite} \quad (4.7a)$$

$$\lim F_{12}(z_0, z) \quad \text{exists and is finite} \quad (4.7b)$$

$$\lim F_{21}(z_0, z) \exp\{-2iw(z)\} = 0 \quad (4.7c)$$

$$\lim F_{11}(z_0, z) \exp\{-2iw(z)\} = 0 \quad (4.7d)$$

where the notation \lim means that z shall tend to Z along the path \mathcal{A} . For the validity of these formulae it is not necessary that the absolute value of $\exp\{iw(z)\}$ increases monotonically along the whole path \mathcal{A} . It is sufficient that there is a point z_1 on \mathcal{A} such that the elements of the matrix $F(z_0, z_1)$ are all finite, that the limit $\mu(z_1, Z)$ is finite, and that the absolute value of $\exp\{iw(z)\}$ increases monotonically and tends to infinity on the part of \mathcal{A} lying between z_1 and Z . This is easily seen by noting that

$$F(z_0, z) = F(z_0, z_1) F(z_1, z).$$

SYMMETRY PROPERTIES OF THE F -MATRIX CONNECTING TWO POINTS ON THE REAL AXIS

We have already made the assumption that the z -plane is cut such that $q(z)^\dagger$ is a single-valued analytic function of z in the region considered. To adapt our treatment to certain physical problems we shall in this chapter further assume that the functions $Q^2(z)$ and $q^2(z)$ are both real on the real axis (the x -axis) of the complex z -plane. The reality of $Q^2(x)$ implies that the Schrödinger equation (3.1) is invariant for complex conjugation in the special case that the variable z is considered to be real. This means that if a function $\psi(x)$ is a solution of (3.1) on the real axis, so is also the complex conjugate function $\psi^*(x)$. This fact allows us to derive certain relations between the elements of the F -matrix connecting any two points x_1 and x_2 on the real axis. Such relations will in the following be referred to as symmetry relations. For their validity it is, however, essential that $Q^2(z)$ has no pole on the real axis between x_1 and x_2 and that cuts emerging from other poles of $Q^2(z)$ in the complex z -plane do not cross the real axis between x_1 and x_2 . This restriction is connected with the fact that the general solution of the differential equation (3.1) is usually not single-valued when z moves around a pole of $Q^2(z)$ and that a solution of the differential equation (3.1), which is real on the real axis to the left of a pole, need not be real on the real axis to the right of the pole and vice versa.

We shall first derive a general matrix equation, from which all symmetry relations of the kind mentioned above, can be obtained, and then we shall give explicit formulae for the three types of relations, which occur, depending on whether $q^2(x_1)$ and $q^2(x_2)$ are both positive, both negative or have different signs. Complex conjugation (without transposing) of the elements of a vector or a matrix will in the following be denoted by an asterisk *. The fixed lower limit in the integral (3.3) defining $w(z)$ will be allowed to be an arbitrary point in the complex plane.

Using the definitions (3.24a, b) of the functions $f_1(z)$ and $f_2(z)$, which are the elements of the row vector $f(z)$, and considering the case that z

lies on the real axis, we easily find that

$$f^*(x) = f(x) B(x) \quad (5.1a)$$

$$\frac{df^*(x)}{dx} = \frac{df(x)}{dx} B(x) \quad (5.1b)$$

where $B(x)$ is a matrix given by

$$B(x) = \frac{q(x)}{|q(x)|} \begin{pmatrix} 0 & \exp\{2\text{Im}[w(x)]\} \\ \exp\{-2\text{Im}[w(x)]\} & 0 \end{pmatrix} \quad \text{if } q^2(x) > 0 \quad (5.2a)$$

and

$$B(x) = \frac{q(x)}{|q(x)|} \begin{pmatrix} \exp\{-2i\text{Re}[w(x)]\} & 0 \\ 0 & \exp\{2i\text{Re}[w(x)]\} \end{pmatrix} \quad \text{if } q^2(x) < 0. \quad (5.2b)$$

The formula (5.1b) follows immediately from (5.1a), since in each region where $q^2(x) > 0$ or $q^2(x) < 0$, the matrix $B(x)$ is obviously constant. We further note that $\det B(x) = -1$ and that $B^{-1}(x) = B^*(x)$ both when $q^2(x) > 0$ and $q^2(x) < 0$.

Let us now assume that $\psi(x)$ is a solution of (3.1). According to (3.25a, b) and (3.26) we then have

$$\psi(x) = f(x) a(x) \quad (5.3a)$$

$$\frac{d\psi(x)}{dx} = \frac{df(x)}{dx} a(x) \quad (5.3b)$$

$$a(x_1) = F(x_1, x_2) a(x_2). \quad (5.4)$$

Taking the complex conjugate of (5.3a, b) and utilizing (5.1a, b), we get

$$\psi^*(x) = f(x) B(x) a^*(x) \quad (5.5a)$$

$$\frac{d\psi^*(x)}{dx} = \frac{df(x)}{dx} B(x) a^*(x). \quad (5.5b)$$

Since we have assumed that $Q^2(x)$ is real, also $\psi^*(x)$ is a solution of (3.1). It must be emphasized, however that the solution which is equal to $\psi^*(x)$ in one interval may differ from $\psi^*(x)$ in another interval, separated from the first interval by one or more poles of $Q^2(z)$. Therefore we exclude such cases as well as cases where cuts from the poles of $Q^2(z)$ cross the real axis. From (5.5a, b) it then follows that everywhere on the real axis $B(x) a^*(x)$ is the a -vector belonging to the solution $\psi^*(x)$. Thus we have

$$B(x_1) a^*(x_1) = F(x_1, x_2) B(x_2) a^*(x_2)$$

which immediately gives

$$\mathbf{a}(x_1) = \mathbf{B}(x_1) \mathbf{F}^*(x_1, x_2) \mathbf{B}^*(x_2) \mathbf{a}(x_2).$$

By comparing this equation with (5.4) and noting that $\mathbf{a}(x_2)$ can be chosen arbitrarily, we obtain the general relation

$$\mathbf{F}(x_1, x_2) = \mathbf{B}(x_1) \mathbf{F}^*(x_1, x_2) \mathbf{B}^*(x_2). \quad (5.6)$$

When the appropriate expressions for $\mathbf{B}(x_1)$ and $\mathbf{B}^*(x_2)$ are introduced in this formula, we obtain the general symmetry relations, which will be given below.

If both x_1 and x_2 lie in regions where $q^2(x) > 0$ (either in the same region or in different such regions), we have the symmetry relations

$$F_{21}(x_1, x_2) = \frac{\frac{q(x_1)}{|q(x_1)|}}{\frac{q(x_2)}{|q(x_2)|}} \exp\{-2 \operatorname{Im}[w(x_2) + w(x_1)]\} F_{12}^*(x_1, x_2) \quad (5.7a)$$

$$F_{22}(x_1, x_2) = \frac{\frac{q(x_1)}{|q(x_1)|}}{\frac{q(x_2)}{|q(x_2)|}} \exp\{2 \operatorname{Im}[w(x_2) - w(x_1)]\} F_{11}^*(x_1, x_2). \quad (5.7b)$$

For the case that both x_1 and x_2 lie in regions where $q^2(x) < 0$ (either in the same region or in different such regions), we have the symmetry relations

$$F_{11}(x_1, x_2) = \frac{\frac{q(x_1)}{|q(x_1)|}}{\frac{q(x_2)}{|q(x_2)|}} \exp\{2i \operatorname{Re}[w(x_2) - w(x_1)]\} F_{11}^*(x_1, x_2) \quad (5.8a)$$

$$F_{12}(x_1, x_2) = \frac{\frac{q(x_1)}{|q(x_1)|}}{\frac{q(x_2)}{|q(x_2)|}} \exp\{-2i \operatorname{Re}[w(x_2) + w(x_1)]\} F_{12}^*(x_1, x_2) \quad (5.8b)$$

$$F_{21}(x_1, x_2) = \frac{\frac{q(x_1)}{|q(x_1)|}}{\frac{q(x_2)}{|q(x_2)|}} \exp\{2i \operatorname{Re}[w(x_2) + w(x_1)]\} F_{21}^*(x_1, x_2) \quad (5.8c)$$

$$F_{22}(x_1, x_2) = \frac{\frac{q(x_1)}{|q(x_1)|}}{\frac{q(x_2)}{|q(x_2)|}} \exp\{-2i \operatorname{Re}[w(x_2) - w(x_1)]\} F_{22}^*(x_1, x_2). \quad (5.8d)$$

Suppose x_1 lies in a region where $q^2(x) < 0$, and x_2 lies in a region where $q^2(x) > 0$. Whether these regions are adjacent or not, we have the symmetry relations

$$F_{12}(x_1, x_2) = \frac{\frac{q(x_1)}{|q(x_1)|}}{\frac{q(x_2)}{|q(x_2)|}} \exp\{2 \operatorname{Im}[w(x_2)] - 2i \operatorname{Re}[w(x_1)]\} F_{11}^*(x_1, x_2) \quad (5.9a)$$

$$F_{21}(x_1, x_2) = \frac{\frac{q(x_1)}{|q(x_1)|}}{\frac{q(x_2)}{|q(x_2)|}} \exp\{-2 \operatorname{Im}[w(x_2)] + 2i \operatorname{Re}[w(x_1)]\} F_{22}^*(x_1, x_2). \quad (5.9b)$$

Except for the elements of the F -matrix the symmetry relations contain only quantities that are independent of x_1 and x_2 . This fact should be emphasized since it is not clear from the notations. In connection with special problems we shall often use special cases of the above general symmetry relations.

The above symmetry relations are a direct consequence of the fact that the function $Q^2(z)$ has been assumed to be real on the real axis. Further symmetry relations exist if $Q^2(z)$ has some kind of symmetry. If for example $Q^2(-z) = Q^2(z)$, the matrix $F(-z_1, -z_2)$ can be expressed in terms of the matrix $F(z_1, z_2)$.

ESTIMATES OF THE F -MATRIX CONNECTING TWO POINTS ON THE REAL AXIS

In this chapter we shall estimate the F -matrix connecting two points on the real axis for some important forms of the function $q^2(x)$. We shall derive the estimates, which will be needed in the following chapters for obtaining the connection formulae and for treating certain physical applications. In some cases different choices of the cuts in the complex z -plane and different choices of the phase of the function $q(z)$ [†] are taken into consideration. We shall retain the possibility of choosing $q^2(z)$ different from $Q^2(z)$. The zeros of $Q^2(z)$ are called transition points. If they lie on the real axis, they are called classical turning points. Analogously we use the name generalized classical turning points for the zeros of $q^2(z)$ on the real axis (the x -axis). A region where $Q^2(x)$ is positive is called a classically allowed region, and a region where $Q^2(x)$ is negative is called a classically forbidden region. Correspondingly we use the names classically allowed and classically forbidden in a generalized sense for the regions where $q^2(x)$ is positive and negative, respectively. For simplicity we shall often use the notions classically allowed region, classically forbidden region, and classical turning point without mentioning that these notions should be understood in the generalized sense. Furthermore, a classical turning point shall be a simple (i.e., not a multiple) zero of $q^2(x)$, if nothing else is explicitly said. In the generalized sense we shall speak of an overdense potential barrier to denote a region of the real axis where $q^2(x)$ is negative. A barrier where the function $q^2(x)$ is positive is said to be underdense.

6.1. Estimates of the F -matrix connecting two points in the same classically allowed region

The points x_1 and x_2 are assumed to lie in the same classically allowed region of the real axis, and the fixed lower limit in the integral (3.3) defining $w(z)$ is chosen to be a point in the same region. If, in the complex z -plane,

there is no cut which crosses the real axis between x_1 and x_2 , the function $w(x)$ is real and the phase of $q(z)^{\frac{1}{2}}$ is constant over the entire interval (x_1, x_2) of the real axis. The symmetry relations (5.7a, b) are thus simplified to

$$F_{22}(x_1, x_2) = F_{11}^*(x_1, x_2) \quad (6.1a)$$

$$F_{12}(x_1, x_2) = F_{21}^*(x_1, x_2). \quad (6.1b)$$

With the help of these formulae we can write the condition $\det \mathbf{F}(x_1, x_2) = 1$ as follows

$$|F_{11}(x_1, x_2)|^2 - |F_{21}(x_1, x_2)|^2 = 1. \quad (6.2)$$

The most convenient path A connecting the points x_1 and x_2 is the real axis. Since the function $w(z)$ is real on this path, we choose $M = 1$ in the basic estimates (4.3) for $\mathbf{F}(x_1, x_2)$, getting

$$|F_{11}(x_1, x_2) - 1| \leq \frac{1}{2}[\exp\{\mu\} - 1] \quad (6.3a)$$

$$|F_{21}(x_1, x_2)| \leq \frac{1}{2}[\exp\{\mu\} - 1]. \quad (6.3b)$$

Furthermore, since ε and w are both real along the path A , we find from (3.22a) by using similar estimates as in chapter 4 that

$$|\operatorname{Re}\{F_{11}(x_1, x_2) - 1\}| \leq \frac{1}{2}[\exp\{\mu\} - 1 - \mu]. \quad (6.4)$$

For completeness we also include estimates of the series used by Olver. Thus from (4.4a, b) we obtain

$$|F_{11}(x_1, x_2) + \exp\{-2i w(x_1)\} F_{21}(x_1, x_2) - 1| \leq \exp\{\mu\} - 1 \quad (6.5a)$$

$$|\exp\{2i w(x_1)\} F_{12}(x_1, x_2) + F_{22}(x_1, x_2) - 1| \leq \exp\{\mu\} - 1. \quad (6.5b)$$

6.2. Estimates of the F -matrix connecting two points in the same classically forbidden region

The points x_1 and x_2 are now assumed to lie in the same classically forbidden region of the real axis, and the fixed lower limit in the integral (3.3) defining $w(z)$ is chosen to be a point in the same region. If, in the complex z -plane, there is no cut crossing the real axis between x_1 and x_2 , the function $w(x)$ is purely imaginary and the phase of $q(z)^{\frac{1}{2}}$ is constant over the whole interval (x_1, x_2) of the real axis, and we have the symmetry relations

$$F_{ij}^*(x_1, x_2) = F_{ij}(x_1, x_2) \quad (6.6)$$

which mean that all the elements of the matrix $F(x_1, x_2)$ are real. For the sake of completeness we also recall the condition (3.19) for the matrix $F(x_1, x_2)$, which reads

$$F_{11}(x_1, x_2) F_{22}(x_1, x_2) - F_{12}(x_1, x_2) F_{21}(x_1, x_2) = 1. \quad (6.7)$$

As in the preceding section the most convenient path A connecting the points x_1 and x_2 is the real axis, since the functions $iq(z)$ and $iw(z)$ are real on this path. Assuming that $iw(z)$ increases monotonically as z moves from x_2 to x_1 along the real axis, we can according to (4.1) use the estimates (4.3) and (4.4) with $M = \frac{1}{2}$, getting

$$|F_{11}(x_1, x_2) - 1| \leq \exp\{\frac{1}{2}\mu\} - 1 \quad (6.8a)$$

$$|F_{12}(x_1, x_2)| \leq [\exp\{\frac{1}{2}\mu\} - 1] \exp\{-2iw(x_2)\} \quad (6.8b)$$

$$|F_{21}(x_1, x_2)| \leq [\exp\{\frac{1}{2}\mu\} - 1] \exp\{2iw(x_1)\} \quad (6.8c)$$

$$|F_{22}(x_1, x_2) - 1| \leq \frac{1}{2}\mu + [\exp\{\frac{1}{2}\mu\} - 1 - \frac{1}{2}\mu] \exp\{2i[w(x_1) - w(x_2)]\} \quad (6.8d)$$

and

$$|F_{11}(x_1, x_2) + \exp\{-2iw(x_1)\} F_{21}(x_1, x_2) - 1| \leq \exp\{\frac{1}{2}\mu\} - 1 \quad (6.9a)$$

$$\begin{aligned} |\exp\{2iw(x_1)\} F_{12}(x_1, x_2) + F_{22}(x_1, x_2) - 1| &\leq \\ &\leq [\exp\{\frac{1}{2}\mu\} - 1] \exp\{2|w(x_1) - w(x_2)|\}. \end{aligned} \quad (6.9b)$$

6.3. Estimates of the F -matrix connecting two points on opposite sides of a classical turning point

In this section we shall be concerned with estimates of the elements of the matrix $F(x_1, x_2)$ when the points x_1 and x_2 lie on the real axis but on opposite sides of a classical turning point, which is assumed to correspond to a simple zero of the function $q^2(x)$. We choose the notations x_1 and x_2 such that the point x_1 lies in the classically forbidden region and the point x_2 in the classically allowed region. We assume that x_1 and x_2 lie far enough from the classical turning point for the JWKB-approximation to be valid in the neighbourhood of x_1 as well as in the neighbourhood of x_2 . As regards the relative positions of the classically forbidden and classically allowed regions with respect to the positive direction of the real axis the two cases shown in fig. 6.1a and fig. 6.2a occur. We cut the z -plane along the real axis and consider the function $q(z)^{\frac{1}{2}}$ on the real axis and in the upper half of the z -plane. In order to be prepared to treat the applications considered

in the following chapters, we shall allow for different choices of the phase of $q(z)^{\frac{1}{2}}$.

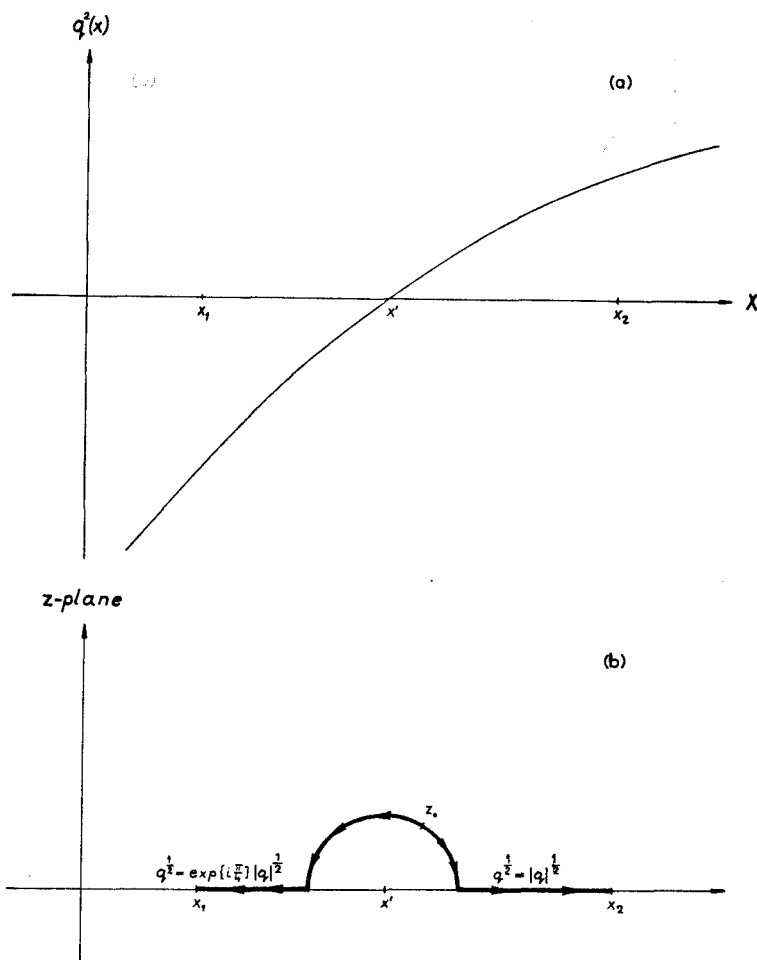


Fig. 6.1

We consider first the case that the phase of $q(z)^{\frac{1}{2}}$ is chosen either as shown in fig. 6.1b or as in fig. 6.2b. The cases in fig. 6.1 and fig. 6.2 can be treated simultaneously, since the difference between these two cases appears only in the signs of certain quantities. In the formulae we shall give both signs, letting the upper signs refer to the case in fig. 6.1 and the lower signs to the

case in fig. 6.2. If, in the definition (3.3) of $w(z)$, we choose the fixed lower limit of the integral to be the classical turning point x' , which means that

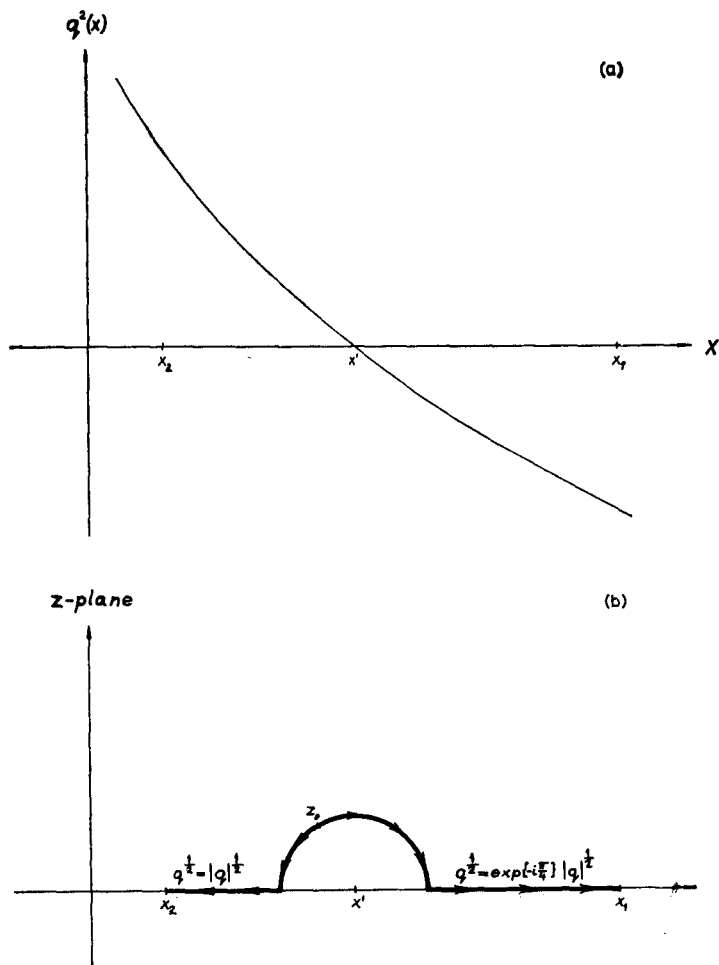


Fig. 6.2

$w(x') = 0$, the symmetry relations (5.9a, b) take the following simple form

$$F_{12}(x_1, x_2) = \pm i F_{11}^*(x_1, x_2) \quad (6.10a)$$

$$F_{21}(x_1, x_2) = \pm i F_{22}^*(x_1, x_2). \quad (6.10b)$$

Using these relations we can write the condition $\det \mathbf{F}(x_1, x_2) = 1$ as follows

$$F_{11}(x_1, x_2) F_{22}(x_1, x_2) + F_{11}^*(x_1, x_2) F_{22}^*(x_1, x_2) = 1. \quad (6.11)$$

In the present case we have to dwell for a while on a consideration of the path Λ to be used. The μ -integral diverges at the classical turning point x' and to obtain useful estimates of the matrix $\mathbf{F}(x_1, x_2)$ we shall choose a path of integration, which avoids the point x' by passing around it in a curve through the complex z -plane. To be able to use the basic estimates, derived in chapter 4, we must know the qualitative behaviour of the absolute value of $\exp\{i\omega(z)\}$ along this curve. We therefore consider the vicinity of the classical turning point x' , where the function $q^2(z)$ is approximately proportional to $z - x'$. It is then easy to see that on a small semi-circle with its center at x' and lying above the real axis, the absolute value of $\exp\{i\omega(z)\}$ has a single minimum. If $q^2(z)$ is equal to $Q^2(z)$ it is also easily found that the μ -integral for the small semi-circle has the value $\frac{5}{24}\pi |\omega(z)|^{-1}$ where z denotes any point on the semi-circle. If other zeros and singularities of the smooth function $q^2(z)$ lie sufficiently far away from x' , the absolute value of $\exp\{i\omega(z)\}$ still has only a single minimum on a suitably chosen curve which gives a wider berth to x' than the just mentioned semi-circle, drawn in the region where $q^2(z)$ is approximately a linear function of $z - x'$. The point where the minimum is attained on this curve is called z_0 . We assume that the curve goes far enough from x' for the μ -integral along it to be small compared to 1. To estimate the elements of the matrix $\mathbf{F}(x_1, x_2)$ we can then use a path of integration Λ joining x_1 and x_2 as shown in fig. 6.1b and fig. 6.2b, respectively. The path Λ runs along the real axis except in the neighbourhood of x' , where Λ coincides with the previously mentioned curve above the real axis. If z moves along Λ from x_1 to x_2 , the absolute value of $\exp\{i\omega(z)\}$ first decreases monotonically from $|\exp\{i\omega(x_1)\}| \gg 1$ to $|\exp\{i\omega(z_0)\}| \ll 1$ and then increases monotonically to $|\exp\{i\omega(x_2)\}| = 1$. The arrows on the path Λ in fig. 6.1b and fig. 6.2b indicate the directions in which the absolute value of $\exp\{i\omega(z)\}$ increases.

We can now apply the basic estimates (4.3) with $M = 1$ to the elements of $\mathbf{F}(x_1, z_0)$ and $\mathbf{F}(x_2, z_0)$. To estimate the elements of $\mathbf{F}(x_1, x_2)$ we consider the 11- and 21-elements of the matrix equation

$$\mathbf{F}(x_1, z_0) = \mathbf{F}(x_1, x_2) \mathbf{F}(x_2, z_0)$$

and use the symmetry relations (6.10a, b), getting

$$F_{11}(x_1, x_2) = \frac{F_{11}(x_1, z_0)}{F_{11}(x_2, z_0) \pm i \frac{F_{11}^*(x_1, x_2)}{F_{11}(x_1, x_2)} F_{21}(x_2, z_0)} \quad (6.12a)$$

$$F_{22}(x_1, x_2) = \frac{\pm i F_{21}^*(x_1, z_0)}{F_{11}^*(x_2, z_0) \pm i \frac{F_{22}^*(x_1, x_2)}{F_{22}(x_1, x_2)} F_{21}^*(x_2, z_0)}. \quad (6.12b)$$

From these formulae, and (4.3a, c) with $M = 1$, we get

$$\begin{aligned} |F_{11}(x_1, x_2) - 1| &\leq \frac{|F_{11}(x_1, z_0) - 1| + |F_{11}(x_2, z_0) - 1| + |F_{21}(x_2, z_0)|}{1 - |F_{11}(x_2, z_0) - 1| - |F_{21}(x_2, z_0)|} \leq \\ &\leq \mu + \text{higher powers of } \mu \end{aligned} \quad (6.13a)$$

$$\begin{aligned} |F_{22}(x_1, x_2)| &\leq \frac{|F_{21}(x_1, z_0)|}{1 - |F_{11}(x_2, z_0) - 1| - |F_{21}(x_2, z_0)|} \leq \\ &\leq |\exp\{2i w(x_1)\}| [\frac{1}{2}\mu + \text{higher powers of } \mu] \end{aligned} \quad (6.13b)$$

if μ is small compared to 1.

The factor $|\exp\{2i w(x_1)\}|$, occurring in the estimate (6.13b), is usually large and increases rapidly when x_1 moves away from the classical turning point x' . From the estimates (6.13a, b) combined with the symmetry relations (6.10a, b) we thus obtain the approximate values $F_{11}(x_1, x_2) \approx 1$ and $F_{12}(x_1, x_2) \approx \pm i$, whereas the elements $F_{22}(x_1, x_2)$ and $F_{21}(x_1, x_2)$, which may be large and even strongly varying, remain undetermined. Consequently it is quite obvious that our power of determining the vector $\mathbf{a}(x_1)$ from a knowledge of $\mathbf{a}(x_2)$ and vice versa must be subject to restrictions. As we shall see in chapter 8, this circumstance shows itself in the one-directional nature of the connection formulae, and problems connected to it will be encountered and discussed in several places in the following treatment.

We shall also estimate the elements of $\mathbf{F}(x_1, x_2)$, assuming $q^2(x)$ to behave as in fig. 6.1a but choosing the phase of $q(z)^{\frac{1}{2}}$ and the lower limit in the integral (3.3) defining $w(z)$ differently from the previous part of this section. For the case to be treated now we refer to fig. 6.3a, which is essentially the same as fig. 6.1a, and to fig. 6.3b, which shows the choice of the phase for $q(z)^{\frac{1}{2}}$ to be used now. To conform with the notations in section 9.1, where the estimates to be derived now shall be used, we denote the classical

turning point by x'' . Choosing the fixed lower limit in the integral (3.3) defining $w(z)$ as a point x' in the classically forbidden region to the left

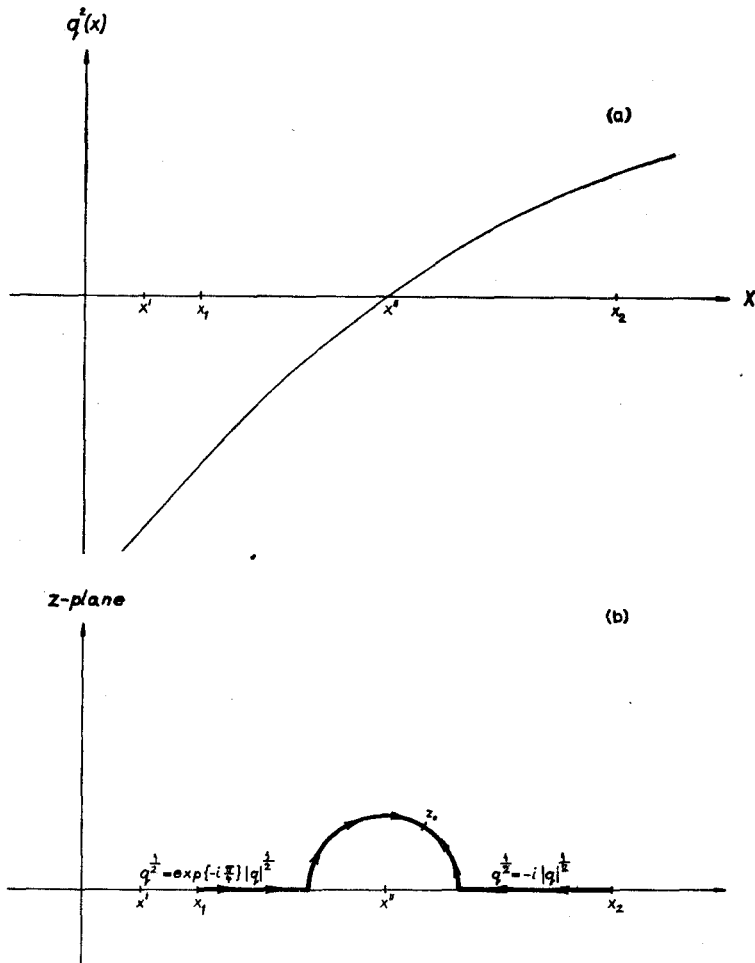


Fig. 6.3

of x'' , we have according to (5.9a, b) the symmetry relations

$$F_{12}(x_1, x_2) = i F_{11}^*(x_1, x_2) \exp \left\{ -2 \int_{x'}^{x''} |q(x)| dx \right\} \quad (6.14a)$$

$$F_{21}(x_1, x_2) = i F_{22}^*(x_1, x_2) \exp \left\{ 2 \int_{x'}^{x''} |q(x)| dx \right\}. \quad (6.14b)$$

Combining these relations with the condition (3.19) for the matrix $F(x_1, x_2)$, we get

$$F_{11}(x_1, x_2) F_{22}(x_1, x_2) + F_{11}^*(x_1, x_2) F_{22}^*(x_1, x_2) = 1. \quad (6.15)$$

Joining x_1 and x_2 by a path A similar to the one considered previously in this section, we find that there is a point z_0 on A such that the absolute value of $\exp\{i w(z)\}$ decreases monotonically as one moves along A from z_0 to x_1 and also as one moves along A from z_0 to x_2 . The arrows on the path A in fig. 6.3b indicate the directions in which the absolute value of $\exp\{i w(z)\}$ is increasing. The basic estimates (4.3) can be used for estimating the elements of $F(z_0, x_1)$ and $F(z_0, x_2)$. To estimate the diagonal elements of $F(x_1, x_2)$ we consider the 12- and 22-elements of the matrix equation

$$F(x_1, z_0) = F(x_1, x_2) F(x_2, z_0).$$

We use the symmetry relations (6.14a, b) and replace the elements of $F(x_1, z_0)$ and $F(x_2, z_0)$ by the elements of $F(z_0, x_1)$ and $F(z_0, x_2)$ according to (3.20). The resulting formulae can be written as follows

$$F_{11}(x_1, x_2) = \frac{-i F_{12}^*(z_0, x_1) \exp\left\{2 \int_{x'}^{x''} |q(x)| dx\right\}}{F_{11}^*(z_0, x_2) - i \frac{F_{11}^*(x_1, x_2)}{F_{11}(x_1, x_2)} F_{12}^*(z_0, x_2) \exp\left\{2 \int_{x'}^{x''} |q(x)| dx\right\}}$$

$$F_{22}(x_1, x_2) = \frac{F_{11}(z_0, x_1)}{F_{11}(z_0, x_2) - i \frac{F_{22}^*(x_1, x_2)}{F_{22}(x_1, x_2)} F_{12}(z_0, x_2) \exp\left\{2 \int_{x'}^{x''} |q(x)| dx\right\}}.$$

Assuming μ to be small compared to 1 and using the estimates (4.3a) and (4.3b) with $M = 1$, we then get

$$|F_{11}(x_1, x_2)| \leq \exp\left\{2 \int_{x_1}^{x''} |q(x)| dx\right\} \left[\frac{1}{2}\mu + \text{higher powers of } \mu\right] \quad (6.16a)$$

$$|F_{22}(x_1, x_2) - 1| \leq \mu + \text{higher powers of } \mu. \quad (6.16b)$$

Comparing these estimates with (6.13a, b), we easily see that the upper bounds agree but belong to different matrix elements. In the present case

$$F_{22}(x_1, x_2) \approx 1 \quad \text{and} \quad F_{21}(x_1, x_2) \approx i \exp\left\{2 \int_{x'}^{x''} |q(x)| dx\right\}$$

whereas $F_{11}(x_1, x_2)$ and $F_{12}(x_1, x_2)$ are undetermined.

We have thought it instructive to derive in detail the estimates of $F(x_1, x_2)$ on the different assumptions made above. Furthermore, we shall need the results from both calculations in the following.

6.4. Estimates of the F -matrix connecting two points on opposite sides of an overdense potential barrier

In this section we shall consider the case that, as shown in fig. 6.4a or fig. 6.5a, there are two classical turning points x' and x'' , each corresponding to a simple zero of $q^2(x)$. The region between x' and x'' is assumed to be classically forbidden, and the regions to the left of x' and to the right of x'' are assumed to be classically allowed. Let x_1 denote a point in the classically allowed region to the left of x' , and let x_2 denote a point in the classically allowed region to the right of x'' . The points x_1 and x_2 are assumed to lie so far from the turning points that the JWKB-approximation may be used in the neighbourhood of x_1 as well as in the neighbourhood of x_2 . We cut the z -plane along the real axis and consider the function $q(z)^\dagger$ on the real axis and in the upper half of the z -plane, choosing the phase of $q(z)^\dagger$ as shown in fig. 6.4b or fig. 6.5b. Choosing in the definition (3.3) of $w(z)$ the fixed lower limit in the integral to be a point in the classically allowed region to the left of the classical turning point x' or possibly this turning point itself, we have the symmetry relations

$$F_{11}(x_1, x_2) = -F_{22}^*(x_1, x_2) \exp\{2K\} \quad (6.17a)$$

$$F_{21}(x_1, x_2) = -F_{12}^*(x_1, x_2) \exp\{2K\} \quad (6.17b)$$

where K is defined by

$$K = i \int_{x'}^{x''} q(z) dz = \int_{x'}^{x''} |q(x)| dx. \quad (6.18)$$

By introducing the symmetry relations (6.17a, b) into the condition $\det F(x_1, x_2) = 1$, we obtain the formula

$$|F_{12}(x_1, x_2)|^2 - |F_{22}(x_1, x_2)|^2 = \exp\{-2K\}. \quad (6.19)$$

We shall first estimate $F_{12}(x_1, x_2)$ and $F_{22}(x_1, x_2)$ for the case that the classical turning points x' and x'' are well separated as in fig. 6.4a. To obtain these estimates we shall use the results obtained in the previous section,

which are valid only if $w(x') = 0$. This particularization will therefore be introduced now. Let x_0 be a point on the real axis between x' and x'' and consider a path A joining x_1 and x_2 and passing through x_0 as shown by the heavy line in fig. 6.4b. Since the turning points x' and x'' are well separated,

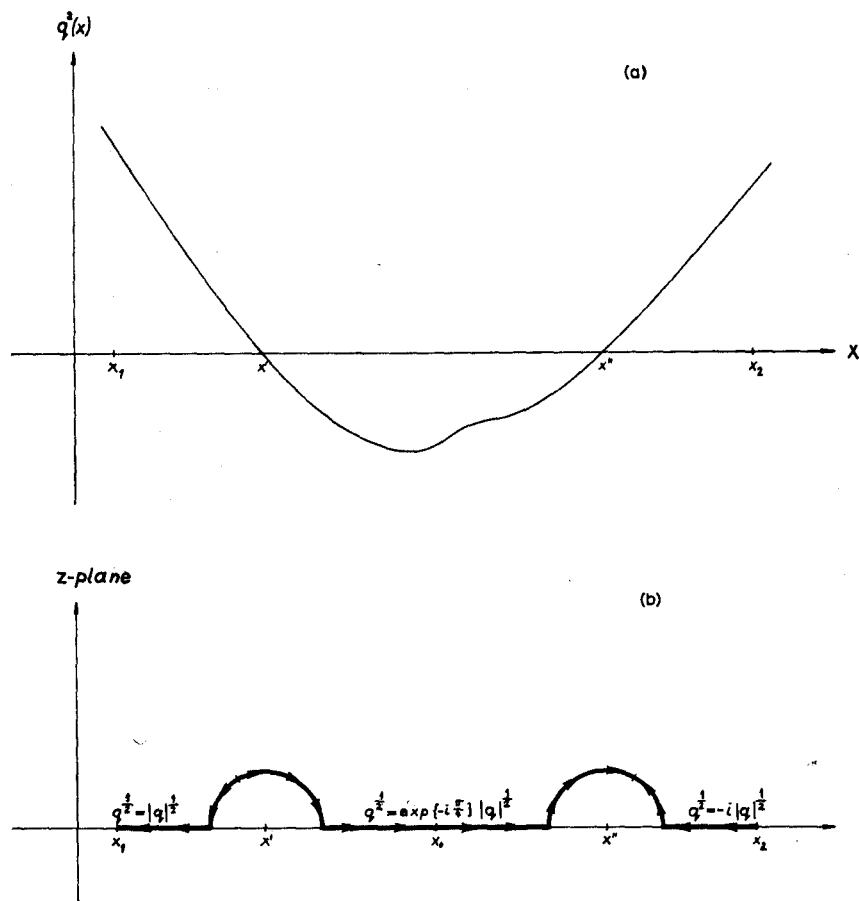


Fig. 6.4

we shall assume that the path A can be chosen such that the μ -integral for the whole path A is small compared to 1 and that the absolute value of $\exp\{i w(z)\}$ has a single minimum between x_1 and x_0 , whereas it has a single maximum between x_0 and x_2 . The directions of increasing $|\exp\{i w(z)\}|$

on Δ are indicated by arrows in fig. 6.4b. Utilizing the formula (3.20) for inverting the F -matrix, we get from the symmetry relations (6.10a, b) and the estimates (6.13a, b)

$$F_{12}(x_1, x_0) = i F_{22}^*(x_1, x_0) \quad (6.20a)$$

$$F_{21}(x_1, x_0) = i F_{11}^*(x_1, x_0) \quad (6.20b)$$

$$|F_{22}(x_1, x_0) - 1| \leq \mu(x_1, x_0) + \text{higher powers of } \mu(x_1, x_0) \quad (6.20c)$$

$$|F_{11}(x_1, x_0)| \leq \exp \left\{ 2 \int_{x'}^{x_0} |q(x)| dx \right\} \times \\ \times \left[\frac{1}{2} \mu(x_1, x_0) + \text{higher powers of } \mu(x_1, x_0) \right]. \quad (6.20d)$$

According to the symmetry relations (6.14a, b) and the estimates (6.16a, b) we similarly have

$$F_{12}(x_0, x_2) = i F_{11}^*(x_0, x_2) \exp \left\{ -2 \int_{x'}^{x''} |q(x)| dx \right\} \quad (6.21a)$$

$$F_{21}(x_0, x_2) = i F_{22}^*(x_0, x_2) \exp \left\{ 2 \int_{x'}^{x''} |q(x)| dx \right\} \quad (6.21b)$$

$$|F_{22}(x_0, x_2) - 1| \leq \mu(x_0, x_2) + \text{higher powers of } \mu(x_0, x_2) \quad (6.21c)$$

$$|F_{11}(x_0, x_2)| \leq \exp \left\{ 2 \int_{x_0}^{x''} |q(x)| dx \right\} \left[\frac{1}{2} \mu(x_0, x_2) + \right. \\ \left. + \text{higher powers of } \mu(x_0, x_2) \right]. \quad (6.21d)$$

From the identity

$$\mathbf{F}(x_1, x_2) = \mathbf{F}(x_1, x_0) \mathbf{F}(x_0, x_2)$$

and the formulae (6.20) and (6.21) we then get the estimates

$$|F_{12}(x_1, x_2) - i| \leq \mu(x_1, x_2) + \text{higher powers of } \mu(x_1, x_2) \quad (6.22a)$$

$$|F_{22}(x_1, x_2) - 1| \leq \mu(x_1, x_2) + \text{higher powers of } \mu(x_1, x_2) \quad (6.22b)$$

which together with the symmetry relations (6.17a, b) determine all the elements of the matrix $\mathbf{F}(x_1, x_2)$ approximately :

$$\mathbf{F}(x_1, x_2) = \begin{pmatrix} -[1 + O(\mu)] \exp\{2K\} & i + O(\mu) \\ [i + O(\mu)] \exp\{2K\} & 1 + O(\mu) \end{pmatrix}. \quad (6.23)$$

Here $\mu = \mu(x_1, x_2)$ is the μ -integral for the whole path A from x_1 to x_2 . Obviously we use the symbol $O(\mu)$ in a slightly different meaning from mathematics, where this symbol is used to denote an upper bound for a function as the independent variable tends towards a certain limit. We shall, however, write $O(\mu)$ to denote a quantity which is at the most of the order of magnitude of μ , even if μ cannot tend to the limit zero.

It is interesting to see how the exponential factors in the estimates (6.20) and (6.21) cancel on estimating the product $F(x_1, x_2) = F(x_1, x_0) F(x_0, x_2)$. Although we know approximately only two of the four elements of each of the matrices $F(x_1, x_0)$ and $F(x_0, x_2)$, we obtain approximate values for all of the elements of $F(x_1, x_2)$.

It should be pointed out that the above expression (6.23) for $F(x_1, x_2)$ cannot be used for determining $a(x_1)$ if

$$a_2(x_2) = -i a_1(x_2) \exp\{2K\} [1 + O(\mu)],$$

because the significant terms of the elements of $F(x_1, x_2)$ then cancel on evaluating the product $F(x_1, x_2) a(x_2)$. The fact that the usefulness of the expression (6.23) for the matrix $F(x_1, x_2)$ fails in this special case is nothing but a reflection of the one-directional nature of the connection formulae.

The estimates (6.22a, b) of $F_{12}(x_1, x_2)$ and $F_{22}(x_1, x_2)$ do not apply if the classical turning points x' and x'' lie close together, for in this case the path A from x_1 to x_2 , passing through x_0 , runs close to x' and x'' , and this implies that the μ -integral along this path is no longer small compared to 1. To treat the case that the points x' and x'' lie close together as in fig. 6.5a, we choose a suitable path A joining the points x_1 and x_2 as shown in fig. 6.5b. The path A coincides with the real axis except in the region of the turning points x' and x'' where A forms a curve above the real axis. We assume that in a certain region containing both x' and x'' and containing also the curved part of the path A above the real axis, the function $q^2(z)$ can be approximated by a quadratic function of z (a parabola). We emphasize that this assumption will be used only in a rather qualitative way, namely to ensure that on the path A the absolute value of $\exp\{i w(z)\}$ has one minimum which is attained at a point called z_1 , and one maximum, which is attained at a point called z_2 lying between z_1 and x_2 on the path A . Such a path A is expected to exist on the rather general assumptions that the classical turning points x' and x'' lie close together and that there are no singularities and no further zeros of $q^2(z)$ in the neighbourhood of x' and x'' . The arrows on the path A in fig. 6.5b indicate the directions in which

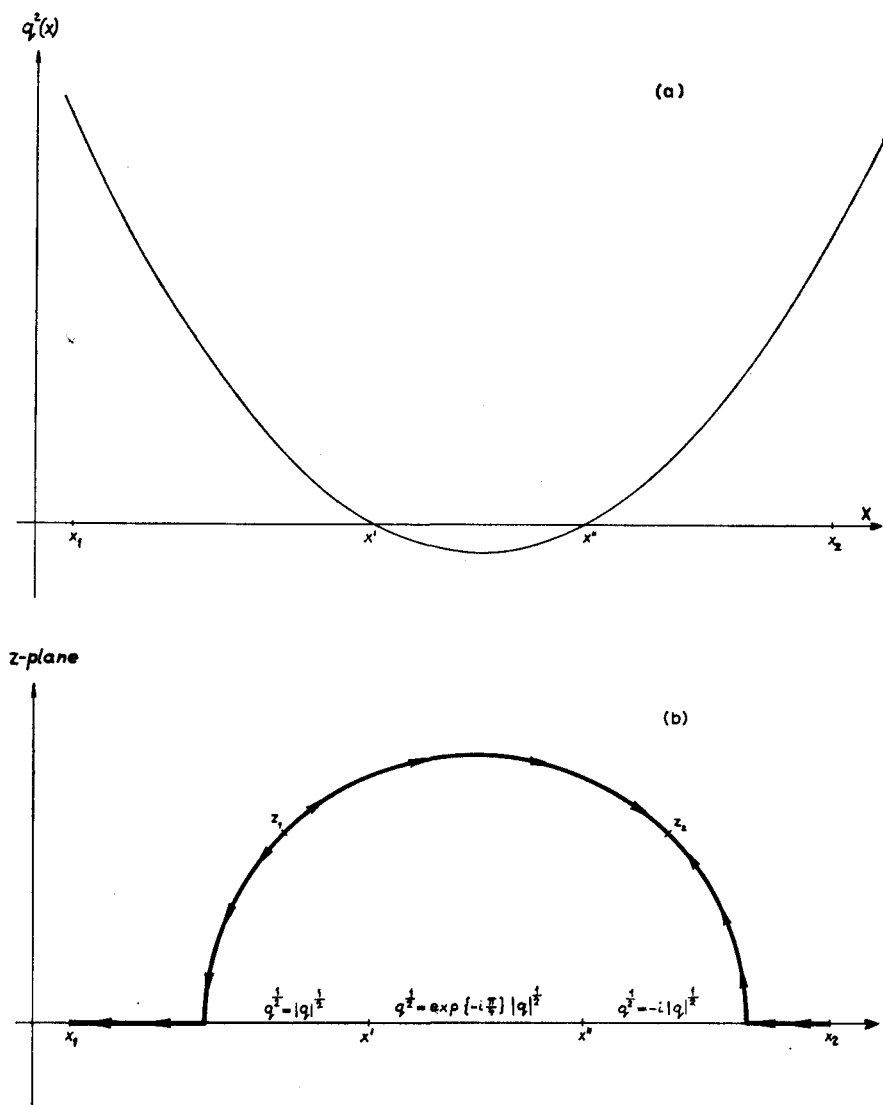


Fig. 6.5

$|\exp\{i w(z)\}|$ increases (or remains constant). In the definition (3.3) of $w(z)$ we shall now choose the fixed lower limit in the integral to be a point in the classically allowed region to the left of the turning point x' or possibly

this turning point itself. As z moves from x_1 to x_2 along A , the absolute value of $\exp\{i w(z)\}$ first decreases monotonically from $|\exp\{i w(x_1)\}| = 1$ to $|\exp\{i w(z_1)\}| < 1$, then increases monotonically to $|\exp\{i w(z_2)\}| > \exp\{K\}$, and finally decreases monotonically to $|\exp\{i w(x_2)\}| = \exp\{K\}$. It is essential to assume that the path A just described can be chosen such that the μ -integral along it is small compared to 1. To estimate the elements of $F(x_1, x_2)$ in the present case we consider the 22-element of the matrix identity

$$F(z_1, z_2) = F(z_1, x_1) F(x_1, x_2) F(x_2, z_2)$$

and use the symmetry relations (6.17a, b) and replace the elements of $F(z_1, z_2)$, $F(z_1, x_1)$, and $F(x_2, z_2)$ by the elements of $F(z_2, z_1)$, $F(x_1, z_1)$, and $F(z_2, x_2)$ according to (3.20), getting

$$F_{11}(z_2, z_1) = A F_{22}(x_1, x_2) - B F_{12}(x_1, x_2) \quad (6.24)$$

where

$$A = F_{11}(x_1, z_1) F_{11}(z_2, x_2) - F_{21}(x_1, z_1) F_{12}(z_2, x_2) \frac{F_{22}^*(x_1, x_2)}{F_{22}(x_1, x_2)} \exp\{2K\}$$

$$B = F_{21}(x_1, z_1) F_{11}(z_2, x_2) - F_{11}(x_1, z_1) F_{12}(z_2, x_2) \frac{F_{12}^*(x_1, x_2)}{F_{12}(x_1, x_2)} \exp\{2K\}.$$

Using the basic estimates (4.3) and remembering that $|\exp\{i w(x_1)\}| = 1$ and $|\exp\{i w(x_2)\}| = \exp\{K\}$ we get the estimates

$$\left| \frac{A - 1}{B} \right| \leq \frac{1}{2} \mu(x_1, z_1) + \frac{1}{2} \mu(z_2, x_2) + \text{higher powers of } \mu(x_1, z_1) \text{ and } \mu(z_2, x_2). \quad (6.25)$$

According to (4.3a) we also have the estimate

$$|F_{11}(z_2, z_1) - 1| \leq \frac{1}{2} \mu(z_1, z_2) + \text{higher powers of } \mu(z_1, z_2). \quad (6.26)$$

From the formula (6.19) it follows that

$$|F_{12}(x_1, x_2)| \leq |F_{22}(x_1, x_2)| + \exp\{-K\}$$

and hence we can write

$$F_{12}(x_1, x_2) = \Theta [|F_{22}(x_1, x_2)| + \exp\{-K\}] \quad (6.27)$$

where Θ is a complex number fulfilling the condition

$$|\Theta| \leq 1. \quad (6.28)$$

Substituting (6.27) into (6.24), we get

$$F_{22}(x_1, x_2) = \frac{F_{11}(z_2, z_1) + B \Theta \exp\{-K\}}{A - B \Theta \frac{|F_{22}(x_1, x_2)|}{F_{22}(x_1, x_2)}}.$$

Using now in this formula (6.25), (6.26), and (6.28), we get the estimate

$$\begin{aligned} |F_{22}(x_1, x_2) - 1| &\leq \frac{|F_{11}(z_2, z_1) - 1| + |A - 1| + |B| [1 + \exp\{-K\}]}{1 - |A - 1| - |B|} \leq \\ &\leq [1 + \frac{1}{2} \exp\{-K\}] [\mu + \text{higher powers of } \mu] \end{aligned}$$

i.e.,

$$F_{22}(x_1, x_2) = 1 + [1 + \frac{1}{2} \exp\{-K\}] O(\mu) \quad (6.29)$$

where $\mu = \mu(x_1, x_2)$ is the μ -integral for the whole path A from x_1 to x_2 . Since $K > 0$, the factor $[1 + \frac{1}{2} \exp\{-K\}]$ in the error term in (6.29) could have been left out, but we have retained it in order to be able to refer later to the estimate (6.29), which in the form given above is useful also in connection with transmission through an underdense potential barrier, where $K < 0$.

From (6.19) and (6.29) we get

$$|F_{12}(x_1, x_2)| = \{1 + \exp\{-2K\}\}^{\frac{1}{2}} [1 + O(\mu)]$$

since $K > 0$. Hence we can write

$$F_{12}(x_1, x_2) = \exp\{i\varphi\} \{1 + \exp\{-2K\}\}^{\frac{1}{2}} [1 + O(\mu)] \quad (6.30)$$

where φ is a real phase, which will be discussed later.

The estimates (6.29) and (6.30) together with the symmetry relations (6.17a, b) give the approximate formula

$$F(x_1, x_2) \approx \begin{pmatrix} -\exp\{2K\} & e^{i\varphi}\{1 + \exp\{-2K\}\}^{\frac{1}{2}} \\ -e^{-i\varphi}\{1 + \exp\{-2K\}\}^{\frac{1}{2}} \exp\{2K\} & 1 \end{pmatrix}, \quad (6.31)$$

where the approximate values of the matrix elements differ from the corresponding exact values by factors $[1 + O(\mu)]$. When $a_1(x_2)$ and $a_2(x_2)$ are given, the matrix (6.31) allows an approximate calculation of $a_\nu(x_1)$ ($\nu = 1, 2$) unless

$$a_1(x_2) = [1 + \exp\{-2K\}]^{\frac{1}{2}-\nu} \exp\{i\varphi - 2K\} a_2(x_2) [1 + O(\mu)].$$

The quantity $\exp\{-2K\}$ in the non-diagonal elements of (6.31) is significant only when $\mu \ll \exp\{-2K\}$, which as a rule is the case only when the turning

points lie close to each other (The parabolic barrier is an exception, see below). Otherwise $\exp\{-2K\}$ should be deleted, whereby the formula (6.31) should become identical to (6.23), if the lower limit in the integral defining $w(z)$ is chosen to be x' also in the matrix $F(x_1, x_2)$ in (6.31). Comparing (6.23) and (6.31) we thus conclude that $\varphi = \frac{1}{2}\pi$ if the turning points are well separated and $w(x') = 0$.

Let us now further consider the phase φ occurring in the non-diagonal elements of the matrix (6.31). In our derivation of (6.31) the lower limit in the integral (3.3) defining $w(z)$ has been allowed to be any point in the classically allowed region to the left of x' . Since $w(x)$ is real in this region, it is thus immediately clear that the phase φ depends on our choice of the lower limit in the integral (3.3), while all other quantities in (6.31) are unaffected. To be able to say something more definite about φ , we shall now choose $w(x') = 0$. In the limiting case when the classical turning points x' and x'' coincide, it follows from the forthcoming formulae (7.13a, b), which are valid if $q^2(z) = Q^2(z)$ that

$$F(x_1, x_2) \approx \begin{pmatrix} 1 & 2i \cos \frac{1}{4}\pi \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 2i \cos \frac{1}{4}\pi & 1 \end{pmatrix} = \begin{pmatrix} -1 & i\sqrt{2} \\ i\sqrt{2} & 1 \end{pmatrix}.$$

Comparing this result with (6.31), we find that if $q^2(z) = Q^2(z)$ the phase φ has approximately the value $\frac{1}{2}\pi$ in the limiting case when K is very small. On the other hand, when K is fairly large we have already found that φ has approximately the value $\frac{1}{2}\pi$ also in this case. Since the same approximate value $\frac{1}{2}\pi$ of the phase φ thus applies both to the limiting case of coinciding classical turning points ($K = 0$) and to the case of well separated classical turning points ($K \gg 1$), one might expect the phase φ in (6.31) to have approximately the value $\frac{1}{2}\pi$ also for all intermediate values of K . To a reasonable degree of approximation this is confirmed by a calculation performed by SOOP [1965].

For the special case that $q^2(z)$ is a polynomial of the second order in z there are no zeros or singularities of $q^2(z)$ in the complex plane. If $x_1 = -\infty$ and $x_2 = +\infty$, we can thus, for any value of $K \geq 0$, let the radius of the semi-circle in fig. 6.5b tend to infinity. The value of μ then tends to zero, if $q^2(z) = Q^2(z)$, and the matrix (6.31) provides for all values of K an exact expression for $F(-\infty, +\infty)$. Furthermore, the value of the phase φ is in this case exactly equal to $\frac{1}{2}\pi$ when $K = 0$, which is easily found from the forthcoming formulae (7.11a, b).

MERZBACHER [1961] has used a matrix formalism for connecting, in the JWKB-approximation, the wave functions on opposite sides of a potential barrier with well separated classical turning points to each other. The matrix connecting $\begin{pmatrix} A \\ B \end{pmatrix}$ and $\begin{pmatrix} F \\ G \end{pmatrix}$ in Merzbacher's equation (7.30) shall in our notations be the matrix

$$F(-\infty, +\infty) \begin{pmatrix} 0 & -i \exp\{-K\} \\ -i \exp\{K\} & 0 \end{pmatrix}.$$

Introducing here the expression (6.23) for $F(-\infty, +\infty)$, we get

$$\begin{pmatrix} [1 + O(\mu)] \exp\{K\} & [i + O(\mu)] \exp\{K\} \\ -[i + O(\mu)] \exp\{K\} & [1 + O(\mu)] \exp\{K\} \end{pmatrix}.$$

Comparing this matrix with the matrix in Merzbacher's equation (7.30), we realize that the quantities $1/(2\theta)$ in Merzbacher's formula are insignificant. The reason why they appear there is that Merzbacher has in his derivation of the formula disregarded the one-sided nature of the formulae connecting the JWKB-solutions on opposite sides of a classical turning point. When $G = iF$ the significant terms in Merzbacher's matrix cancel on calculating A and B , and the results obtained are quite unreliable as is confirmed by the following example.

For the special case of a parabolic potential barrier we have found that $F(-\infty, +\infty)$ is exactly given by (6.31) for all values of K . Let us thus introduce (6.31) for $F(-\infty, +\infty)$ in the above matrix product and, assuming K to be large, expand the square roots occurring to the first order in $\exp\{-2K\}$. We then obtain the following matrix

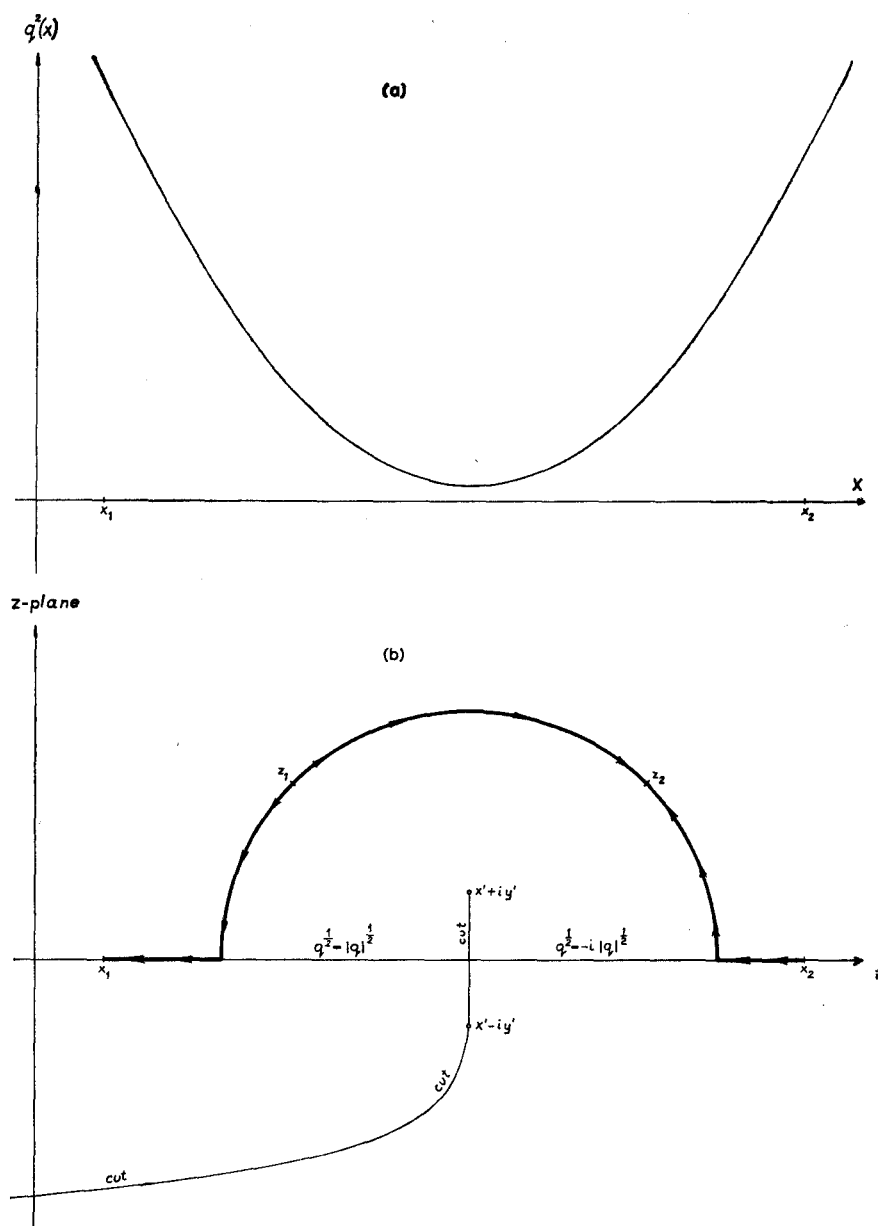
$$\begin{pmatrix} -i e^{i\varphi} [\exp\{K\} + \frac{1}{2} \exp\{-K\}] & i \exp\{K\} \\ -i \exp\{K\} & i e^{-i\varphi} [\exp\{K\} + \frac{1}{2} \exp\{-K\}] \end{pmatrix}$$

where the phase φ is approximately equal to $\frac{1}{2}\pi$, since $w(x') = 0$. The terms containing $\exp\{-K\}$ are now significant. We find, however, that the corresponding terms containing $1/\theta$ in Merzbacher's matrix are not in agreement with the above result. This confirms again that they are unjustifiable.

6.5. Estimates of the F -matrix connecting two points on opposite sides of an underdense potential barrier

In this section we shall be concerned with an underdense potential barrier, i.e. we shall assume that $q^2(x)$ as shown in fig. 6.6a or fig. 6.7a is positive along the whole real axis but that there are two complex conjugate zeros of $q^2(z)$ lying close to this axis. These zeros are denoted by $x' \pm iy'$ where y' is positive but small, and we assume that all other zeros and singularities of $q^2(z)$ lie fairly far away from the real axis.

We shall first choose the cuts in the complex z -plane in such a way that the present underdense barrier can be treated analogously to the overdense



barrier of fig. 6.5. For this purpose we cut the complex z -plane as shown in fig. 6.6b along a line emerging from $x' + iy'$ passing through $x' - iy'$ and continuing towards infinity in the lower half of the z -plane. We choose the phase of $q(z)^{\frac{1}{2}}$ according to fig. 6.6b, i.e., such that $q(z)^{\frac{1}{2}}$ is real and positive on the real axis to the left of the cut, and we choose the fixed lower limit in the integral (3.3) defining $w(z)$ to be a point on the real axis to the left of the cut. If x_1 and x_2 are two points on the real axis on opposite sides of the cut, and if $x_1 < x_2$, we have according to (5.7) the symmetry relations

$$F_{11}(x_1, x_2) = -F_{22}^*(x_1, x_2) \exp\{2K\} \quad (6.32a)$$

$$F_{21}(x_1, x_2) = -F_{12}^*(x_1, x_2) \exp\{2K\}, \quad (6.32b)$$

the quantity K being defined by the formula

$$K = i \int_{x' - iy'}^{x' + iy'} q(z) dz \quad (6.33)$$

where the path of integration joining the two zeros $x' \pm iy'$ shall cross the real axis to the left of the cut in the complex z -plane. Since $q(z)$ is real on the real axis, we have $q(z^*) = q^*(z)$, and we see that the quantity K is real. Furthermore, assuming the zeros $x' \pm iy'$ to lie so close to each other that it is permissible to approximate $q^2(z)$ by a quadratic expression in z in a small region containing both of these zeros, one easily finds that K is negative. Introducing the symmetry relations (6.32a, b) into the relation $\det \mathbf{F}(x_1, x_2) = 1$, we get

$$|F_{12}(x_1, x_2)|^2 - |F_{22}(x_1, x_2)|^2 = \exp\{-2K\}. \quad (6.34)$$

Except for the definition of K , the symmetry relations (6.32a, b) and the formula (6.34) in the present section are the same as the symmetry relations (6.17a, b) and the formula (6.19) in the previous section of this chapter. To estimate $\mathbf{F}(x_1, x_2)$ for the present case illustrated by fig. 6.6 we can proceed in a similar way as in the latter part of section 6.4, where $\mathbf{F}(x_1, x_2)$ was estimated for the case illustrated by fig. 6.5. With only minor changes the treatment given there and leading to the estimates (6.29) and (6.30) can be applied step by step in the case corresponding to fig. 6.6. The result is again the formulae (6.29) and (6.30) with the only change that K is now defined according to (6.33) and is therefore negative and that in (6.30) the error $O(\mu)$ is to be replaced by $\exp\{K\} O(\mu)$.

To discuss the value of the phase φ in (6.30) for the present case we shall assume that the Stokes' line (i.e., the line along which the differential $d w$

is purely imaginary) joining the zeros $x' \pm iy'$ lies to the left of the cut in fig. (6.6b), and we shall choose the fixed lower limit in the integral (3.3) defining $w(z)$ to be the point where this Stokes' line crosses the real axis. Suppose first that the zeros $x' \pm iy'$ lie so far from the real axis that not only the μ -integral along the path A shown in fig. 6.6b but also the μ -integral along the real axis between x_1 and x_2 is small compared to 1. One can then use matrix multiplication and the formulae (6.1) and (6.3), valid on each side of the cut, to estimate $F(x_1, x_2)$. When the result is compared with (6.30) one finds that $\varphi \approx \frac{1}{2}\pi$. Suppose next that $y' = 0$. As was found at the end of section 6.4, we have $\varphi \approx \frac{1}{2}\pi$ also in this case, provided $q^2(z) = Q^2(z)$. It is reasonable to expect that the phase φ has roughly the value $\frac{1}{2}\pi$ also throughout the intermediate range of values of y' . This is confirmed by calculations performed by SOOP [1965].

The same reasons as mentioned at the end of section 6.4 lead to the conclusion that the formulae $F_{22}(-\infty, +\infty) = 1$ and $|F_{12}(-\infty, +\infty)| = \{1 + \exp\{-2K\}\}^{\frac{1}{2}}$ are exactly valid if $q^2(z)$ is equal to $Q^2(z)$ and is a polynomial of the second order in z .

As already mentioned, we chose the cut in the complex z -plane according to fig. 6.6b in order to obtain as close an analogy as possible to the treatment of the overdense potential barrier of fig. 6.5. With no such an a priori intention it might seem more natural to avoid cuts crossing the real axis and to keep the phase of $q^{\frac{1}{2}}(z)$ constant along this axis. To allow for this point of view and also to illustrate the fact that various treatments are often possible, we shall derive the estimates of the elements of $F(x_1, x_2)$ also for this case. The function $q^2(x)$ is represented by fig. 6.7a, which is the same as fig. 6.6a. The cuts in the complex z plane are, however, now made as shown in fig. 6.7b. The phase of $q(z)^{\frac{1}{2}}$ is chosen such that this function is positive on the real axis, and the constant lower limit in the integral (3.3) defining $w(z)$ is chosen to be a point x_0 on the real axis. We want to estimate $F(x_1, x_2)$, where x_1 is a point to the left of the potential barrier, and x_2 is a point to the right of the potential barrier. A direct path from x_1 to x_2 must pass in the neighbourhood of the zeros $x' \pm iy'$ and hence have a large μ -integral. Therefore such a path is not convenient for estimating $F(x_1, x_2)$. However, letting $x_1 + i0$ denote a point on the upper lip of the cut, which emerges from $x' + iy'$, approaches the real axis, and continues at an infinitesimal distance above the real axis to the left of x' , we can obtain a satisfactory estimate for the matrix $F(x_1 + i0, x_2)$, since the points $x_1 + i0$ and x_2 can be joined by a convenient path (shown in fig. 6.7b) which does

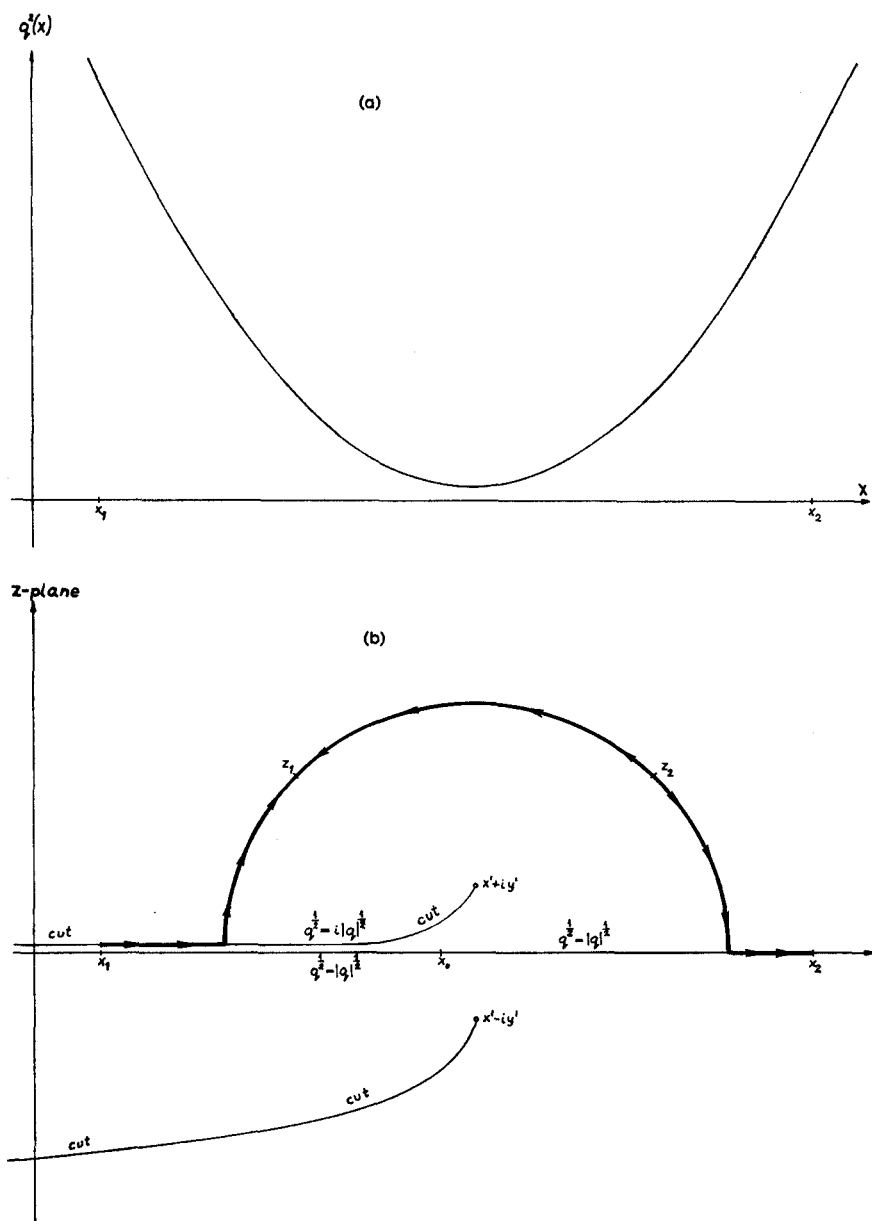


Fig. 6.7

not pass close to the zeros $x' \pm iy'$. The matrix $F(x_1, x_1 + i0)$ is easily obtained in a very simple form, and estimates of the elements of the matrix $F(x_1, x_2)$ can then be calculated from the formula

$$F(x_1, x_2) = F(x_1, x_1 + i0) F(x_1 + i0, x_2). \quad (6.35)$$

Let us first consider the matrix $F(x_1, x_1 + i0)$. Since all solutions of the differential equation (3.1) are one-valued as z moves around a zero of $Q^2(z)$ or $q^2(z)$ in a closed loop, it follows from the definition (3.28) that

$$W_\psi(x_1 + i0) = W_\psi(x_1).$$

The formula (3.39) therefore gives

$$F(x_1, x_1 + i0) = W_f^{-1}(x_1) W_f(x_1 + i0).$$

Using the definitions (3.29), (3.24a, b), and (3.3), we then get

$$F(x_1, x_1 + i0) = \begin{pmatrix} 0 & -i \exp\{-\alpha\} \\ -i \exp\{\alpha\} & 0 \end{pmatrix} \quad (6.36)$$

where

$$\alpha = 2i w(x' + iy') = 2i \int_{x_0}^{x'+iy'} q(z) dz. \quad (6.37)$$

The imaginary part of α depends on x_0 , but the real part of α is independent of x_0 and is given by the formula

$$\operatorname{Re}\{\alpha\} = K \quad (6.38)$$

where K is defined by (6.33) and is negative also for the present choice of cut in the z -plane and phase of $q(z)$.

We next turn our attention to the matrix $F(x_1 + i0, x_2)$. The elements of this matrix obey the symmetry relations

$$F_{22}(x_1 + i0, x_2) = -F_{11}^*(x_1 + i0, x_2) \exp\{2K\} \quad (6.39a)$$

$$F_{21}(x_1 + i0, x_2) = -F_{12}^*(x_1 + i0, x_2) \exp\{2K\}. \quad (6.39b)$$

Combining these symmetry relations with the relation $\det F(x_1 + i0, x_2) = 1$, we get

$$|F_{12}(x_1 + i0, x_2)|^2 - |F_{11}(x_1 + i0, x_2)|^2 = \exp\{-2K\}. \quad (6.40).$$

The points $x_1 + i0$ and x_2 are joined by a path A as shown in fig. 6.7b. On this path the absolute value of $\exp\{i w(z)\}$ has one maximum (attained

at a point called z_1) and one minimum (attained at a point called z_2). The directions of increasing $|\exp\{i w(z)\}|$ on the path A in fig. 6.7b are indicated by arrows. Considering the 11-element of the matrix identity

$$F(z_1, z_2) = F(z_1, x_1 + i0) F(x_1 + i0, x_2) F(x_2, z_2)$$

and using the symmetry relations (6.39a, b), we get

$$F_{11}(z_1, z_2) = C F_{11}(x_1 + i0, x_2) + D F_{12}(x_1 + i0, x_2) \quad (6.41)$$

where

$$C = F_{11}(z_1, x_1 + i0) F_{11}(x_2, z_2) + \\ - F_{12}(z_1, x_1 + i0) F_{21}(x_2, z_2) \frac{F_{11}^*(x_1 + i0, x_2)}{F_{11}(x_1 + i0, x_2)} \exp\{2K\}$$

$$D = F_{11}(z_1, x_1 + i0) F_{21}(x_2, z_2) + \\ - F_{12}(z_1, x_1 + i0) F_{11}(x_2, z_2) \frac{F_{12}^*(x_1 + i0, x_2)}{F_{12}(x_1 + i0, x_2)} \exp\{2K\}.$$

From these definitions and the basic estimates (4.3) we get

$$\left. \begin{array}{l} |C - 1| \\ |D| \end{array} \right\} \leq \frac{1}{2} \mu(x_1 + i0, z_1) + \frac{1}{2} \mu(z_2, x_2) + \\ + \text{higher powers of } \mu(x_1 + i0, z_1) \text{ and } \mu(z_2, x_2). \quad (6.42)$$

According to (4.3a) we also have the estimate

$$|F_{11}(z_1, z_2) - 1| \leq \frac{1}{2} \mu(z_1, z_2) + \text{higher powers of } \mu(z_1, z_2). \quad (6.43)$$

From the formula (6.40) it follows that

$$|F_{12}(x_1 + i0, x_2)| \leq |F_{11}(x_1 + i0, x_2)| + \exp\{-K\}$$

and hence we can write

$$F_{12}(x_1 + i0, x_2) = \Theta \{ |F_{11}(x_1 + i0, x_2)| + \exp\{-K\} \} \quad (6.44)$$

where

$$|\Theta| \leq 1. \quad (6.45)$$

Substituting (6.44) into (6.41), we get

$$F_{11}(x_1 + i0, x_2) = \frac{F_{11}(z_1, z_2) - \Theta D \exp\{-K\}}{C + \Theta D \frac{|F_{11}(x_1 + i0, x_2)|}{F_{11}(x_1 + i0, x_2)}}.$$

Using the formulae (6.42), (6.43), and (6.45), we get

$$|F_{11}(x_1 + i0, x_2) - 1| \leq \\ \leq [1 + \frac{1}{2} \exp\{-K\}] [\mu(x_1 + i0, x_2) + \text{higher powers of } \mu(x_1 + i0, x_2)]$$

i.e.,

$$F_{11}(x_1 + i0, x_2) = 1 + [1 + \frac{1}{2} \exp\{-K\}] O(\mu) \quad (6.46)$$

where $\mu = \mu(x_1 + i0, x_2)$ is the μ -integral for the whole path from $x_1 + i0$ to x_2 in fig. 6.7b. The formula (6.46) shows that $F_{11}(x_1 + i0, x_2)$ is close to 1 unless the absolute value of the negative quantity K is too large. From (6.40) and (6.46) it follows that

$$F_{12}(x_1 + i0, x_2) = \exp\{i\varphi\} \{1 + \exp\{-2K\}\}^{\frac{1}{2}} [1 + \exp\{K\} O(\mu)] \quad (6.47)$$

where φ is a real phase. Summarizing the results contained in the estimates (6.46), (6.47), and the symmetry relations (6.39a, b), we get the approximate formula

$$F(x_1 + i0, x_2) \approx \\ \approx \begin{pmatrix} 1 & \{1 + \exp\{2K\}\}^{\frac{1}{2}} \exp\{-K + i\varphi\} \\ -\{1 + \exp\{2K\}\}^{\frac{1}{2}} \exp\{K - i\varphi\} & -\exp\{2K\} \end{pmatrix}$$

which is valid provided the absolute value of the negative quantity K is not too large. The quantity $\exp\{2K\}$ in the square root in the non-diagonal elements is significant only when $|K|$ is so small that

$$\exp\{K\} \gg \mu(x_1 + i0, x_2).$$

To obtain the matrix $F(x_1, x_2)$ we now use (6.35), (6.36), (6.46), and (6.47). Remembering also the formula (6.38) and the fact that K is negative, we get

$$F_{21}(x_1, x_2) = -i \exp\{\alpha\} [1 + \exp\{-K\} O(\mu)] \quad (6.48)$$

$$F_{22}(x_1, x_2) = \exp\{i(\varphi - \frac{1}{2}\pi + \text{Im } \alpha)\} [1 + \exp\{2K\}]^{\frac{1}{2}} [1 + \exp\{K\} O(\mu)] \quad (6.49)$$

where μ still denotes the μ -integral for the path connecting $x_1 + i0$ and x_2 in fig. 6.7b. The other two elements of $F(x_1, x_2)$ can be obtained from the symmetry relations (6.1a, b).

Until now our treatment of the case in fig. 6.7 is valid for any choice of the point x_0 on the real axis, but in the following discussion of the value of the phase φ we shall choose x_0 to be the point where the Stokes' line, joining the points $x' \pm iy'$, crosses the real axis. When y' is "small" this

point is $x_0 \approx x'$. Our special choice of x_0 implies that α is real and equal to K , and hence the formulae (6.48), (6.49) and (6.1a, b) give

$$F(x_1, x_2) \approx \begin{pmatrix} \{1 + \exp\{2K\}\}^{\frac{1}{2}} \exp\{-i(\varphi - \frac{1}{2}\pi)\} & i \exp\{K\} \\ -i \exp\{K\} & \{1 + \exp\{2K\}\}^{\frac{1}{2}} \exp\{i(\varphi - \frac{1}{2}\pi)\} \end{pmatrix}. \quad (6.50)$$

In the limiting case when $y' = 0$, i.e., $K = 0$, it follows from the forthcoming formulae (7.13a, b), valid if $q^2(z) = Q^2(z)$, that

$$F(x_1 + i0, x_2) \approx \begin{pmatrix} 1 & 0 \\ 2i \cos \frac{1}{4}\pi & 1 \end{pmatrix} \begin{pmatrix} 1 & 2i \cos \frac{1}{4}\pi \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & i\sqrt{2} \\ i\sqrt{2} & -1 \end{pmatrix}.$$

Comparing this result with (6.47), we find that, if $q^2(z) = Q^2(z)$, the phase φ has approximately the value $\frac{1}{2}\pi$ in the limiting case when the points $x' \pm iy'$ coincide, i.e. when $K = 0$. In the other limiting case when the distance between the zeros $x' \pm iy'$ is so large that the μ -integral along the real axis between x_1 and x_2 is small compared to 1, the matrix $F(x_1, x_2)$ must be approximately equal to the unit matrix according to (6.3) and (6.1). Since the matrix on the right-hand side of (6.50) actually approaches the unit matrix as $K \rightarrow -\infty$ if $\varphi = \frac{1}{2}\pi$, the phase φ must be approximately equal to $\frac{1}{2}\pi$ also in this limiting case. Thus we have $\varphi \approx \frac{1}{2}\pi$ in the limiting case when the zeros $x' \pm iy'$ coincide as well as in the limiting case when these zeros are very well separated. We may expect that φ has roughly the same value also in the intermediate cases. It should then be possible to use the formula (6.50) with $\varphi = \frac{1}{2}\pi$ as a rough interpolation formula throughout the whole region of negative values of K . It must, however, be emphasized that as a rule the quantity $\exp\{2K\}$ in the factor $\{1 + \exp\{2K\}\}^{\frac{1}{2}}$ appearing in the diagonal elements of (6.50) is significant only for rather small values of $|K|$.

In the special case that the barrier is parabolic and $q^2(z) = Q^2(z)$, the formula (6.50) tends to exactness for all values of $K (\leq 0)$ when $x_1 \rightarrow -\infty$ and $x_2 \rightarrow +\infty$.

**PROPERTIES OF THE F -MATRIX
IN THE REGION AROUND A WELL
ISOLATED ZERO OR POLE OF $Q^2(z)$**

In this chapter we shall in general not restrict ourselves to the case that the function $Q^2(z)$ is real on the real axis. We shall consider the F -matrix connecting certain points around a well isolated zero or pole of the function $Q^2(z)$. The function $q(z)$, which appears in the definition (3.3) of $w(z)$, will be chosen conveniently for the absolute value of $\exp \{i w(z)\}$ to vary in such a way that we can apply the basic estimates (4.3) to the elements of the above mentioned F -matrix. For the case of a zero or of a simple pole of $Q^2(z)$ it is suitable to choose $q^2(z)$ to be equal to $Q^2(z)$. We shall also treat the case that $Q^2(z)$ has a pole of the second order with a residue that is different from zero and not too small in absolute value. In this case it is convenient to choose for $q^2(z)$ the function which one obtains by omitting in the expression for $Q^2(z)$ the term containing z^{-2} . In all cases to be treated in the present chapter we shall choose the lower limit in the integral (3.3) defining $w(z)$ to be the zero or the pole itself, which implies that $w(z)$ is equal to zero at the zero or pole. From this point there emerge certain diverging lines on which $w(z)$ is purely imaginary and other diverging lines on which $w(z)$ is real. These lines will be called Stokes' lines and anti-Stokes' lines, respectively. This terminology is slightly more general than the one usually used, since it allows for the possibility that the function $q^2(z)$ may be different from the function $Q^2(z)$. Our basic estimates (4.3) show that the F -matrix connecting two points on the same anti-Stokes' line is approximately a unit matrix when the two points both lie so far away from the zero or pole that the μ -integral along the part of the anti-Stokes' line connecting the two points is small compared to 1. It is our purpose in this chapter to derive approximate formulae for the F -matrix connecting two points lying on different anti-Stokes' lines emerging from a zero or pole of $Q^2(z)$.

7.1. Auxiliary formulae

Let us consider two adjacent anti-Stokes' lines emerging from a well isolated zero or simple pole of $q^2(z)$. The function $w(z)$ is real but of opposite sign on these two lines. In the neighbourhood of a zero of the order n of $q^2(z)$ the angle between adjacent anti-Stokes' lines is $2\pi/(n+2)$. From a simple pole of $q^2(z)$ there emerges a single line on which $w(z)$ is real. If the complex z -plane is cut along this line, the function $w(z)$ has opposite signs on the two lips of the cut, and these lips may therefore be considered as two adjacent anti-Stokes' lines separated by an angle of 2π . For the general case of either a zero of any order n of $q^2(z)$ or of a simple pole of $q^2(z)$ we consider two adjacent anti-Stokes' lines, and we let z_ν and $z_{\nu+2}$ be two points on these lines lying so far away from the zero or pole that the points z_ν and $z_{\nu+2}$ can be joined by a curve along which the μ -integral (4.2) is small compared to 1. Since the zero is well isolated a simple calculation indicates that this path can be chosen such that it consists of two parts $z_\nu z_{\nu+1}$ and $z_{\nu+1} z_{\nu+2}$ along each of which the absolute value of $\exp\{i w(z)\}$ is monotonic. On the path $z_\nu z_{\nu+1} z_{\nu+2}$ the absolute value of $\exp\{i w(z)\}$ has either a single minimum or a single maximum, namely at the point $z_{\nu+1}$. Fig. 7.1a and fig. 7.1b show two adjacent anti-Stokes' lines emerging from a zero of $q^2(z)$ of the order $n = 3$. The Stokes' line emerging from the same point into the region between the two anti-Stokes' lines is also drawn. The arrows on the path $z_\nu z_{\nu+1} z_{\nu+2}$ in fig. 7.1a and fig. 7.1b indicate the directions in which the absolute value of $\exp\{i w(z)\}$ increases. As z moves along this path, the absolute value of $\exp\{i w(z)\}$ has at $z_{\nu+1}$ a minimum in fig. 7.1a but a maximum in fig. 7.1b. For the case that $q^2(z)$ has a pole of the first order we have analogously fig. 7.2a and fig. 7.2b, where the heavy line represents two anti-Stokes' lines with infinitesimal separation emerging from the pole and lying on the opposite lips of a cut in the complex z -plane.

For the case shown in fig. 7.1a or fig. 7.2a we combine the two equations corresponding to the 11- and 21-components of the matrix equation

$$F(z_{\nu+2}, z_{\nu+1}) = F(z_{\nu+2}, z_\nu) F(z_\nu, z_{\nu+1})$$

with the condition

$$\det F(z_{\nu+2}, z_\nu) = 1$$

and get the formulae

$$F_{11}(z_{\nu+2}, z_\nu) = \frac{F_{11}(z_{\nu+2}, z_{\nu+1})}{F_{11}(z_\nu, z_{\nu+1})} - \frac{F_{21}(z_\nu, z_{\nu+1})}{F_{11}(z_\nu, z_{\nu+1})} F_{12}(z_{\nu+2}, z_\nu)$$

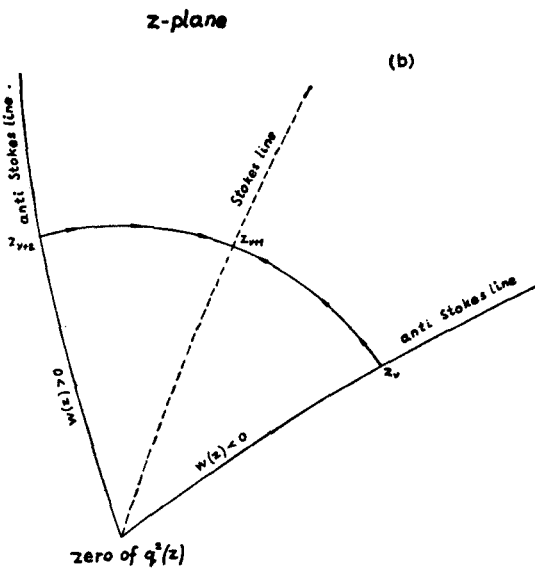
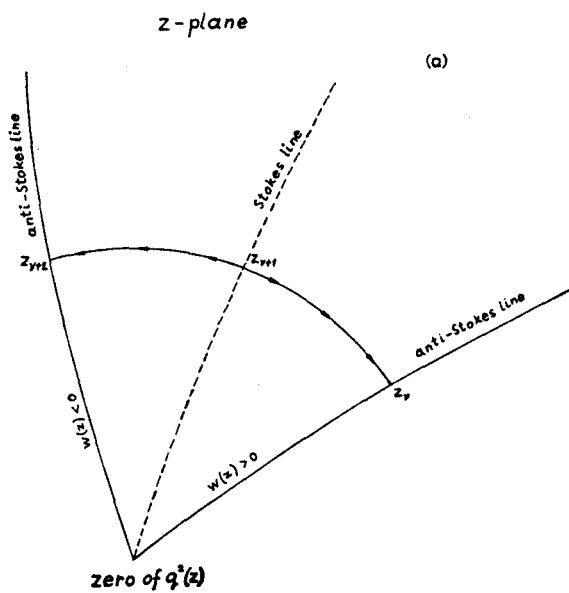


Fig. 7.1

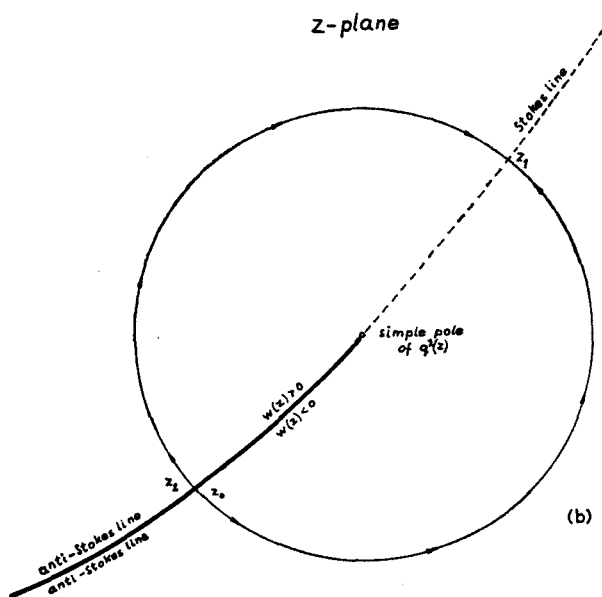
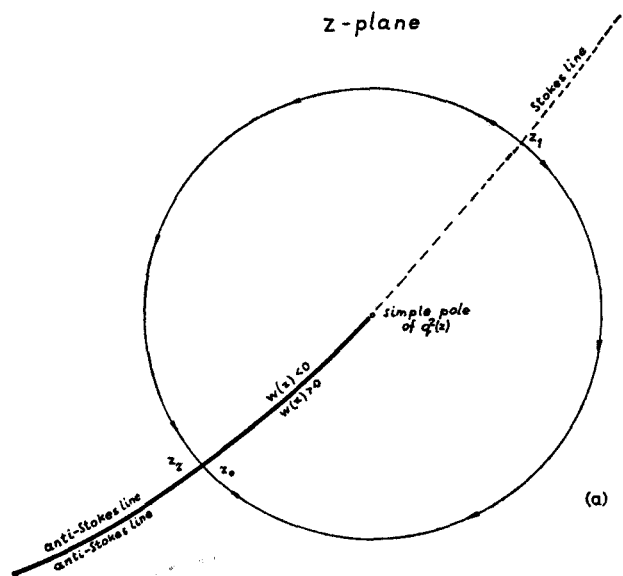


Fig. 7.2

$$F_{22}(z_{\nu+2}, z_{\nu}) = \frac{F_{11}(z_{\nu}, z_{\nu+1})}{F_{11}(z_{\nu+2}, z_{\nu+1})} + \frac{F_{21}(z_{\nu+2}, z_{\nu+1})}{F_{11}(z_{\nu+2}, z_{\nu+1})} F_{12}(z_{\nu+2}, z_{\nu})$$

$$F_{21}(z_{\nu+2}, z_{\nu}) = \frac{F_{21}(z_{\nu+2}, z_{\nu+1})}{F_{11}(z_{\nu}, z_{\nu+1})} - \frac{F_{21}(z_{\nu}, z_{\nu+1})}{F_{11}(z_{\nu+2}, z_{\nu+1})} +$$

$$- \frac{F_{21}(z_{\nu}, z_{\nu+1}) F_{21}(z_{\nu+2}, z_{\nu+1})}{F_{11}(z_{\nu}, z_{\nu+1}) F_{11}(z_{\nu+2}, z_{\nu+1})} F_{12}(z_{\nu+2}, z_{\nu})$$

from which, by means of the basic estimates (4.3) we get

$$F_{11}(z_{\nu+2}, z_{\nu}) = 1 + O(\mu) + O(\mu) F_{12}(z_{\nu+2}, z_{\nu}) \quad (7.1a)$$

$$F_{22}(z_{\nu+2}, z_{\nu}) = 1 + O(\mu) + O(\mu) F_{12}(z_{\nu+2}, z_{\nu}) \quad (7.1b)$$

$$F_{21}(z_{\nu+2}, z_{\nu}) = O(\mu) + O(\mu^2) F_{12}(z_{\nu+2}, z_{\nu}) \quad (7.1c)$$

where μ denotes the μ -integral (4.2) along the path $z_{\nu} z_{\nu+1} z_{\nu+2}$.

For the case shown in fig. 7.1b or fig. 7.2b we combine the two equations corresponding to the 11- and 12-components of the matrix equation

$$F(z_{\nu+1}, z_{\nu}) = F(z_{\nu+1}, z_{\nu+2}) F(z_{\nu+2}, z_{\nu})$$

with the condition

$$\det F(z_{\nu+2}, z_{\nu}) = 1$$

and get the formulae

$$F_{11}(z_{\nu+2}, z_{\nu}) = \frac{F_{11}(z_{\nu+1}, z_{\nu})}{F_{11}(z_{\nu+1}, z_{\nu+2})} - \frac{F_{12}(z_{\nu+1}, z_{\nu+2})}{F_{11}(z_{\nu+1}, z_{\nu+2})} F_{21}(z_{\nu+2}, z_{\nu})$$

$$F_{22}(z_{\nu+2}, z_{\nu}) = \frac{F_{11}(z_{\nu+1}, z_{\nu+2})}{F_{11}(z_{\nu+1}, z_{\nu})} + \frac{F_{12}(z_{\nu+1}, z_{\nu})}{F_{11}(z_{\nu+1}, z_{\nu})} F_{21}(z_{\nu+2}, z_{\nu})$$

$$F_{12}(z_{\nu+2}, z_{\nu}) = \frac{F_{12}(z_{\nu+1}, z_{\nu})}{F_{11}(z_{\nu+1}, z_{\nu+2})} - \frac{F_{12}(z_{\nu+1}, z_{\nu+2})}{F_{11}(z_{\nu+1}, z_{\nu})} +$$

$$- \frac{F_{12}(z_{\nu+1}, z_{\nu}) F_{12}(z_{\nu+1}, z_{\nu+2})}{F_{11}(z_{\nu+1}, z_{\nu}) F_{11}(z_{\nu+1}, z_{\nu+2})} F_{21}(z_{\nu+2}, z_{\nu})$$

from which we get, by means of the estimates (4.3)

$$F_{11}(z_{\nu+2}, z_{\nu}) = 1 + O(\mu) + O(\mu) F_{21}(z_{\nu+2}, z_{\nu}) \quad (7.2a)$$

$$F_{22}(z_{\nu+2}, z_{\nu}) = 1 + O(\mu) + O(\mu) F_{21}(z_{\nu+2}, z_{\nu}) \quad (7.2b)$$

$$F_{12}(z_{\nu+2}, z_{\nu}) = O(\mu) + O(\mu^2) F_{21}(z_{\nu+2}, z_{\nu}). \quad (7.2c)$$

7.2. Properties of the F -matrix in the region around a well isolated zero of the first order for $Q^2(z)$

In this section we shall derive estimates of the F -matrices connecting points on different anti-Stokes' lines emerging from a simple zero of $Q^2(z)$. The matrices will be estimated for the general case that $Q^2(z)$ may be complex even on the real axis and that the zero of $Q^2(z)$ may lie anywhere in the complex plane. With more restricted assumptions, however, the

z -plane

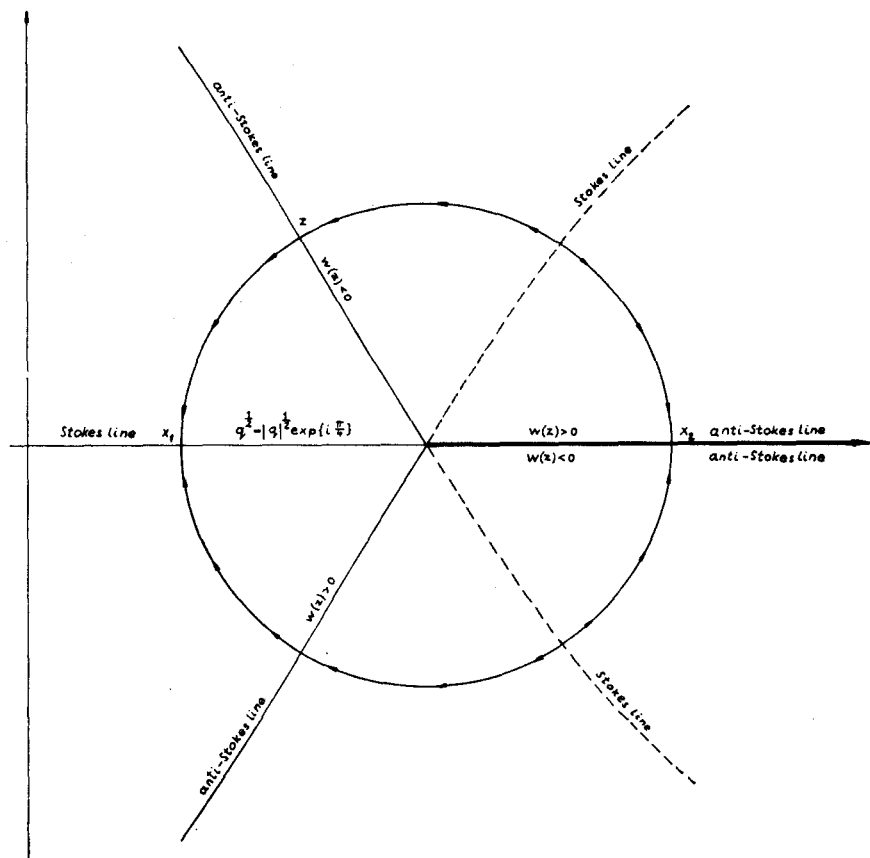


Fig. 7.3

derivation is algebraically simpler. This is the reason why we shall first treat the following important and very frequently arising case separately.

Thus we first assume that the function $Q^2(z)$ is real on the real axis and that there is on this axis a well isolated simple zero of the function $Q^2(z)$. The region to the left of the zero is assumed to be classically forbidden, and the region to the right of the zero is assumed to be classically allowed. We choose $q^2(z)$ to be equal to $Q^2(z)$ and the fixed lower limit in the integral (3.3) defining $w(z)$ to be the zero itself. We cut the complex z -plane along the part of the real axis which lies to the right of the zero as is indicated by the heavy line in fig. 7.3. The choice of phase for $q^{\dagger}(z)$ is also shown in the figure, and three points (x_1 , z , and x_2) are indicated there, x_1 lying on the real axis in the classically forbidden region, z lying on the anti-Stokes' line in the upper half of the complex plane, and x_2 lying on the upper lip of the cut along the real axis in the classically allowed region. We assume that x_1 , z , and x_2 lie sufficiently far from the zero of $Q^2(z)$ for the μ -integral to be small along the path circumscribing the zero through these points as shown in fig. 7.3. The arrows on this path indicate the directions in which the absolute value of $\exp\{i w(z)\}$ increases if the zero is well isolated. It will be recalled that we have given in section 6.3 symmetry relations which can be used here. The choice of phase for $q^{\dagger}(z)$ in fig. 7.3 conforms with that in fig. 6.1b. The notations x_1 and x_2 are also analogous in these two figures. Thus the symmetry relations (6.10a, b) with the upper signs are valid in the present case. Introducing (6.10a) into the equation obtained from the 12-element of the matrix identity

$$F(x_1, z) = F(x_1, x_2) F(x_2, z)$$

and using the estimate (6.13a) for $F_{11}(x_1, x_2)$, the estimate (4.3b) for $F_{12}(x_1, z)$, and the formula (3.20) for the elements of $F(x_2, z)$, we get

$$F_{11}(z, x_2) = O(\mu) - [i + O(\mu)] F_{12}(z, x_2) \quad (7.3)$$

where μ denotes the μ -integral (4.2) along the path $x_1 z x_2$. Using (7.1a, b, c) we obtain expressions for $F_{11}(z, x_2)$, $F_{22}(z, x_2)$, and $F_{21}(z, x_2)$ in terms of $F_{12}(z, x_2)$ and the μ -integral for the path $z x_2$. Combining these formulae with the above formula (7.3) and neglecting terms that are at the most of the order of magnitude of the μ -integral for the path $x_1 z x_2$, we get the approximate formula

$$F(z, x_2) \approx \begin{pmatrix} 1 & i \\ 0 & 1 \end{pmatrix}. \quad (7.4)$$

Matrices connecting points on other pairs of anti-Stokes' lines are derived

analogously. For the explicit expressions we refer to the formulae (7.5) below.

We shall next consider the more general case that the function $Q^2(z)$ need not be real on the real axis and that there is a well isolated simple zero of $Q^2(z)$ lying anywhere in the complex z -plane. As previously we choose $q^2(z)$ to be equal to $Q^2(z)$ and the fixed lower limit in the integral (3.3) defining $w(z)$ to be the zero itself. We cut the complex z -plane along an anti-Stokes' line (the heavy line in fig. 7.4) emerging from the zero consider-

z -plane

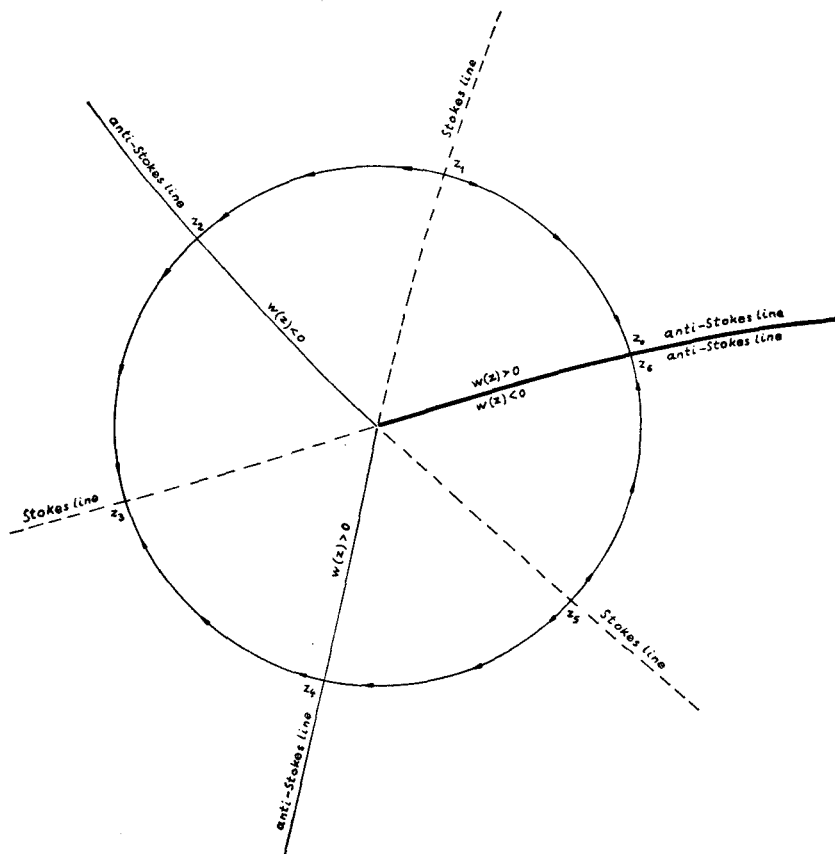


Fig. 7.4

ed, and we assume that the phase of $q(z)$ has been chosen such that the signs of $w(z)$ on the two lips of the heavy line in fig. 7.4, which are two anti-

Stokes' lines with infinitesimal separation, are those indicated in fig. 7.4. The arrows on the path through the points $z_0, z_1, \dots, z_5, z_6$ around the zero indicate the directions in which the absolute value of $\exp\{i w(z)\}$ increases. In the general case which we are now treating there are no symmetry relations to be used. Instead we utilize the fact that any solution of the differential equation (3.1) is one-valued as z moves around a point where $Q^2(z)$ is equal to zero. We have already used this property of the solutions to derive the formula (6.36). Similarly one can obtain an exact formula for $F(z_0, z_6)$. This formula, which one obtains by replacing in (6.36) α by 0, is

$$F(z_0, z_6) = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}.$$

Let us now consider the 11- and 12- elements of the matrix equation

$$F(z_3, z_2) F(z_2, z_0) F(z_0, z_6) = F(z_3, z_4) F(z_4, z_6).$$

For the elements of the matrices $F(z_2, z_0)$ and $F(z_4, z_6)$ we use the formulae (7.1a, b, c) and (3.20), and for the elements of the matrix $F(z_0, z_6)$ we use the above formula. Furthermore, the basic estimates (4.3) apply to $F(z_3, z_2)$ and $F(z_3, z_4)$. From the above matrix equation one can thus determine $F_{12}(z_2, z_0)$ and $F_{12}(z_6, z_4)$. Similarly one can also determine the previously considered element $F_{12}(z_2, z_0)$ and the element $F_{21}(z_4, z_2)$ from the 11- and 21-elements of the matrix equation

$$F(z_2, z_0) F(z_0, z_6) F(z_6, z_5) = F(z_2, z_4) F(z_4, z_5).$$

The final result is the approximate formulae

$$F(z_2, z_0) \approx \begin{pmatrix} 1 & i \\ 0 & 1 \end{pmatrix} \quad (7.5a)$$

$$F(z_4, z_2) \approx \begin{pmatrix} 1 & 0 \\ i & 1 \end{pmatrix} \quad (7.5b)$$

$$F(z_6, z_4) \approx \begin{pmatrix} 1 & i \\ 0 & 1 \end{pmatrix} \quad (7.5c)$$

where we have neglected terms of at the most the order of magnitude of the μ -integral for the whole path from z_0 to z_6 around the zero of $Q^2(z)$.

Finally we remark that the elements of the matrix $F(z_3, z_0)$ can be estimated by means of the matrix equation

$$F(z_3, z_0) = F(z_3, z_2) F(z_2, z_0),$$

the approximate formula (7.5a) for $F(z_2, z_0)$, and the basic estimates (4.3) for $F(z_3, z_2)$. It is found that $F_{11}(z_3, z_0) \approx 1$ and $F_{12}(z_3, z_0) \approx i$, whereas the values of $F_{21}(z_3, z_0)$ and $F_{22}(z_3, z_0)$ cannot be determined within the JWKB-approximation. We recall the corresponding result obtained in section 6.3 for the special case that the function $Q^2(z)$ is real on the real axis and that the zero of $Q^2(z)$ lies on this axis. Compare especially the estimates (6.13a, b) and the symmetry relations (6.10a, b).

7.3. Properties of the F -matrix in the region around a well isolated zero of the order n for $Q^2(z)$

We shall first give an exact formula for the F -matrix connecting any point z with the corresponding point z' lying on the next sheet of the Riemann surface and obtained by moving z in the positive sense along a path encircling a well isolated zero of the order n for the function $Q^2(z)$. This function need not be real on the real axis, and the zero may lie anywhere in the complex z -plane. We choose the function $q^2(z)$ to be equal to $Q^2(z)$ and the fixed lower limit in the integral (3.3) defining $w(z)$ to be the zero itself. Since for the differential equation (3.1) any solution $\psi(z)$ as well as its derivative $\psi'(z)$ is single-valued as z moves in a loop around a zero of any order for the function $Q^2(z)$, one finds by means of (3.39), (3.28), (3.29), (3.24a, b), and (3.3) that

$$F(z', z) = \begin{pmatrix} i^n & 0 \\ 0 & i^n \end{pmatrix} \quad \text{if } n \text{ is even} \quad (7.6a)$$

$$F(z', z) = \begin{pmatrix} 0 & i^n \\ i^n & 0 \end{pmatrix} \quad \text{if } n \text{ is odd.} \quad (7.6b)$$

These formulae are exactly valid, independent of the value of z . We have already in chapter 6 and also previously in the present chapter obtained essentially the inverse of the matrix (7.6b) for the special case of a simple zero, i.e. for $n = 1$.

We shall now for a while specialize our treatment and consider the case that

$$Q^2(z) = A z^n \quad (7.7)$$

where n is a positive integer and A is a complex constant. For this function $Q^2(z)$ the differential equation (3.1) is invariant for the transformation $z \rightarrow z \exp \{2\pi i/(n+2)\}$ and therefore it is natural that the angle $2\pi/(n+2)$

shall play an important rôle in the following considerations. We choose the function $q^2(z)$ to be equal to $Q^2(z)$ and $w(z)$ to be equal to zero at the origin. For the present treatment it is convenient to assume that we have available the whole Riemann surface on which $q^{\dagger}(z)$ is a one-valued function.

We shall first consider the F -matrix connecting any two points z_0 and z joined by a path which does not pass through the origin. We rotate the points z_0 and z as well as the path joining these two points through an angle $2\pi/(n+2)$ in the positive sense around the origin. Using (3.22a, b, c, d) and the formulae

$$w\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}\right) = -w(z)$$

$$\varepsilon\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}\right) = \varepsilon(z)$$

which are obtained from (3.3), (3.5), and (7.7), we find that

$$F_{11}\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}, z_0 \exp\left\{\frac{2\pi i}{n+2}\right\}\right) = F_{22}(z, z_0) \quad (7.8a)$$

$$F_{22}\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}, z_0 \exp\left\{\frac{2\pi i}{n+2}\right\}\right) = F_{11}(z, z_0) \quad (7.8b)$$

$$F_{12}\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}, z_0 \exp\left\{\frac{2\pi i}{n+2}\right\}\right) = F_{21}(z, z_0) \quad (7.8c)$$

$$F_{21}\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}, z_0 \exp\left\{\frac{2\pi i}{n+2}\right\}\right) = F_{12}(z, z_0). \quad (7.8d)$$

Repeated application of these formulae gives

$$F\left(z \exp\left\{\frac{4\pi i}{n+2}\right\}, z_0 \exp\left\{\frac{4\pi i}{n+2}\right\}\right) = F(z, z_0). \quad (7.9)$$

The formulae (7.8) and (7.9) give an important piece of information on the F -matrix for the present case.

Assuming still $Q^2(z)$ to be given by the special formula (7.7) and $q(z)$ as well as $w(z)$ to be defined in the same way as previously, we shall next consider the matrix $F(z \exp\{2\pi i/(n+2)\}, z)$, where $z (\neq 0)$ is any point on the Riemann surface. By considering the power series expansion of the solution of the differential equation (3.1) in the neighbourhood of the origin

one easily finds that there exists a special solution $\psi(z)$ of the differential equation (3.1) such that

$$\psi\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}\right) = \exp\{i\alpha\} \psi(z)$$

$$\psi'\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}\right) = \exp\left\{i\left(\alpha - \frac{2\pi}{n+2}\right)\right\} \psi'(z)$$

where α is a constant. There is one solution $\psi(z)$ for which $\alpha = 0$ and another for which $\alpha = 2\pi/(n+2)$. According to (3.25a, b) the above formulae for ψ and ψ' can be written as follows

$$f\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}\right) a\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}\right) = \exp\{i\alpha\} f(z) a(z)$$

$$f'\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}\right) a\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}\right) = \exp\left\{i\left(\alpha - \frac{2\pi}{n+2}\right)\right\} f'(z) a(z).$$

Introducing into these equations the expressions

$$f\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}\right) = -i \exp\left\{\frac{\pi i}{n+2}\right\} f(z) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$f'\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}\right) = -i \exp\left\{-\frac{\pi i}{n+2}\right\} f'(z) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which follow from the definitions (3.24a, b) of f_1 and f_2 , and remembering the definition (3.29) of the matrix $W_f(z)$, we arrive at the equation

$$W_f(z) \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} a\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}\right) - i \exp\left\{i\left(\alpha - \frac{\pi}{n+2}\right)\right\} a(z) \right] = 0$$

from which we easily obtain the relation

$$a\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}\right) = i \exp\left\{i\left(\alpha - \frac{\pi}{n+2}\right)\right\} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} a(z).$$

Rewriting the left-hand side of this formula by means of (3.26), we get

$$\left[F\left(z \exp\left\{\frac{2\pi i}{n+2}\right\}, z\right) - i \exp\left\{i\left(\alpha - \frac{\pi}{n+2}\right)\right\} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right] a(z) = 0.$$

The quantities $a_1(z)$ and $a_2(z)$ cannot be zero simultaneously at any point z , since according to (3.26) this would imply that $a_1(z)$ and $a_2(z)$ were both identically equal to zero, which in turn would imply that the special solution $\psi(z)$ considered were also identically equal to zero, contrary to our previous assumptions. The determinant of the above system of linear and homogeneous

equations for $a_1(z)$ and $a_2(z)$ must therefore be equal to zero, i.e.

$$\det \left[F \left(z \exp \left\{ \frac{2\pi i}{n+2} \right\}, z \right) - i \exp \left\{ i \left(\alpha - \frac{\pi}{n+2} \right) \right\} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right] = 0.$$

Combining this equation with the formula

$$\det F \left(z \exp \left\{ \frac{2\pi i}{n+2} \right\}, z \right) = 1$$

we easily get

$$F_{12} \left(z \exp \left\{ \frac{2\pi i}{n+2} \right\}, z \right) + F_{21} \left(z \exp \left\{ \frac{2\pi i}{n+2} \right\}, z \right) = 2i \cos \left(\alpha - \frac{\pi}{n+2} \right).$$

Substituting here either of the two possible values of α , i.e. either $\alpha = 0$ or $\alpha = 2\pi/(n+2)$, we get

$$F_{12} \left(z \exp \left\{ \frac{2\pi i}{n+2} \right\}, z \right) + F_{21} \left(z \exp \left\{ \frac{2\pi i}{n+2} \right\}, z \right) = 2i \cos \frac{\pi}{n+2}. \quad (7.10)$$

As this is an exact relation for the case when $q^2(z) = Q^2(z)$ is given by (7.7), it remains valid also in the neighbourhood of the origin, although the μ -integral for the path from z to $z \exp\{2\pi i/(n+2)\}$ is then large.

In the relation (7.10) the point z is allowed to be an arbitrary point. Let us, however, now assume that z lies on one of the anti-Stokes' lines emerging from the origin. The point $z \exp\{2\pi i/(n+2)\}$ is then on an adjacent anti-Stokes' line, and the formulae (7.1a, b, c) or (7.2a, b, c), depending on whether $w(z)$ is positive or negative, apply to the matrix $F(z \exp\{2\pi i/(n+2)\}, z)$. Combining these formulae with the relation (7.10) and omitting the error terms $O(\mu)$, we obtain the following approximate formulae

$$F \left(z \exp \left\{ \frac{2\pi i}{n+2} \right\}, z \right) \approx \begin{pmatrix} 1 & 2i \cos \frac{\pi}{n+2} \\ 0 & 1 \end{pmatrix} \quad (7.11a)$$

$$F \left(z \exp \left\{ \frac{2\pi i}{n+2} \right\}, z \right) \approx \begin{pmatrix} 1 & 0 \\ 2i \cos \frac{\pi}{n+2} & 1 \end{pmatrix} \quad (7.11b)$$

which apply if $w(z)$ is positive or negative, respectively. Since there are no zeros or singularities of $Q^2(z)$ in the complex plane, we can let the absolute value of z tend to infinity. The μ -integral then tends to zero and consequently the formulae (7.11a, b) tend to exactness as $|z| \rightarrow \infty$.

Let us now consider the more general case when $Q^2(z)$ has not the simple form (7.7) but has still a well isolated zero of the order n . The relation (7.10) is then no longer exactly valid but can be used approximately in a certain region in the neighbourhood of the zero considered. We shall assume that this region extends so far out from the zero that it contains a closed curve around the zero with a μ -integral much smaller than 1. The points where this closed curve crosses the anti-Stokes' lines emerging from the zero are denoted by $z_0, z_2, \dots, z_{2n}, z_{2(n+1)},$ and $z_{2(n+2)}$. This last point is the point corresponding to z_0 but lying on the next Riemann sheet. See fig. 7.4 where the case $n = 1$ is illustrated. The basic estimates (4.3) show that the matrix $F(z_{\nu+2}, z_\nu)$ is approximately independent of the positions of the points z_ν and $z_{\nu+2}$ on their respective anti-Stokes' lines, provided these points do not move too close to the zero. According to (7.10) we then have the approximate relation

$$F_{12}(z_{\nu+2}, z_\nu) + F_{21}(z_{\nu+2}, z_\nu) \approx 2i \cos \frac{\pi}{n+2}. \quad (7.12)$$

We emphasize that this formula cannot represent a good approximation unless the zero lies sufficiently well isolated. The presence of another zero or a singularity of $Q^2(z)$ close to the zero considered introduces considerable changes in the formula (7.12). Combining (7.12) with (7.1a - c) or (7.2a - c), we find the approximate formulae

$$F(z_{\nu+2}, z_\nu) \approx \begin{pmatrix} 1 & 2i \cos \frac{\pi}{n+2} \\ 0 & 1 \end{pmatrix} \quad (7.13a)$$

$$F(z_\nu, z_{\nu+2}) \approx \begin{pmatrix} 1 & 0 \\ 2i \cos \frac{\pi}{n+2} & 1 \end{pmatrix} \quad (7.13b)$$

which apply if $w(z_\nu)$ is positive or negative, respectively. The formulae (7.13a, b) agree with (7.11a, b). We notice, however, that the derivation

of (7.11a, b) is rigorous and allows us to determine definite limits of error, whereas in the derivation of (7.13a, b) we utilize the approximate formula (7.12) in which the error has not been estimated. The important case $n = 1$ has been rigorously treated in the previous section, and the reader is referred to the derivations of (7.4) and (7.5a, b, c) for this case.

The results obtained in the present and the previous section together with the basic estimates (4.3) clearly show the appearance of the Stokes' phenomenon in the region around a well isolated zero of $Q^2(z)$.

7.4. Properties of the F -matrix in the region around a well isolated pole of the first or second order for $Q^2(z)$

In this section we shall assume that inside a certain region around the origin the function $Q^2(z)$ is given by the formula

$$Q^2(z) = -\frac{l(l+1)}{z^2} + \frac{B}{z} + \sum_{\nu=0}^{\infty} b_{\nu} z^{\nu} \quad (7.14)$$

where $l, B, b_0, b_1, b_2, \dots$ are constants. The number l , which may also be zero, will later, namely in the applications in chapter 11, be restricted to non negative integers, but for the moment we shall only assume that $2l+1$ is not a negative integer. For estimating the elements of the F -matrix it is important to know how the absolute value of $\exp\{i\omega(z)\}$ varies. In order to obtain a convenient qualitative behaviour of $|\exp\{i\omega(z)\}|$ in the region around the pole we shall choose

$$q^2(z) = Q^2(z) + \frac{l(l+1)}{z^2} = \frac{B}{z} + \sum_{\nu=0}^{\infty} b_{\nu} z^{\nu} \quad (7.15)$$

and we shall assume that the absolute value of the constant B is large enough that a closed curve exists, encircling the pole, for which the μ -integral is small compared to 1 although the curve runs in the region where the behaviour of the function $q^2(z)$ is still determined by the term B/z in (7.15). The convenience of this assumption is apparent from the fact that, if $q^2(z) = B/z$, the μ -integral for a circle with its centre at the origin and its radius equal to $|z|$ is inversely proportional to $|Bz|^{\frac{1}{2}}$. We choose the fixed lower limit in the integral (3.3) defining $w(z)$ to be the pole itself. From the pole there then emerges a single curve on which $w(z)$ is real. If the complex z -plane is cut along this line, the two lips of the cut form two anti-Stokes'

lines, as has been mentioned in section 7.1. On the above mentioned closed curve ($z_0 z_1 z_2$ in fig. 7.2a and fig. 7.2b) encircling the pole, the absolute value of the function $\exp\{i w(z)\}$ has either a single minimum or a single maximum depending on the choice of the phase of $q(z)$, and therefore on the signs of $w(z)$ along the two anti-Stokes' lines emerging from the pole. See fig. 7.2a and fig. 7.2b, where the arrows on the loop around the pole indicate the directions in which the absolute value of $\exp\{i w(z)\}$ increases. We can therefore use the formulae (7.1a, b, c) or (7.2a, b, c) for expressing the matrix $F(z_2, z_0)$ in terms of one of its elements. For obtaining approximate expressions for all of the elements of the matrix $F(z_2, z_0)$ we need a further relation between the elements of this matrix. To this purpose we shall derive an exact and very general relation, which is analogous to (7.10). It applies to the matrix $F(z', z)$, where z is any point in the complex plane and z' is the point arrived at after moving from z in the positive sense along a loop crossing no cut and enclosing the origin but no other pole or zero of $q^2(z)$. The points z and z' thus lie infinitesimally near each other but on opposite sides of a cut emerging from the pole or in other words, on two successive Riemann sheets.

When $Q^2(z)$ is given by (7.14) and $2l + 1$ is not a negative integer, there exists a special solution $\psi(z)$ of the differential equation (3.1) which for small values of $|z|$ behaves as a constant times z^{l+1} . For this special solution $\psi(z)$ we obviously have

$$\psi(z') = \exp\{2\pi i l\} \psi(z)$$

$$\psi'(z') = \exp\{2\pi i l\} \psi'(z).$$

According to (3.25a, b) these relations give

$$f(z') a(z') = \exp\{2\pi i l\} f(z) a(z)$$

$$f'(z') a(z') = \exp\{2\pi i l\} f'(z) a(z).$$

With $q^2(z)$ given by (7.15), one finds from the definition (3.3) of w and the definitions (3.24a, b) of f_1 and f_2 the following formulae

$$f(z') = i f(z) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$f'(z') = i f'(z) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

which apply if $B \neq 0$ and $w(0) = 0$. From the last four equations and the

definition (3.29) of the matrix $W_f(z)$ we get the formula

$$W_f(z) \left\{ i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathbf{a}(z') - \exp\{2\pi i l\} \mathbf{a}(z) \right\} = 0$$

which immediately gives

$$\mathbf{a}(z') = -i \exp\{2\pi i l\} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathbf{a}(z). \quad (7.16)$$

Rewriting the left-hand side of this formula by means of (3.26), we get

$$\left\{ \mathbf{F}(z', z) - i \exp\{(2l+1)\pi i\} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\} \mathbf{a}(z) = 0. \quad (7.17)$$

The functions $a_1(z)$ and $a_2(z)$ cannot be equal to zero simultaneously, for according to (3.26) this would imply that they were identically equal to zero, which is contradictory to the assumption that $\psi(z)$ shall not be identically equal to zero. Thus it follows from (7.17) that

$$\det \left\{ \mathbf{F}(z', z) - i \exp\{(2l+1)\pi i\} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\} = 0.$$

Combining this formula with the condition that the determinant of the matrix $\mathbf{F}(z', z)$ is equal to 1, we get

$$F_{12}(z', z) + F_{21}(z', z) = 2i \cos[(2l+1)\pi]. \quad (7.18)$$

This is an exact and general relation which is valid wherever z lies, if only $q^2(z)$ is chosen according to (7.15) and $B \neq 0$, $w(0) = 0$, and if one does not cross any cut in the complex z -plane as one moves around the origin from z to z' along a curve encircling no other pole or zero of $q^2(z)$.

We shall now assume that the points z and z' lie on the anti-Stokes' lines just as the points z_0 and z_2 , respectively, in fig. 7.2a and 7.2b.

Combining (7.18) with (7.1a, b, c) we then get

$$\mathbf{F}(z', z) \approx \begin{pmatrix} 1 & 2i \cos[(2l+1)\pi] \\ 0 & 1 \end{pmatrix} \quad (7.19a)$$

for the case in fig. 7.2a, and combining (7.18) with (7.2a, b, c), we get

$$\mathbf{F}(z', z) \approx \begin{pmatrix} 1 & 0 \\ 2i \cos[(2l+1)\pi] & 1 \end{pmatrix} \quad (7.19b)$$

for the case in fig. 7.2b. In the approximate formulae (7.19a, b) we have left out terms which (if the number l is real) are at the most of the order of the μ -integral (4.2) along the loop connecting the points z and z' .

Substituting (7.19a) or (7.19b), respectively, into (7.17), we obtain

$$\frac{a_1(z)}{a_2(z)} \approx \exp\{-2\pi i \sigma(l + \frac{1}{2})\} \quad (7.20)$$

where

$$\sigma = \begin{cases} +1 & \text{for the case in fig. 7.2a} \\ -1 & \text{for the case in fig. 7.2b.} \end{cases} \quad (7.21)$$

Substituting (3.24a, b) and (7.20) into (3.25a), and remembering that $a_1(z)$ and $a_2(z)$ are approximately constant when z lies on the anti-Stokes' line considered and not too close to the pole, we find that

$$\psi(z) \approx \text{const. } q(z)^{-\frac{1}{2}} \cos[w(z) - \sigma(l + \frac{1}{2})\pi]. \quad (7.22)$$

In order to obtain also the value of the constant factor on the right-hand side of this formula, when the power series expansion of $\psi(z)$ is known for small values of $|z|$, we can proceed as follows.

Another solution of the differential equation (3.1) is

$$\bar{\psi}(z) = \psi(z) \int^z [\psi(z')]^{-2} dz'. \quad (7.23)$$

The solutions $\psi(z)$ and $\bar{\psi}(z)$ are linearly independent since

$$\det W_\psi = \begin{vmatrix} \psi(z) & \psi'(z) \\ \bar{\psi}(z) & \bar{\psi}'(z) \end{vmatrix} = 1. \quad (7.24)$$

The difference between the two roots of the indicial equation is $2l+1$, and thus the behaviour of $\bar{\psi}(z)$ as one moves around the pole from z to z' (which need no longer lie on the anti-Stokes' lines) depends upon whether $2l+1$ is an integer or not. If, in the latter case, the fixed lower limit of the integral in (7.23) is chosen conveniently, both cases are covered by the formulae

$$\begin{aligned} \bar{\psi}(z') &= \exp\{-2\pi il\} \{\bar{\psi}(z) + 2\pi ic \psi(z)\} \\ \bar{\psi}'(z') &= \exp\{-2\pi il\} \{\bar{\psi}'(z) + 2\pi ic \psi'(z)\} \end{aligned}$$

where c is a certain constant. If $2l+1$ is not an integer, c is equal to zero. If, however, $2l+1$ is an integer, c is the residue of the function $[\psi(z)]^{-2}$ at the origin and is thus determined by the power series expansion of $\psi(z)$ for small values of $|z|$. In exceptional cases c may be equal to zero also when $2l+1$ is an integer. For the special case that $l=0$ the constant c is equal to B if $\psi(z)$ is normalized such that $\psi(z)/z \rightarrow 1$ as $z \rightarrow 0$. The a -coefficients corresponding to the function $\bar{\psi}(z)$ are denoted by $\bar{a}_1(z)$ and $\bar{a}_2(z)$. In a

similar way as we have derived the formula (7.16) we obtain

$$\bar{a}(z') = -i \exp\{-2\pi i l\} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} [\bar{a}(z) + 2\pi i c a(z)]. \quad (7.25)$$

Introducing (7.16) and (7.25) into the definition (3.30) of $A(z')$, we can express $A(z')$ in terms of $a(z)$ and $\bar{a}(z)$. Using (3.30), (3.36), and (7.24), we can also express $A^{-1}(z)$ in terms of $a(z)$ and $\bar{a}(z)$. Because of the formula (3.38) we can then express also $F(z', z)$ in terms of $a(z)$ and $\bar{a}(z)$. We shall consider only the case when $2l+1$ is an integer. In this special but important case the resulting formula for the matrix $F(z', z)$ can be simplified by means of (3.36) and (7.24) with the result that the elements of $F(z', z)$ do not depend on $\bar{a}_1(z)$ and $\bar{a}_2(z)$ but only on $a_1(z)$ and $a_2(z)$. The formulae thus obtained when $2l+1$ is an integer are

$$F_{11}(z', z) = -4\pi i c (-1)^{2l+1} [a_2(z)]^2 \quad (7.26a)$$

$$F_{22}(z', z) = 4\pi i c (-1)^{2l+1} [a_1(z)]^2 \quad (7.26b)$$

$$F_{12}(z', z) = (-1)^{2l+1} \{i + 4\pi i c a_1(z) a_2(z)\} \quad (7.26c)$$

$$F_{21}(z', z) = (-1)^{2l+1} \{i - 4\pi i c a_1(z) a_2(z)\}. \quad (7.26d)$$

We emphasize that the a -coefficients appearing in these formulae refer to a special solution $\psi(z)$ which behaves as a constant times z^{l+1} in the neighbourhood of the pole. We also see that for the special case that $2l+1$ is an integer we can obtain the formula (7.18) as a consequence of (7.26c, d). Let us now assume that $c \neq 0$. From (7.26a, b, c, d) it is then easily seen that the elements of the matrix $F(z', z)$ in general vary rapidly with z except when z lies on the line where $w(z)$ is real, for, unless this is the case, $a_1(z)$ or $a_2(z)$ in general varies rapidly with z . Assuming z and z' to lie on this line, and comparing the formulae (7.26a, b, c, d) with the approximate formulae (7.19a) and (7.19b), respectively, we find that

$$a_1(z) \approx \frac{1}{2}(\sigma\pi c)^{-\frac{1}{2}} \exp\{-i\sigma(l + \frac{3}{4})\pi\} \quad (7.27a)$$

$$a_2(z) \approx \frac{1}{2}(\sigma\pi c)^{-\frac{1}{2}} \exp\{+i\sigma(l + \frac{3}{4})\pi\} \quad (7.27b)$$

where σ is still defined by (7.21). The sign of $(\sigma\pi c)^{-\frac{1}{2}}$ shall be the same in (7.27a) and in (7.27b). This sign depends on the sign of $\psi(z)$. Substituting the formulae (3.24a, b) and (7.27a, b) into (3.25a), we find that on the anti-Stokes' line and sufficiently far away from the pole at the origin,

the function $\psi(z)$ is given by the following approximate formula

$$\psi(z) \approx (\sigma \pi c)^{-\frac{1}{2}} q(z)^{-\frac{1}{2}} \cos[w(z) - \sigma(l + \frac{3}{4})\pi]. \quad (7.28)$$

We recall the definition of c as the residue of $[\psi(z)]^{-2}$ at $z = 0$, and we emphasize again that the formula (7.28) applies to the case when $2l + 1$ is an integer and to the special solution $\psi(z)$ which behaves as a constant times z^{l+1} for sufficiently small values of $|z|$. Furthermore, we have assumed that the constant B is fairly large and that $w(0) = 0$. Knowing $\psi(z)$ for small values of $|z|$, we can, except for the sign, obtain $\psi(z)$ on the "left lip" of the cut in fig. 7.2a or fig. 7.2b sufficiently far away from the origin by means of the approximate formula (7.28). This formula will be used in chapter 11.

THE WAVE FUNCTION IN A REGION OF THE REAL AXIS WHERE THERE IS AT THE MOST ONE CLASSICAL TURNING POINT

Also in this chapter we shall allow $q^2(z)$ to be different from $Q^2(z)$, but for simplicity we shall use the concepts "classically allowed region", "classically forbidden region", and "classical turning point" in their generalized sense as introduced in the beginning of chapter 6, without stating this explicitly. Furthermore, when speaking of a classical turning point, we shall in the present chapter exclude the possibility of a multiple root of the equation $q^2(z) = 0$ at the point considered.

8.1. Estimate of the accuracy of the JWKB-approximation in a classically allowed region

We shall now consider the special case that the whole interval (x_0, x) as well as the fixed lower limit in the integral (3.3) defining $w(x)$ belongs to a region of the real axis which is classically allowed in the generalized sense. It is not an essential restriction to consider only real wave functions $\psi(x)$, which according to (3.35a, b) and (3.24a, b) means that the quantities $a_1(x)$ and $a_2(x)$ are complex conjugate, provided $q(x)^{-\frac{1}{2}}$ is chosen to be real. Using a convenient normalization we can then write

$$a_1(x_0) = \frac{1}{2} \exp\{i\gamma_0\} \quad (8.1a)$$

$$a_2(x_0) = \frac{1}{2} \exp\{-i\gamma_0\} \quad (8.1b)$$

where γ_0 is a real number. Introducing these relations into the formula $\psi(x_0) = f(x_0) \mathbf{a}(x_0)$ and noting that $f(x_0)$ is given by (3.23) and (3.24a, b), we get

$$\psi(x_0) = q(x_0)^{-\frac{1}{2}} \cos[w(x_0) + \gamma_0]. \quad (8.2)$$

Proceeding similarly as above, remembering that $\mathbf{a}(x) = \mathbf{F}(x, x_0) \mathbf{a}(x_0)$, and using the symmetry relations (6.1a, b), we obtain for $\psi(x)$ the expression

$$\psi(x) = A(x) q(x)^{-\frac{1}{2}} \cos[w(x) + \gamma(x)] \quad (8.3)$$

where the positive function $A(x)$ and the real function $\gamma(x)$ are defined by

$$A(x) \exp\{i\gamma(x)\} = F_{11}(x, x_0) \exp\{i\gamma_0\} + F_{12}(x, x_0) \exp\{-i\gamma_0\}. \quad (8.4)$$

From this formula, the symmetry relation (6.1b), and the estimates (6.3a, b) we get

$$\begin{aligned} |A - 1| &\leq |A \exp\{i(\gamma - \gamma_0)\} - 1| = \\ &= |F_{11}(x, x_0) - 1 + F_{12}(x, x_0) \exp\{-2i\gamma_0\}| \leq \exp\{\mu\} - 1 \end{aligned} \quad (8.5a)$$

$$\begin{aligned} |\sin(\gamma - \gamma_0)| &= A^{-1} |\operatorname{Im}\{F_{11}(x, x_0) + F_{12}(x, x_0) \exp\{-2i\gamma_0\}\}| \leq \\ &\leq A^{-1} [\exp\{\mu\} - 1]. \end{aligned} \quad (8.5b)$$

If $\mu \ll 1$ we thus have $A \approx 1$ and $\gamma(x) \approx \gamma_0$, and from (8.3) we obtain the usual JWKB-approximation for $\psi(x)$. From the above estimates we realize that the error in the amplitude as well as in the phase of this approximate wave function is at the most of the order of magnitude μ if $\mu \ll 1$

8.2. Estimate of the accuracy of the JWKB-approximation in a classically forbidden region

We shall next consider the special case that the whole interval (x_0, x) of the real axis belongs to a region which is classically forbidden in the generalized sense, and we shall choose x_0 as the fixed lower limit in the integral (3.3) defining $w(x)$. If the real quantity $iw(x)$ is increasing from x_0 to x we can according to (3.41) write the wave function as follows

$$\begin{aligned} \psi(x) &= a_1(x_0) q(x)^{-\frac{1}{2}} \exp\{|w(x)\}| [1 + \eta_1(x)] + \\ &\quad + a_2(x_0) q(x)^{-\frac{1}{2}} \exp\{-|w(x)\}| [1 + \eta_2(x)] \end{aligned} \quad (8.6)$$

where the symbols $\eta_1(x)$ and $\eta_2(x)$ are introduced to simplify the writing, their definitions being obvious from (3.41). According to (6.9a, b) we have

$$|\eta_1(x)| \leq \exp\{\frac{1}{2}\mu\} - 1 \quad (8.7a)$$

$$|\eta_2(x)| \leq [\exp\{\frac{1}{2}\mu\} - 1] \exp\{2|w(x)|\} \quad (8.7b)$$

μ being the μ -integral from x_0 to x along the real axis. We recall the fact that the two terms with the coefficients $a_1(x_0)$ and $a_2(x_0)$ in the formula (8.6) for $\psi(x)$ represent two linearly independent solutions of the differential equation (3.1). As long as $\mu \ll 1$ the first term in (8.6) with $\eta_1(x)$ neglected is,

according to (8.7a), an approximate solution of the wave equation. The second term in (8.6) with $\eta_2(x)$ neglected does not in general have this property, since according to (8.7b) the absolute value of $\eta_2(x)$ may increase very rapidly as x moves away from x_0 , i.e., as $|w(x)|$ increases rapidly.

In a classically forbidden region it is interesting and important to know whether the decreasing term of the JWKB-approximation is really significant although the increasing term is also present. According to (8.6) the error in the decreasing term of the JWKB-approximation is negligible if

$$|\eta_2(x)| \ll 1.$$

According to (8.7b) this condition is fulfilled if

$$[\exp\{\frac{1}{2}\mu\} - 1] \exp\{2|w(x)|\} \ll 1. \quad (8.8a)$$

From (8.6) we next find that the error in the increasing term of the JWKB-approximation is small compared to the decreasing term if

$$|a_1(x_0)| \exp\{|w(x)|\} |\eta_1(x)| \ll |a_2(x_0)| \exp\{-|w(x)|\}.$$

According to (8.7a) this condition is fulfilled if

$$[\exp\{\frac{1}{2}\mu\} - 1] \exp\{2|w(x)|\} \ll \left| \frac{a_2(x_0)}{a_1(x_0)} \right|. \quad (8.8b)$$

Thus, in an interval (x_0, x) of a classically forbidden region where the conditions (8.8a) and (8.8b) are both fulfilled, one can be sure that the decreasing term in the JWKB-approximation is significant.

For any choice of the fixed lower limit in the integral (3.3) defining $w(x)$ there are sufficient conditions analogous to (8.8a, b) for the significance of both terms in the JWKB-approximation. From these conditions we can draw the following conclusions. Suppose that in a classically forbidden region the JWKB-approximation has been fitted to an exact wave function at a given point x_0 and that both terms of the JWKB-approximation are of a similar order of magnitude at this point. If x moves from x_0 in one direction, both terms of the JWKB-approximation are first of similar order of magnitude, and as long as this is the case and $\mu \ll 1$, both terms are significant, but as soon as one of the terms becomes small enough compared to the other term, only the larger term is significant. The corresponding assertion is true if x moves from x_0 in the other direction, but then the rôle of the terms is interchanged, because the term that is large on one side of x_0 is small on the other side.

8.3. The connection formulae for the JWKB-approximations of the same wave function on opposite sides of a classical turning point

Since we have already in chapter 6 estimated the elements of the F -matrix connecting two points on the real axis and lying on opposite sides of a generalized classical turning point, it is now an easy and quite straightforward procedure to derive approximate connection formulae for the wave function $\psi(x)$ as well as upper bounds for the errors involved. The turning point is denoted by x' , and this point is chosen as the fixed lower limit in the integral (3.3) defining $w(z)$. We cut the z -plane along the real axis and consider only the real axis and the upper half of the z -plane, choosing the phase of $q(z)^\dagger$ as shown in fig. 6.1b or in fig. 6.2b. We shall treat the two cases illustrated in these two figures simultaneously, letting the upper signs refer to the case in fig. 6.1 and the lower signs to the case in fig. 6.2.

We shall first assume that we know the wave function $\psi(x)$ and its derivative at a point x_2 in the classically allowed region, and we want to determine the value of the same wave function at a point x_1 in the classically forbidden region. Writing

$$a_1(x_2) = [\tfrac{1}{2}(A+B) \pm \tfrac{1}{2}(A-B)] \exp\{\pm \tfrac{1}{4}i\pi\} \quad (8.9a)$$

$$a_2(x_2) = [\tfrac{1}{2}(A+B) \mp \tfrac{1}{2}(A-B)] \exp\{\mp \tfrac{1}{4}i\pi\} \quad (8.9b)$$

and substituting these a -coefficients and the expressions (3.23) and (3.24a, b) for $f(x_2)$ into the formula $\psi(x_2) = f(x_2) a(x_2)$, we get

$$\begin{aligned} \psi(x_2) = & A |q(x_2)|^{-\frac{1}{2}} \exp\{i[|w(x_2)| + \tfrac{1}{4}\pi]\} + \\ & + B |q(x_2)|^{-\frac{1}{2}} \exp\{-i[|w(x_2)| + \tfrac{1}{4}\pi]\}. \end{aligned} \quad (8.10a)$$

A convenient expression for the desired quantity $\psi(x_1)$ is obtained quite analogously when use is also made of the formula $a(x_1) = F(x_1, x_2) a(x_2)$ and of the symmetry relations (6.10a, b). The result is

$$\begin{aligned} \psi(x_1) = & \{(A+B) + [\tfrac{1}{2}(A+B) \pm \tfrac{1}{2}(A-B)] \times \\ & \times [F_{11}(x_1, x_2) - 1 \pm i \exp\{-2iw(x_1)\} F_{22}^*(x_1, x_2)]\} + \\ & + [\tfrac{1}{2}(A+B) \mp \tfrac{1}{2}(A-B)] \times \\ & \times [F_{11}^*(x_1, x_2) - 1 \mp i \exp\{-2iw(x_1)\} F_{22}(x_1, x_2)] \{ |q(x_1)|^{-\frac{1}{2}} \exp\{|w(x_1)|\} \}. \end{aligned} \quad (8.11)$$

From this formula and the estimates (6.13a, b) we then get

$$\psi(x_1) = \{(A+B) + (|A| + |B|) O(\mu)\} |q(x_1)|^{-\frac{1}{2}} \exp\{|w(x_1)|\}. \quad (8.10b)$$

If the wave function is real on the real axis, the coefficients $a_1(x_2)$ and $a_2(x_2)$ are complex conjugate and hence the quantities A and B are complex conjugate according to (8.9a, b). With a convenient normalization of the wave function we can then write

$$A = \frac{1}{2} \exp\{i(\gamma - \frac{1}{2}\pi)\}$$

$$B = \frac{1}{2} \exp\{-i(\gamma - \frac{1}{2}\pi)\}$$

where γ is a real phase, and the formulae (8.10a, b) become

$$\psi(x_2) = |q(x_2)|^{-\frac{1}{2}} \cos[|w(x_2)| + \gamma - \frac{1}{4}\pi] \quad (8.12a)$$

$$\psi(x_1) = [\sin \gamma + O(\mu)] |q(x_1)|^{-\frac{1}{2}} \exp\{|w(x_1)|\}. \quad (8.12b)$$

Obviously it is not always possible to obtain the JWKB-approximation for the wave function in the classically forbidden region from a knowledge of the wave function in the classically allowed region, but if the quotient $(A+B)/(|A| + |B|)$ is not close to zero, i.e. if γ is not close to a multiple of π , it is actually possible, since the term containing $O(\mu)$ can then be neglected in (8.10b) and (8.12b).

We shall now assume that we know the wave function $\psi(x)$ and its derivative at a point x_1 in the classically forbidden region, and we want to determine the same wave function at a point x_2 in the classically allowed region. It is not an essential restriction to assume the wave function to be real on the real axis, and therefore we write

$$a_1(x_1) = C \exp\{\pm \frac{1}{4}i\pi\} \quad (8.13a)$$

$$a_2(x_1) = D \exp\{\pm \frac{1}{4}i\pi\} \quad (8.13b)$$

where C and D are real numbers. Introducing these expressions for the a -coefficients into the formula $\psi(x_1) = f(x_1) a(x_1)$ and using for $f(x_1)$ the formulae (3.23) and (3.24a, b), we get

$$\psi(x_1) = C |q(x_1)|^{-\frac{1}{2}} \exp\{|w(x_1)|\} + D |q(x_1)|^{-\frac{1}{2}} \exp\{-|w(x_1)|\}. \quad (8.14a)$$

To obtain $\psi(x_2)$ we proceed in a similar way using also the formula $a(x_2) = F(x_2, x_1) a(x_1)$, the formula (3.20) for inverting the F -matrix, and the symmetry relations (6.10a, b). Remembering that C and D are real numbers, we get

$$\psi(x_2) = 2c |q(x_2)|^{-\frac{1}{2}} \cos[|w(x_2)| + \gamma - \frac{1}{4}\pi] \quad (8.15)$$

where the positive number c and the real number γ are defined by

$$c \exp\{\pm i\gamma\} = \pm i C F_{22}(x_1, x_2) + D F_{11}^*(x_1, x_2). \quad (8.16)$$

From this definition and the estimates (6.13a, b) we get

$$\begin{aligned} \left| \frac{c \exp\{\pm i\gamma\}}{D} - 1 \right| &\leq |F_{11}(x_1, x_2) - 1| + \left| \frac{C}{D} F_{22}(x_1, x_2) \right| \leq \\ &\leq \mu + \text{higher powers of } \mu + \\ &+ \left| \frac{C \exp\{|w(x_1)|\}}{D \exp\{-|w(x_1)|\}} \right| [\frac{1}{2}\mu + \text{higher powers of } \mu]. \quad (8.17) \end{aligned}$$

This inequality gives useful information on c and γ only if C and D fulfil the condition that

$$|C \exp\{|w(x_1)|\}| \lesssim |D \exp\{-|w(x_1)|\}| \quad (8.18)$$

where the symbol \lesssim means that the quantity on the left-hand side shall be at the most of the same order of magnitude as the quantity on the right-hand side. Assuming this condition to be fulfilled, we get from (8.17) the estimate

$$c \exp\{\pm i\gamma\} = D[1 + O(\mu)]$$

from which we conclude that

$$\begin{aligned} c &= |D| [1 + O(\mu)] \\ \cos \gamma &= \frac{D}{|D|} [1 + O(\mu)] \\ \sin \gamma &= O(\mu). \end{aligned}$$

With the aid of these estimates the formula (8.15) gives

$$\psi(x_2) = 2D[1 + O(\mu)] |q(x_2)|^{-\frac{1}{2}} \cos[|w(x_2)| - \frac{1}{4}\pi + O(\mu)]. \quad (8.14b)$$

The problem of obtaining an approximate expression for the wave function in the classically allowed region from a knowledge of the wave function in the classically forbidden region can obviously be solved within the JWKB-approximation only if the condition (8.18) is fulfilled, i.e. only if on the right-hand side of (8.14a) the first term is at the most of the same order of magnitude as the second term. If this condition is fulfilled, however, the formula (8.14b) applies and the JWKB-approximation for $\psi(x_2)$ is obtained by neglecting $O(\mu)$ in (8.14b).

It should be pointed out that in the above treatment it is not essential to assume the wave function and its derivative to be exactly known at the starting point. An approximate knowledge of the wave function and its derivative at this point means in general that A and B (or γ) or C and D are only approximately known, but this is sufficient for our purpose, as is easily seen from the formulae (8.10a, b), (8.12a, b), and (8.14a, b). This fact is obviously of great importance for the usefulness of the previous formulae in applications where the wave function is only approximately known at the starting point.

We shall now summarize the above results and write more explicitly the connection formulae obtained. To indicate the permitted direction for tracing a solution across a turning point we use an arrow, a symbol which was introduced for this purpose by LANGER [1934] and which has been used by several authors, e.g. in the textbooks on quantum mechanics by KEMBLE [1937], SCHIFF [1949], and MESSIAH [1959]. Omitting the error term $O(\mu)$, we get from (8.10a, b) the connection formula

$$A|q(x)|^{-\frac{1}{2}} \exp\{i[|w(x)| + \frac{1}{4}\pi]\} + B|q(x)|^{-\frac{1}{2}} \exp\{-i[|w(x)| + \frac{1}{4}\pi]\} \rightarrow \\ \rightarrow (A + B)|q(x)|^{-\frac{1}{2}} \exp\{|w(x)|\} \quad (8.19)$$

where A and B are arbitrary constants subject only to the restriction that $(A + B)/(|A| + |B|)$ must not be close to zero. From (8.12a, b) we similarly get the connection formula

$$|q(x)|^{-\frac{1}{2}} \cos[|w(x)| + \gamma - \frac{1}{4}\pi] \rightarrow \sin \gamma |q(x)|^{-\frac{1}{2}} \exp\{|w(x)|\} \quad (8.20)$$

where γ is a real constant subject only to the restriction of not being close to a multiple of π . From (8.14a, b) we finally obtain the connection formula

$$|q(x)|^{-\frac{1}{2}} \exp\{-|w(x)|\} \rightarrow 2|q(x)|^{-\frac{1}{2}} \cos[|w(x)| - \frac{1}{4}\pi] \quad (8.21)$$

which can be used also when there is an exponentially increasing term present in the left member, provided this exponential fulfils the condition (8.18). This extension of the validity of (8.21) is very important and useful, e.g. in the treatment of penetration through a potential barrier.

The above results have been derived for a special choice of the phase of $q(z)^{\frac{1}{2}}$, but the final connection formulae are independent of this choice and are valid quite generally, if only the lower limit in the integral (3.3) defining $w(x)$ coincides with the classical turning point x' . However, also this restriction can easily be removed by replacing in the final connection formulae $|w(x)|$ by $|w(x) - w(x')|$.

The meaning of the arrow \rightarrow used in the above connection formulae is that, if a given wave function $\psi(x)$ is closely approximated by the left member on one side of the turning point, then it is closely approximated by the right member on the other side of the turning point. The converse, however, is in general not true. It is immediately obvious that the formulae (8.19) and (8.20) cannot be used in the reverse direction. If the wave function can be approximated by the right member of (8.19) in a classically forbidden region, we know the value of $A + B$, but from this knowledge we cannot determine A and B separately. Similarly, the phase γ cannot be determined by fitting a given wave function to the right member of (8.20), since $\sin \gamma$ appears there only as a multiplying factor. The fact that we cannot draw any inference as to the wave function in the classically allowed region from the knowledge that it can be approximated by an exponentially increasing term in the classically forbidden region, is also understood if we remember that the neglected decreasing exponential, which is insignificant in the classically forbidden region, has a quite decisive influence on the wave function in the classically allowed region. Similar arguments illustrate the one-directional nature of the connection formula (8.21). From (8.20) and (8.21) we realize that the wave function in the classically forbidden region is fairly insensitive to small changes in the phase of the wave function in the classically allowed region, except when these changes take place in the neighbourhood of the value which corresponds to an exponentially decreasing wave function in the classically forbidden region. For this special wave function the quantity γ is close to zero but is not precisely known to us. Even very small departures of γ from this unknown value cause the increasing exponential to appear and completely change the wave function on the other side of the turning point. From the knowledge that the wave function is closely approximated by the right member of (8.21) in a classically allowed region, we cannot infer that it is closely approximated by the left member in the classically forbidden region, because we do not know whether or not the error in the phase causes the increasing exponential to appear and completely spoil the agreement between the left member of (8.21) and the wave function.

The connection formula (8.20), usually with γ chosen equal to $\frac{1}{2}\pi$, and the connection formula (8.21) are currently used in the literature. The connection formula (8.19) is usually not given explicitly, but it can easily be derived from (8.20). In fact, by replacing in (8.20) γ by $\gamma + \frac{1}{2}\pi$, and adding to the resulting formula the formula (8.20) multiplied by $\pm i$, we obtain, after both members of the final formula have been divided by the common

factor $\exp\{\pm i\gamma\}$, the connection formulae

$$|q(x)|^{-\frac{1}{2}} \exp\{\pm i(|w(x)| + \frac{1}{2}\pi)\} \rightarrow |q(x)|^{-\frac{1}{2}} \exp\{|w(x)|\}$$

which are equivalent to (8.19). It is therefore astonishing that the allowed connections contained in the formula (8.19) are so often overlooked, whereas many authors, especially when treating barrier penetration problems, use instead formally unsatisfactory formulae obtained by obscure arguments, which in typical cases proceed as follows. In more or less satisfactory ways the authors first obtain the connection formula (8.20) with $\gamma = \frac{1}{2}\pi$ and the connection formula (8.21). Some authors also mention the one-sided nature of these formulae, but then they use some impossible argument to make the reader think that the connection formulae may also be used in the wrong direction. Using the connection formula (8.21) in the wrong direction and the connection formula (8.20) with $\gamma = \frac{1}{2}\pi$ they then obtain connection formulae similar to our formula (8.19) with $B = 0$ and the further factor $[1 + \frac{1}{2}i \exp\{-2|w(x)|\}]$ on the right-hand side of (8.19) or with $A = 0$ and the further factor $[1 - \frac{1}{2}i \exp\{-2|w(x)|\}]$ on the right-hand side of (8.19). These factors are insignificant compared to the inherent inaccuracy of the JWKB-approximation. In barrier penetration problems many authors then proceed across the next classical turning point by using the connection formula (8.21) in the allowed direction and the formula (8.20) with $\gamma = \frac{1}{2}\pi$ in the wrong direction. The insignificant terms in the classically forbidden region then give rise to insignificant terms in the next classically allowed region. Although these terms are unimportant numerically, it is unsatisfactory, misleading, and unnecessarily complicated that they occur in the formulae. This fact will be further illustrated in connection with the treatment of barrier transmission in the next chapter.

As already mentioned in chapter 1 there have been and still are controversial discussions on the one-sided nature of the connection formulae (HEADING [1962], H. JEFFREYS [1956], LANGER [1934]). H. JEFFREYS [1956], when arguing against Langer, has remarked that despite the one-sided nature of the connection formulae it is possible to solve with good approximation certain boundary value problems with boundary conditions on opposite sides of a classical turning point by means of the JWKB-approximation. We shall here discuss a special problem of this kind which has been considered by H. JEFFREYS [1956]. Contrary to HEADING [1962] (cf. his p. 12), we believe that Jeffreys's treatment of the problem is right, but we find it illuminating to show in a very direct way that the boundary conditions can be satisfied without violating the one-sided nature of the connection formulae. The problem amounts to obtaining an approximate solution of the wave equation subject to the boundary conditions of being equal to zero at a given point x_1 in the classically forbidden region as well as at a given point x_2 in the classically allowed region. Choosing the lower limit in the integral (3.3) defining $w(x)$ to be the classical turning point x' , we write the JWKB-approximation of the desired solution in the classically forbidden region as follows

$$\psi(x) = C|q(x)|^{-\frac{1}{2}} \exp\{|w(x)|\} + D|q(x)|^{-\frac{1}{2}} \exp\{-|w(x)|\}. \quad (8.22)$$

The condition that the wave function $\psi(x)$ shall be equal to zero for $x = x_1$ gives

$$C = -D \exp\{-2|w(x_1)|\}. \quad (8.23)$$

Since therefore the two terms on the right-hand side of (8.22) are of the same order of magnitude in the neighbourhood of x_1 , it follows from the result obtained at the end of section 8.2 that the desired wave function is approximately equal to the expression on the right-hand side of (8.22) throughout the classically forbidden region except in the neighbourhood of the classical turning point. It should, however, be remembered that it is only in a certain region around x_1 that both terms on the right-hand side of (8.22) are significant. Now that an approximate formula for the wave function in the classically forbidden region has been obtained, we shall turn our attention to the wave function and the boundary condition in the classically allowed region. According to (8.23) the condition (8.18) for the validity of the connection formula (8.14a, b) is fulfilled, and, except in the neighbourhood of the classical turning point, the wave function in the classically allowed region is therefore approximately given by the formula

$$\psi(x) = 2D |q(x)|^{-\frac{1}{2}} \cos[|w(x)| - \frac{1}{2}\pi]. \quad (8.24)$$

The boundary condition that the wave function $\psi(x)$ shall be equal to zero for $x = x_2$ then gives the approximate "quantization condition"

$$|w(x_2)| + \frac{1}{2}\pi \approx n\pi \quad (8.25)$$

where n is an integer. Thus we have shown how the boundary value problem considered by Jeffreys can be solved approximately in a simple and direct way without violating any connection formula.

BARRIER TRANSMISSION

Although barrier transmission problems have been treated by means of the JWKB-method for a very long time, there are still questions that remain to be answered or elucidated. For instance, the misconceptions concerning the connection formulae, mentioned in the preceding chapter, often occur in the literature on barrier transmission problems.

In the treatment to be given in sections 9.1 and 9.2 below we shall derive exact expressions for the transmission and reflection coefficients in terms of the F -matrix connecting points on opposite sides of the potential barrier. This matrix has been considered in detail for both overdense and underdense potential barriers in sections 6.4 and 6.5. For a thorough understanding of the present chapter a detailed study of these sections is necessary.

If the energy of the incident particle lies below the peak of the potential barrier, and the two classical turning points, denoted by x' and x'' ($> x'$), are well separated, it is well known that in the JWKB-approximation the transmission coefficient is

$$T = \exp \left\{ -2 \int_{x'}^{x''} |Q(x)| dx \right\}. \quad (9.1)$$

There are, however, some unsatisfactory features in the derivations that are presented in most text books. For the case that the kinetic energy of the incident particle is only slightly less than the energy corresponding to the top of the barrier KEMBLE [1935] has obtained the following formula for the transmission coefficient

$$T = \left[1 + \exp \left\{ 2 \int_{x'}^{x''} |Q(x)| dx \right\} \right]^{-1}. \quad (9.2)$$

This formula is quite correct in the JWKB-approximation, but Kemble's way of obtaining it is not satisfactory. The formula (9.2) can obviously be used also when the kinetic energy of the incident particle lies well below the

top of the barrier, but in this case the term 1 is not only very small compared to the exponential function but is in general insignificant. In the special case of a parabolic potential the formula is, however, exact.

The problem of calculating the reflection coefficient for the case that the kinetic energy of the incident particle lies above the top of the potential barrier (the super-barrier case) has recently been much discussed, especially in the Russian literature. It is a rather vast problem, and we shall consider it only in a special case. If $Q^2(z)$ has two complex conjugate zeros $x_0 \pm iy'$ (where $y' > 0$) close to the real axis, the transmission coefficient is given by the simple approximate formula

$$T = \left[1 + \exp \left\{ -2 \int_{x_0 - iy'}^{x_0 + iy'} |Q(x_0 + iy)| dy \right\} \right]^{-1} \quad (9.3)$$

which has been given by KEMBLE [1935], [1937]. This formula is exactly valid for the parabolic potential. For other potentials the exponential function in (9.3) is usually significant only when the kinetic energy of the incident particle lies only slightly above the top of the barrier. As a rough approximation the formula can be used also for larger values of the energy of the incident particle, since, as this energy increases, the transmission coefficient calculated by formula (9.3) rapidly approaches the correct value 1.

In sections 9.1 and 9.2 below we shall treat the cases of sub-barrier and super-barrier transmission separately, but first we shall say a few words about the probability current and the condition to be imposed on $q^2(x)$ in order that the JWKB-functions $f_1(x)$ and $f_2(x)$ may be interpreted as waves propagating in opposite directions.

The probability current S is given by the formula

$$S = \frac{\hbar}{2mi} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right) = \frac{\hbar}{m} \frac{d(\arg \psi)}{dx} |\psi|^2, \quad (9.4)$$

where m is the mass of the particle, and \hbar is Planck's constant divided by 2π .

Expressing in (9.4) ψ and $d\psi/dx$ according to (3.25a, b) in terms of the JWKB-functions and the a -coefficients, and assuming $q^2(x)$ to be any real function, we get

$$S = \begin{cases} \frac{\hbar}{m} q (|a_1 f_1|^2 - |a_2 f_2|^2) & \text{when } q^2(x) > 0 \\ \frac{\hbar}{m} q (a_1 f_1 a_2^* f_2^* - a_1^* f_1^* a_2 f_2) & \text{when } q^2(x) < 0. \end{cases} \quad (9.5)$$

We shall assume that the function $q^2(x)$ is positive for sufficiently large values of $|x|$ and that the function $\varepsilon(x)q(x)$ tends to zero so rapidly as $|x| \rightarrow \infty$ that the μ -integral converges also if the path extends to infinity. Since the imaginary part of $w(x)$ is constant in each region of the real axis where $q^2(x) > 0$, we easily conclude from estimates similar to those leading to the basic estimates in chapter 4 that the limit $F(x, +\infty)$ exists and is finite if $q^2 > 0$ in the whole interval $(x, +\infty)$. Similarly the limit $F(-\infty, x)$ is seen to exist and be finite if $q^2 > 0$ in the whole interval $(-\infty, x)$. Using matrix multiplication we then conclude that the limits $F(-\infty, z)$, $F(z, +\infty)$, and $F(-\infty, +\infty)$ exist and are finite if z lies elsewhere on the real axis or in the complex plane but does not coincide with a singularity or zero of $q^2(z)$. From this result it follows according to (3.16) that the four limits $a_1(\pm\infty)$ and $a_2(\pm\infty)$ exist and are finite. Thus the fact that the μ -integral is finite even if the path proceeds to infinity implies that for large values of $|x|$ the JWKB-functions $f_1(x)$ and $f_2(x)$ approach two linearly independent solutions of the differential equation (3.1). As $x \rightarrow \pm\infty$ the functions $f_1(x)$ and $f_2(x)$ may then be interpreted as waves proceeding in opposite directions. The absolute values of the corresponding probability currents, which are

$$\frac{\hbar}{m} |a_1 \exp\{i w\}|^2 \quad \text{and} \quad \frac{\hbar}{m} |a_2 \exp\{-i w\}|^2$$

according to (9.5) and (3.24a, b), lead to the simple formulae for the reflection and transmission coefficients, which will be used below in sections 9.1 and 9.2.

9.1. Barrier penetration when the kinetic energy of the incident particle lies below the energy corresponding to the top of the barrier

The behaviour of the function $q^2(x)$ on the real axis is assumed to be as shown in fig. 6.4a or fig. 6.5a. The z -plane is cut along the real axis, and the function $q(z)^\dagger$ is defined on the real axis and in the upper half of the z -plane, with the phase chosen as shown in fig. 6.4b or fig. 6.5b. The fixed lower limit in the integral (3.3) defining $w(z)$ is chosen to be the left classical turning point x' . The wave function $\psi(x)$ is given by the formula (3.25a). Far to the left of the barrier $f_1(x)$ represents a wave travelling from left to right, and $f_2(x)$ represents a wave travelling from right to left. Far to the right of the barrier the opposite is true. The potential barrier causes a wave

incident from the left to be partly reflected and partly transmitted. Far to the right of the barrier there shall be only an outgoing wave, and therefore $a_1(+\infty) = 0$. Hence the formula (3.16) gives

$$a_1(z) = F_{12}(z, +\infty) a_2(+\infty) \quad (9.6a)$$

$$a_2(z) = F_{22}(z, +\infty) a_2(+\infty). \quad (9.6b)$$

For $x < x'$ the function $w(x)$ is real, and for $x > x''$ the same function has the constant imaginary part $-iK$, where K is a positive quantity defined by (6.18), i.e.

$$K = \int_{x'}^{x''} |q(x)| dx. \quad (9.7)$$

Remembering the discussion of the incoming and outgoing waves, given above, we therefore realize that the reflection coefficient R and the transmission coefficient T are given by the formulae

$$R = \left| \frac{a_2(-\infty)}{a_1(-\infty)} \right|^2 \quad (9.8a)$$

$$T = \left| \frac{a_2(+\infty)}{a_1(-\infty)} \right| \exp\{-2K\}. \quad (9.8b)$$

Because of (9.6a, b) these formulae give

$$R = \left| \frac{F_{22}(-\infty, +\infty)}{F_{12}(-\infty, +\infty)} \right|^2 \quad (9.9a)$$

$$T = \frac{\exp\{-2K\}}{|F_{12}(-\infty, +\infty)|^2}. \quad (9.9b)$$

Using here (6.19), we get

$$R = \frac{|F_{22}(-\infty, +\infty)|^2 \exp\{2K\}}{1 + |F_{22}(-\infty, +\infty)|^2 \exp\{2K\}} \quad (9.10a)$$

$$T = \frac{1}{1 + |F_{22}(-\infty, +\infty)|^2 \exp\{2K\}}. \quad (9.10b)$$

These formulae confirm that

$$R + T = 1. \quad (9.11)$$

The matrix $F(x_1, x_2)$ considered in section 6.4 corresponds to the present matrix $F(-\infty, +\infty)$, if we put $x_1 = -\infty$ and $x_2 = +\infty$. The estimates (6.22b) and (6.29) thus apply to $F_{22}(-\infty, +\infty)$. We recall that the derivation of (6.22b) is adapted to the case when the classical turning points are

well separated and the derivation of (6.29) to the case when they lie close to each other. The reader is referred, however, to section 6.4 for more details on the validity of these formulae. The matrix element $F_{22}(-\infty, +\infty)$ is found to be approximately equal to 1 according to both of the estimates (6.22b) and (6.29). Thus we obtain from (9.10a, b) the following approximate formulae for R and T , valid whether the classical turning points are well separated or lie close together

$$R \approx \frac{\exp\{2K\}}{1 + \exp\{2K\}} \quad (9.12a)$$

$$T \approx \frac{1}{1 + \exp\{2K\}}. \quad (9.12b)$$

The relative errors in these approximate expressions for R and T are at the most of the orders of magnitude $\mu \exp\{-2K\}$ and μ , respectively. It is satisfactory that the approximate formulae (9.12a, b) fulfill the requirement (9.11) exactly. We also remark that if the classical turning points are well separated we have in general the inequality $\exp\{-2K\} \ll \mu$ which, according to (9.10a, b) and (6.22b), implies that the term 1 in the denominator on the right-hand side of (9.12b) is in general not significant in this case. This term is, however, very important when the classical turning points lie so close together that $\exp\{-2K\} \gg \mu$.

As far as we know KEMBLE [1935] was the first to give the formula (9.12b), with $q^2(z) = Q^2(z)$, for the transmission coefficient for the case that the energy of the incident particle is close to the energy corresponding to the top of the potential barrier. He gave, however, no satisfactory proof of this formula.

If the shape of the potential barrier is exactly parabolic and $q^2(z) = Q^2(z)$, we have $F_{22}(-\infty, +\infty) = 1$ according to the remarks at the end of section 6.4. From (9.10a, b) we then find that in this special case the formulae (9.12a, b) are exact. In particular the term 1 in the denominator on the right-hand side of (9.12b) is significant. From the physical point of view an exactly parabolic potential barrier is unrealistic, since for such a barrier the particle velocity tends to infinity as $x \rightarrow \pm \infty$. Nevertheless the problem of penetration through an exactly parabolic barrier is of interest and has been treated by MILLER and GOOD [1953], and in a different way by B.S. JEFFREYS [1961] who transforms the original differential equation to a confluent hypergeometric differential equation and obtains the transmission coefficient from the asymptotic expression of its solution.

The exact validity of (9.12a, b) for the parabolic potential barrier when $q^2(z) = Q^2(z)$ indicates that if the actual barrier has approximately parabolic shape in an interval which contains both of the classical turning points and which is large compared to the distance between these turning points, and if outside this interval the function $Q^2(x)$ attains the limiting value $Q^2(\pm\infty)$ very smoothly, the formulae (9.12a, b) should be extremely accurate and the term 1 in the denominator on the right-hand side of (9.12b) may be significant even if the classical turning points do not lie close together.

We shall now turn to a discussion of the wave function $\psi(x)$ on the real axis. Substituting (3.24a, b) for $f(x)$ and (9.6a, b) for $a(x)$ in the formula (3.25a) for $\psi(x)$, and remembering that in the integral (3.3) defining $w(z)$ the fixed lower limit shall be x' , we get

$$\begin{aligned} \psi(x) = a_2(+\infty) q(x)^{-\frac{1}{2}} & \left[F_{12}(x, +\infty) \exp \left\{ i \int_{x'}^x q(\xi) d\xi \right\} + \right. \\ & \left. + F_{22}(x, +\infty) \exp \left\{ -i \int_{x'}^x q(\xi) d\xi \right\} \right] \quad (9.13) \end{aligned}$$

where the phase of $q(x)^{\frac{1}{2}}$ is to be taken from fig. 6.4b or fig. 6.5b. In the following discussion we let μ denote the μ -integral from x to $+\infty$ along a convenient path which does not pass close to the classical turning points x' and x'' . If x lies to the right of the potential barrier we have, according to the basic estimates (4.3), the formulae

$$F_{22}(x, +\infty) = 1 + O(\mu) \quad (9.14a)$$

$$F_{12}(x, +\infty) = \exp \{-2K\} O(\mu) \quad (9.14b)$$

where K is given by (9.7). Substituting (9.14a, b) into (9.13), we get the formula

$$\psi(x) = i a_2(+\infty) |q(x)|^{-\frac{1}{2}} \exp \left\{ -K + i \int_{x''}^x |q(\xi)| d\xi \right\} [1 + O(\mu)] \quad (9.15)$$

which is valid for $x > x''$. On the other hand, if x lies to the left of the potential barrier, we have, according to (6.22a, b) if $\exp\{-2K\} \ll \mu$, or according to (6.29) and (6.30) if the turning points lie close together, the formulae

$$F_{22}(x, +\infty) = 1 + O(\mu) \quad (9.16a)$$

$$F_{12}(x, +\infty) = \exp \{i\varphi\} [1 + \exp \{-2K\}]^{\frac{1}{2}} [1 + O(\mu)] \quad (9.16b)$$

where φ is a real phase. In the case of well separated classical turning points as well as in the case of coinciding classical turning points $\varphi \approx \frac{1}{2}\pi$. Substituting (9.16a, b) into (9.13) and taking the phase of $q(x)^\dagger$ from fig. 6.4b or fig. 6.5b, we get the formula

$$\begin{aligned} \psi(x) = & i a_2(+\infty) |q(x)|^{-\dagger} \left[\exp \left\{ -i \left(\frac{1}{2}\pi + \int_{x'}^x |q(\xi)| d\xi \right) \right\} [1 + O(\mu)] + \right. \\ & \left. + [1 + \exp\{-2K\}]^\dagger \exp \left\{ i \left(\varphi + \int_{x'}^x |q(\xi)| d\xi \right) \right\} [1 + O(\mu)] \right] \quad (9.17) \end{aligned}$$

which is valid for $x < x'$. Finally, if x lies in the classically forbidden region between two well separated classical turning points, we have, according to (6.21), the formulae

$$F_{22}(x, +\infty) = 1 + O(\mu) \quad (9.18a)$$

$$F_{12}(x, +\infty) = \exp \left\{ -2 \int_{x'}^x |q(\xi)| d\xi \right\} O(\mu). \quad (9.18b)$$

Substituting these formulae into (9.13) and taking into account the phase of $q(x)^\dagger$, we obtain the formula

$$\psi(x) = \exp\{\frac{1}{4}i\pi\} a_2(+\infty) |q(x)|^{-\dagger} \exp \left\{ - \int_{x'}^x |q(\xi)| d\xi \right\} [1 + O(\mu)] \quad (9.19)$$

which is valid for $x' < x < x''$, provided the classical turning points are well separated.

Normalizing $\psi(x)$ conveniently by putting $a_2(+\infty) = \exp\{K - \frac{1}{4}i\pi\}$ and considering the case that the classical turning points are well separated, we can summarize the above formulae for the wave function $\psi(x)$ as follows

$$\psi(x) \approx |q(x)|^{-\dagger} \exp \left\{ i \left[\int_{x''}^x |q(\xi)| d\xi + \frac{1}{4}\pi \right] \right\} \quad \text{for } x > x'' \quad (9.20a)$$

$$\psi(x) \approx |q(x)|^{-\dagger} \exp \left\{ \int_x^{x''} |q(\xi)| d\xi \right\} \quad \text{for } x' < x < x'' \quad (9.20b)$$

$$\psi(x) \approx 2 \exp\{K\} |q(x)|^{-\dagger} \cos \left[\int_x^{x'} |q(\xi)| d\xi - \frac{1}{4}\pi \right] \quad \text{for } x < x'. \quad (9.20c)$$

It is a quite straight-forward procedure to obtain these JWKB-expressions in a simpler way, namely by starting from the outgoing wave (9.20a) and

using the connection formulae (8.19) and (8.21). From the JWKB-formulae (9.20) for the wave function, the transmission coefficient T is immediately obtained as $T \approx \exp\{-2K\}$, which is in agreement with (9.12b) when $\exp\{2K\} \gg 1$.

In most text books (see for instance those by BOHM [1961] and by MERZBACHER [1961]) where the barrier penetration problem for the case of well separated turning points is treated with the aid of the JWKB-method, the authors use the connection formulae (8.20), with $\gamma = \frac{1}{2}\pi$, and (8.21) without paying sufficient attention to their one-sided nature. As we mentioned at the end of section 8.3, the approximate expressions for the wave function inside and to the left of the potential barrier, which they then obtain from the knowledge of the outgoing wave, are correct from the numerical point of view but contain insignificant terms which should be left out. Such expressions are therefore unsatisfactory as is also the whole approach based on the use of the connection formulae in forbidden directions. Since the problem can be treated in a simple and straight-forward way after the connection formulae have been formulated in a precise and convenient way, it is astonishing how much confusion there has been and still is concerning the problem of barrier penetration and the one-sided nature of the connection formulae. Cf. the review given by HEADING [1962].

As already mentioned in section 8.3, Jeffreys and Langer have had different opinions on questions related to the one-sided nature of the connection formulae, and to illuminate these questions JEFFREYS [1956] has treated different boundary value problems for wave equations with classical turning points by expanding the desired solution in terms of certain linearly independent basic solutions. One such problem, involving only one turning point, was discussed at the end of section 8.3. Another, involving two classical turning points, is the problem of barrier penetration. Jeffreys's treatment has recently been criticized by Heading (HEADING [1962]), but we believe that Heading (cf. p. 12 in Heading's book) has misunderstood Jeffreys, whose treatment is perfectly right (apart from some misprints) although unnecessarily complicated and not very straight-forward. Furthermore, Jeffreys's treatment does not give anything beyond that which can be obtained in a simpler and more direct way from the one-sided connection formulae if they have been formulated in a convenient way. We can derive precisely those formulae for the basic solutions (called y_1, y_2 and y_3, y_4), from which H. JEFFREYS [1956] starts his analysis of the barrier penetration problem, by means of our formulae (8.3), (8.5a, b), (8.6), (8.7a), (8.12a, b), and (8.14a, b) with due regard to the condition (8.18). By means of these formulae we can, however, equally well construct the desired solution of the boundary value problem directly without using Jeffreys's basic solutions.

9.2. Super-barrier transmission when the kinetic energy of the incident particle lies slightly above the energy corresponding to the top of the barrier

When the kinetic energy of the particles coming in towards a potential barrier is larger than the height of the barrier, the function $Q^2(x)$ is positive

along the whole real axis, and from the usual JWKB-formulae one obtains the value 1 for the transmission coefficient T and the value 0 for the reflection coefficient R . These are the limiting values which T and R approach as the energy of the incident particles increases to become much larger than the height of the barrier. If, however, this energy lies only slightly above the barrier, the above-mentioned limiting values are poor approximations for T and R . This is quite natural, since there are then two complex conjugate zeros of $Q^2(z)$ near the real axis, and thus for the unmodified JWKB-method the μ -integral along this axis is not small.

The problem concerning the transmission of particles with energies near to the energy of the top of an underdense potential barrier will first be treated briefly, analogously to the corresponding problem for an overdense potential barrier in section 9.1. The function $q^2(x)$ is assumed to be similar to $Q^2(x)$ and thus to be positive along the whole real axis. Since the solutions $\psi(z)$ of the differential equation (3.1) are single-valued as z moves around a zero of $Q^2(z)$ or of $q^2(z)$, we may cut the complex z -plane as indicated in fig. 6.6b. The phase of $q(z)^{\frac{1}{2}}$, also indicated in fig. 6.6b, is chosen such that on the real axis far to the left of the cut $f_1(x)$ represents an incoming wave, i.e. a wave travelling from left to right. We choose the fixed lower limit in the integral (3.3) defining $w(z)$ as described in the beginning of section 6.5. The close analogy between the overdense and underdense potential barrier in the present treatment stands out clearly on comparing fig. 6.5b and fig. 6.6b. The behaviour of the absolute value of $\exp\{i w\}$ is essentially the same on the similar paths of integration from x_1 to x_2 in the two cases. The only difference is that in fig. 6.5b there are two generalized classical turning points x' and x'' on the real axis, whereas in fig. 6.6b there are two complex conjugate zeros of $q^2(z)$, namely $x' \pm iy'$. This, however, is not essential to our procedure of treating these problems. Thus our treatment of the barrier penetration problem in the beginning of section 9.1, which leads to the formulae (9.12a, b), can for the present case of transmission through an underdense barrier be taken over almost step by step with the only modification that instead of referring to the results obtained in section 6.4 we shall now refer to the corresponding results discussed in the beginning of section 6.5. One finds that the reflection and transmission coefficients, R and T , are given exactly by the formulae (9.10a, b) and approximately by the formulae (9.12a, b), where K is now defined according to (6.33) and is therefore negative. This fact makes the relative errors in the approximate formulae (9.12a, b) for R and T different

from the corresponding errors mentioned in section 9.1. For the present case of super-barrier transmission the formulae (9.12a, b) give R and T , respectively, with a relative error that is at the most of the order of magnitude $\mu \exp\{|K|\}$ and $\mu \exp\{-|K|\}$, respectively. As the energy of the incident particle is assumed to be only slightly larger than the height of the barrier, the quantity $\exp\{|K|\}$ is of the order of magnitude of 1, and the relative errors in our approximate formulae for R and T are small since $\mu(-\infty, +\infty)$ is assumed to be small compared to 1. For larger values of the energy of the incident particle the relative error in the approximate formula for the reflection coefficient may be large unless the potential barrier has a shape that is closely parabolic over a large region around the top and is elsewhere very smooth. If this is the case and $q^2(z) = Q^2(z)$, we may expect the formulae (9.12a, b) to be very accurate. The reason is that for a parabolic potential barrier these formulae are exact also for super-barrier transmission provided $q^2(z) = Q^2(z)$.

The alternative way of treating the underdense potential barrier, which will be considered now, is in some respects more convenient from the physical point of view. We choose the cuts in the complex z -plane such that they do not cross the real axis, and we define the phase of $q(z)^\dagger$ such that this function is real and positive on the real axis. Furthermore, we choose the fixed lower limit in the integral (3.3) defining $w(z)$ as a point x_0 on the real axis. This implies that $w(z)$ is real on the real axis, and consequently, far away from the barrier, the function $f_1(x)$, defined by (3.24a), represents a wave travelling in the positive direction of the real axis, whereas the function $f_2(x)$, defined by (3.24b), represents a wave travelling in the negative direction of the real axis. Assuming the incident wave to be travelling in the positive direction of the real axis, we can have only an outgoing wave for large positive values of x , and we must therefore have $a_2(+\infty) = 0$. From (3.26) we then get

$$a_1(z) = F_{11}(z, +\infty) a_1(+\infty) \quad (9.21a)$$

$$a_2(z) = F_{21}(z, +\infty) a_1(+\infty). \quad (9.21b)$$

Since $w(x)$ is real along the whole real axis, the reflection and transmission coefficients, R and T , are simply

$$R = \left| \frac{a_2(-\infty)}{a_1(-\infty)} \right|^2 \quad (9.22a)$$

$$T = \left| \frac{a_1(+\infty)}{a_1(-\infty)} \right|^2. \quad (9.22b)$$

Because of (9.21a, b) and (6.2) these formulae give

$$R = \left| \frac{F_{21}(-\infty, +\infty)}{F_{11}(-\infty, +\infty)} \right|^2 = 1 - \left| \frac{1}{F_{11}(-\infty, +\infty)} \right|^2 \quad (9.23a)$$

$$T = \left| \frac{1}{F_{11}(-\infty, +\infty)} \right|^2. \quad (9.23b)$$

If the potential barrier is smooth and the energy of the incident particle lies well above the top of the barrier, the μ -integral (4.2) along the entire real axis is in general small. We can then use the estimate (4.3a) in (9.23a, b), getting

$$R = O(\mu) \quad (9.24a)$$

$$T = 1 - O(\mu) \quad (9.24b)$$

where μ denotes the μ -integral (4.2) along the whole real axis. However, if the energy of the incident particle lies only slightly above the top of the potential barrier, the estimate (4.3a) of $F_{11}(-\infty, +\infty)$ does not give a useful result since, due to the presence of zeros of $q^2(z)$ close to the real axis, the μ -integral along this axis is no longer small. To estimate the matrix $F(-\infty, +\infty)$ we must then use a more convenient path of integration. Let us assume that close to the real axis there are two complex conjugate simple zeros of $q^2(z)$, which we denote by $x' \pm iy'$, where y' is positive but "small". We cut the complex z -plane by a curve going from $x' + iy'$ towards the real axis and continuing in the negative direction of the real axis as a straight line at an infinitesimal distance above the real axis. The z -values on the upper side of this straight line are denoted by $x + i0$. In the lower half of the z -plane we introduce a cut from the point $x' - iy'$ towards infinity along a curve, which does not cross the real axis. The cuts now described are shown in fig. 6.7b. If the function $q^2(z)$ has singularities or further zeros, we introduce cuts also from these points towards infinity. The matrix $F(-\infty, +\infty)$ can then be calculated approximately in the way that has been described in the latter part of section 6.5. The resulting formulae are (6.48) and (6.49). Using these formulae and also (6.38) and (3.20), we get

$$|F_{21}(-\infty, +\infty)|^2 = [1 + \exp\{-K\} O(\mu)] \exp\{2K\} \quad (9.25a)$$

$$|F_{11}(-\infty, +\infty)|^2 = [1 + \exp\{K\} O(\mu)] [1 + \exp\{2K\}] \quad (9.25b)$$

where μ now denotes the μ -integral between $-\infty + i0$ and $+\infty$ along the

path shown in fig. 6.7b. Substituting (9.25a, b) into (9.23a, b), and noting that K , which is given by (6.33), i.e. by

$$K = i \int_{x'-iy'}^{x'+iy'} q(z) dz = \operatorname{Re} \left\{ 2i \int_{x_0}^{x'+iy'} q(z) dz \right\}, \quad (9.26)$$

is negative, we get the approximate formulae

$$R \approx \frac{1}{1 + \exp\{2|K|\}} \quad (9.27a)$$

$$T \approx \frac{1}{1 + \exp\{-2|K|\}}. \quad (9.27b)$$

Here the relative error in R is at the most of the order of magnitude $\mu \exp\{|K|\}$, and the relative error in T is at the most of the order of magnitude $\mu \exp\{-|K|\}$. We remark that the approximate formulae (9.27a, b) fulfil the condition $R + T = 1$, and we recall that the formulae are exact in the case of a parabolic potential barrier, provided $q^2(z) = Q^2(z)$.

BOUND STATES

In this chapter we shall consider the case of a potential well. We allow for the possibility of choosing $q^2(z)$ different from $Q^2(z)$, but we assume that these two functions are similar in shape. Thus on the real axis the func-

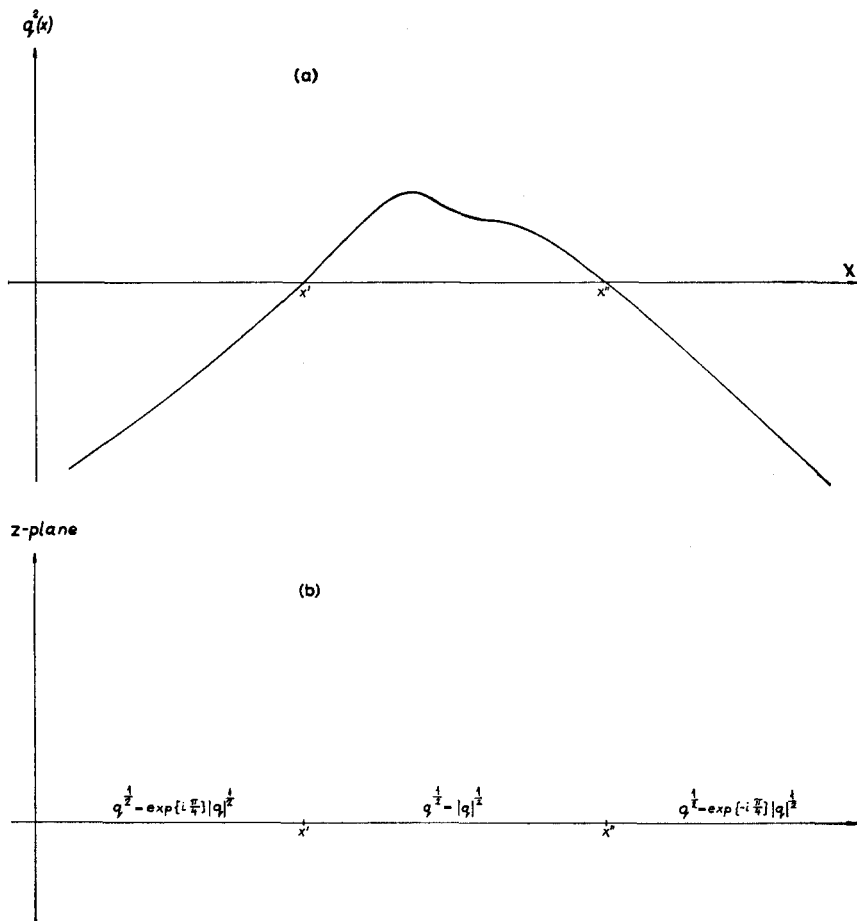


Fig. 10.1

tion $q^2(x)$, which is shown in fig. 10.1a, is positive between the generalized classical turning points x' and x'' , whereas $q^2(x)$ is negative to the left of x' and to the right of x'' . We cut the complex z -plane along the real axis and use only this axis and the upper half of the z -plane. The phase of the function $q(z)^\dagger$ is chosen such that the values of $q(z)^\dagger$ on the different parts of the real axis are those given in fig. 10.1b. We assume that the absolute value of $\exp\{i w(x)\}$ in the classically forbidden regions increases monotonically and tends to infinity as x moves along the real axis to $+\infty$ or to $-\infty$, respectively. This is obviously true irrespective of how the fixed lower limit in the integral (3.3) defining $w(z)$ is chosen. We shall assume that the function $\varepsilon(x)q(x)$ behaves for $x \rightarrow +\infty$ such that the μ -integral (4.2) along a part of the real axis extending to $+\infty$ is convergent, and we shall also make the corresponding assumption for $x \rightarrow -\infty$.

Since the wave functions of bound states must satisfy boundary conditions at $x = \pm\infty$, a rigorous treatment of such states according to the JWKB-method requires the consideration of certain limiting properties, as x tends to $\pm\infty$, of the F -matrix and the a -coefficients. We shall devote the first part of this chapter to these questions. In the latter part we shall consider the quantization condition for bound states.

Letting z_0 be any point where $q(z)$ has neither a singularity nor a zero, we have according to (4.7a, b, c, d) the following limiting properties for the matrix $\mathbf{F}(z_0, x)$

$$\lim_{x \rightarrow \pm\infty} F_{22}(z_0, x) \text{ exist and are finite} \quad (10.1a)$$

$$\lim_{x \rightarrow \pm\infty} F_{12}(z_0, x) \text{ exist and are finite} \quad (10.1b)$$

$$\lim_{x \rightarrow \pm\infty} F_{21}(z_0, x) \exp\{-2i w(x)\} = 0 \quad (10.1c)$$

$$\lim_{x \rightarrow \pm\infty} F_{11}(z_0, x) \exp\{-2i w(x)\} = 0. \quad (10.1d)$$

The corresponding limiting properties of the a -coefficients are according to (4.6a, b) as follows

$$\lim_{x \rightarrow \pm\infty} a_1(x) \text{ exist and are finite} \quad (10.2a)$$

$$\lim_{x \rightarrow \pm\infty} a_2(x) \exp\{-2i w(x)\} = 0. \quad (10.2b)$$

If $a_1(+\infty)$ is different from zero, it follows from (3.25a), (3.24a, b), and (10.2a, b) that

$$\lim_{x \rightarrow +\infty} \frac{\psi(x)}{a_1(+\infty)f_1(x)} = 1. \quad (10.3a)$$

If $a_1(-\infty)$ is different from zero, one similarly finds

$$\lim_{x \rightarrow -\infty} \frac{\psi(x)}{a_1(-\infty)f_1(x)} = 1. \quad (10.3b)$$

We shall assume that the integrals

$$\int_0^{+\infty} |f_1(x)|^2 dx \quad (10.4a)$$

$$\int_{-\infty}^0 |f_1(x)|^2 dx \quad (10.4b)$$

are both divergent. From (10.3a, b) it then follows that the integral

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx$$

is also divergent if at least one of the limits $a_1(+\infty)$ and $a_1(-\infty)$ is different from zero. If the wave function $\psi(x)$ is to represent a bound state, both of the limits $a_1(+\infty)$ and $a_1(-\infty)$ must consequently be equal to zero.

We shall now assume that the limit $a_1(+\infty)$ is equal to zero, and we shall show that on this assumption the limit of $a_2(x)$ as $x \rightarrow +\infty$ exists and is finite, and we shall also express the a -coefficients and the wave function ψ at any point z in terms of this limiting value. Letting in (3.26) the variable z be real and tend to $+\infty$, and noting the existence of the limits (10.1a, b) and (10.2a), we obtain, with due regard to (3.20), the formula

$$a_1(+\infty) = F_{11}(+\infty, z_0) a_1(z_0) + F_{12}(+\infty, z_0) a_2(z_0). \quad (10.5)$$

Introducing here the assumption $a_1(+\infty) = 0$, and using the inversion formula (3.20), we get

$$\frac{a_1(z_0)}{a_2(z_0)} = \frac{F_{12}(z_0, +\infty)}{F_{22}(z_0, +\infty)}. \quad (10.6)$$

Using this formula and the rules for matrix multiplication, we find from

(3.26) the formulae

$$a_1(z) = \frac{a_2(z_0)}{F_{22}(z_0, +\infty)} F_{12}(z, +\infty) \quad (10.7a)$$

$$a_2(z) = \frac{a_2(z_0)}{F_{22}(z_0, +\infty)} F_{22}(z, +\infty). \quad (10.7b)$$

From the last formula we see that the limit of $a_2(z)$ as z approaches $+\infty$ along the real axis exists and is equal to $a_2(z_0)/F_{22}(z_0, +\infty)$. The formulae (10.7a, b) can therefore be written as follows

$$a_1(z) = F_{12}(z, +\infty) a_2(+\infty) \quad (10.8a)$$

$$a_2(z) = F_{22}(z, +\infty) a_2(+\infty). \quad (10.8b)$$

Thus we have rigorously proved a result which may be expected intuitively by merely inspecting (3.26). Substituting (10.8a, b) into (3.25a), and using (3.24a, b) and (3.20), we get

$$\psi(z) = a_2(+\infty) f_2(z) [1 + \eta(z)] \quad (10.9)$$

where

$$\eta(z) = F_{11}(+\infty, z) - 1 - F_{12}(+\infty, z) \exp\{2i w(z)\}. \quad (10.10)$$

If z lies on the real axis to the right of x'' we can estimate the elements of the F -matrix appearing in (10.10) by means of the basic estimates (4.3a, b) with $M = \frac{1}{2}$, getting

$$|\eta(x)| \leq 2[\exp\{\frac{1}{2}\mu(x, +\infty)\} - 1] \quad \text{for } x'' < x < +\infty \quad (10.11)$$

where $\mu(x, +\infty)$ denotes the μ -integral (4.2) along the real axis between x and $+\infty$. According to (10.9) and (10.11) we have

$$\psi(x) = a_2(+\infty) f_2(x) [1 + O(\mu)] \quad \text{for } x'' < x < +\infty \quad (10.12)$$

if $\mu = \mu(x, +\infty)$ is small compared to 1.

Similarly, if the limit $a_1(-\infty)$ is equal to zero, one can show that the limit $a_2(-\infty)$ exists and is finite, and one can derive formulae similar to (10.6), (10.7a, b), (10.8a, b), (10.9), (10.10), (10.11), and (10.12) but with $+\infty$ replaced by $-\infty$ and the inequality $x'' < x < +\infty$ in (10.11) and (10.12) replaced by $-\infty < x < x'$.

The rest of this chapter will be devoted to considerations concerning quantization conditions for bound states. Under the assumptions specified

on pp. 103-104 we have found that if the wave function $\psi(x)$ corresponds to a bound state, the limits $a_1(\pm\infty)$ are both equal to zero and that the limits $a_2(\pm\infty)$ exist and are finite and must both be different from zero in order that the wave function $\psi(x)$ shall not be identically equal to zero. Combining formula (10.6), which is valid if $a_1(+\infty) = 0$, with the corresponding formula obtained by starting from the condition $a_1(-\infty) = 0$, we get

$$\frac{F_{12}(z_0, -\infty)}{F_{22}(z_0, -\infty)} = \frac{F_{12}(z_0, +\infty)}{F_{22}(z_0, +\infty)}$$

where z_0 is any point in the complex plane. Because of the inversion formula (3.20) and the rule for matrix multiplication the last formula is equivalent to

$$F_{12}(-\infty, +\infty) = 0 \quad (10.13)$$

which is thus an exact quantization condition. It can also be obtained directly from (10.8a) by letting z tend to $-\infty$ along the real axis and remembering that for bound states $a_1(-\infty) = 0$, whereas $a_2(+\infty) \neq 0$. We shall also obtain other forms for the quantization condition. From (10.8b) and the corresponding formula obtained by replacing $+\infty$ by $-\infty$, we get

$$F_{22}(-\infty, +\infty) = \frac{F_{22}(z, +\infty)}{F_{22}(z, -\infty)} \quad (10.14a)$$

$$F_{22}(+\infty, -\infty) = \frac{F_{22}(z, -\infty)}{F_{22}(z, +\infty)}. \quad (10.14b)$$

According to the inversion rule (3.20) we have

$$F_{22}(+\infty, -\infty) = F_{11}(-\infty, +\infty)$$

and thus the relations (10.14a, b) give

$$F_{11}(-\infty, +\infty) F_{22}(-\infty, +\infty) = 1. \quad (10.15a)$$

Combining this condition with the general relation $\det \mathbf{F}(x_1, x_2) = 1$, and letting $x_1 \rightarrow -\infty$ and $x_2 \rightarrow +\infty$, we get

$$\lim_{\substack{x_1 \rightarrow -\infty \\ x_2 \rightarrow +\infty}} F_{12}(x_1, x_2) F_{21}(x_1, x_2) = 0. \quad (10.15b)$$

Analogously to (10.13), the conditions (10.14a), (10.14b), (10.15a), and (10.15b) are quantization conditions, selecting the energies for which bound states exist.

For such energy eigen-values the conditions (10.14a, b) are furthermore convenient for obtaining estimates of $F_{11}(-\infty, +\infty)$ and $F_{22}(-\infty, +\infty)$.

For that purpose we choose z in (10.14a, b) to be a point x on the real axis between x' and x'' in fig. 10.1b. As has been mentioned in chapter 3, the diagonal elements of the F -matrix do not depend on the choice of the fixed lower limit in the integral (3.3) defining $w(z)$. Independently of how this lower limit of integration has been chosen we can therefore use the estimate (6.13a) which gives

$$|F_{11}(\pm \infty, x) - 1| \leq \mu(x, \pm \infty) + \text{higher powers of } \mu(x, \pm \infty)$$

where $x' < x < x''$, and $\mu(x, \pm \infty)$ denotes the μ -integral (4.2) from x to $\pm \infty$ along such a path as is shown in fig. 6.1b or fig. 6.2b. Using these estimates in (10.14a, b), and remembering the inversion rule (3.20), we get

$$\left. \begin{aligned} |F_{11}(-\infty, +\infty) - 1| \\ |F_{22}(-\infty, +\infty) - 1| \end{aligned} \right\} \leq \mu(-\infty, +\infty) + \text{higher powers of } \mu(-\infty, +\infty) \quad (10.16)$$

where $\mu(-\infty, +\infty)$ denotes the μ -integral (4.2) from $-\infty$ to $+\infty$ along a path, the two parts of which, namely those from $-\infty$ to x and from x to $+\infty$, possess the properties described and used in section 6.3. It is emphasized that the estimates (10.16) have been derived on the assumption that the energy is that of a bound state.

We shall now proceed by taking account of the symmetry relations. If x_1 and x_2 denote any two points on the real axis such that $x_1 < x'$ and $x_2 > x''$, the symmetry relations (5.8a, d) require that

$$F_{11}(x_1, x_2) \exp \left\{ -i \left[\int_{x'}^{x''} |q(x)| dx - \frac{1}{2} \pi \right] \right\} \text{ is real} \quad (10.17a)$$

and

$$F_{22}(x_1, x_2) \exp \left\{ i \left[\int_{x'}^{x''} |q(x)| dx - \frac{1}{2} \pi \right] \right\} \text{ is real.} \quad (10.17b)$$

From these conditions it immediately follows that

$$F_{11}(x_1, x_2) F_{22}(x_1, x_2) \text{ is real.} \quad (10.18a)$$

Since $\det F(x_1, x_2) = 1$, we also find that

$$F_{12}(x_1, x_2) F_{21}(x_1, x_2) \text{ is real.} \quad (10.18b)$$

We must remember that the symmetry relations are valid not only when the energy assumes one of its eigen-values but for all energies. We thus

notice that (10.15a, b) are special cases of (10.18a, b), applicable when the energy assumes one of its eigen-values and $x_1 \rightarrow -\infty$ and $x_2 \rightarrow +\infty$. Let us return to the symmetry relations (10.17a, b) and note that they can be written as follows

$$\int_{x'}^{x''} |q(x)| dx = (r + \frac{1}{2})\pi + \arg F_{11}(x_1, x_2) \quad (10.19a)$$

$$\int_{x'}^{x''} |q(x)| dx = (s + \frac{1}{2})\pi - \arg F_{22}(x_1, x_2) \quad (10.19b)$$

where r and s are integers. We notice that the arguments of $F_{11}(x_1, x_2)$ and $F_{22}(x_1, x_2)$ do not depend on the positions of the points x_1 and x_2 in their respective regions of the real axis. Since (10.19a, b) are equivalent to the symmetry relations (10.17a, b), they are, of course, valid for all energies.

Starting from the symmetry relation (10.19b), for $x_1 = -\infty$ and $x_2 = +\infty$, and introducing the quantization condition in the form (10.14a), we get

$$\int_{x'}^{x''} |q(x)| dx = (s + \frac{1}{2})\pi - \arg \frac{F_{22}(z, +\infty)}{F_{22}(z, -\infty)}. \quad (10.20)$$

This equation must be exactly fulfilled for any value of z , if the energy is that of a bound state. It is convenient for estimating the accuracy of the semi-classical quantization condition, since the correction term appears in a closed form. Estimating this term as in the derivation of (10.16), or combining (10.16) and (10.19b), we get

$$\int_{x'}^{x''} |q(x)| dx = (s + \frac{1}{2})\pi + O[\mu(-\infty, +\infty)], \quad (10.21)$$

where $\mu(-\infty, +\infty)$ is assumed to be small compared to 1. From (10.21) we get the well-known semi-classical quantization condition

$$\int_{x'}^{x''} |q(x)| dx \approx (s + \frac{1}{2})\pi. \quad (10.22)$$

The accuracy of this approximate quantization condition is in general expected to increase with increasing energy of the bound state, since the μ -integral for an appropriate path is expected to be smaller as this energy increases. See, however, the discussion in chapter 11.

The usual method, found in most text-books, for deriving the semi-classical quantization condition is to equate inside the potential well the two

expressions for the wave function of the bound state, obtained by using the connection formula (8.21) at both of the classical turning points.

The semi-classical quantization condition is in general only approximately valid. However, in the special case of the linear harmonic oscillator it is exact provided $q^2(x) = Q^2(x)$. We shall now prove this well-known fact utilizing our results above. To simplify the notations we shall assume that the classical turning points lie symmetrically with respect to the origin (i.e., that $x' = -x''$), which is no essential restriction. In (10.14a) we shall choose the point z equal to iR , where R is a positive number ($> x''$) which we shall later allow to tend to infinity. We consider a path \mathcal{A} , which runs along the real axis from $-\infty$ to $-R$, then forms a semi-circle in the upper half-plane from $-R$ to $+R$, and again follows the real axis from $+R$ to $+\infty$. For the linear harmonic oscillator the function $Q^2(z)$ is a polynomial of the second order in z with a negative coefficient for the highest power of z . The absolute value of $\exp\{i w(z)\}$ then increases monotonically as z moves from iR to $-\infty$ or from iR to $+\infty$ along \mathcal{A} . For each one of these two parts of the path \mathcal{A} the quantity μ tends to zero as R tends to infinity, since the absolute value of the function $\varepsilon(z)q(z)$ tends to zero as a constant times $|z|^{-3}$ when $|z| \rightarrow \infty$. From (3.20) and (4.3a) we therefore get

$$\lim_{R \rightarrow \infty} F_{22}(iR, -\infty) = 1$$

$$\lim_{R \rightarrow \infty} F_{22}(iR, +\infty) = 1.$$

Using these two formulae in (10.14a) with $z = iR$, we immediately get

$$F_{22}(-\infty, +\infty) = 1.$$

Combining this formula with the symmetry relation (10.19b), we see that the semi-classical quantization condition with $q^2(x) = Q^2(x)$ is exact in the special case of the harmonic oscillator. This fact has long been well known, but the above proof illustrates it from a new point of view.

THE RADIAL EQUATION OF MOTION FOR A PARTICLE IN A CENTRAL FIELD OF FORCE

Let us consider a particle of mass m moving with the energy E in a spherically symmetric potential $V(r)$. If the wave function ψ corresponds to a definite orbital angular momentum with the quantum number l , and if the radial factor of ψ is denoted by $\chi(r)/r$, the Schrödinger equation for the motion of the particle gives the differential equation

$$\frac{d^2 \chi}{dr^2} + Q^2(r) \chi = 0 \quad (11.1)$$

where

$$Q^2(r) = \frac{2m}{\hbar^2} [E - V(r)] - \frac{l(l+1)}{r^2} \quad (11.2)$$

and \hbar denotes Planck's constant h divided by 2π . We shall consider both the unmodified JWKB-method when $q^2(r)$ is chosen as

$$q^2(r) = Q^2(r) = \frac{2m}{\hbar^2} [E - V(r)] - \frac{l(l+1)}{r^2} \quad (11.3)$$

and two different modifications when $q^2(r)$ is chosen as

$$q^2(r) = Q^2(r) - \frac{1}{4r^2} = \frac{2m}{\hbar^2} [E - V(r)] - \frac{(l+\frac{1}{2})^2}{r^2} \quad (11.4)$$

or as

$$q^2(r) = Q^2(r) + \frac{l(l+1)}{r^2} = \frac{2m}{\hbar^2} [E - V(r)]. \quad (11.5)$$

The first modification, i.e. (11.4), obviously corresponds to the well-known replacement of $l(l+1)$ by $(l+\frac{1}{2})^2$ in the usual JWKB-formulae, and the second modification, i.e. (11.5), corresponds to the omission of the centrifugal term in these formulae.

To begin with it may be of some interest to determine those functions $Q^2(r)$ for which the unmodified or either of the above mentioned two

kinds of modified JWKB-functions are exact solutions of the differential equation (11.1).

First we recall the result found in chapter 2 that the unmodified JWKB-functions are exact solutions of the differential equation (11.1) if and only if

$$Q^2(r) = (Ar + B)^{-4} \quad (11.6)$$

where A and B are arbitrary constants.

Next we shall determine the functions $Q^2(r)$ for which the modified JWKB-functions based on the choice (11.4) of $q^2(r)$ are exact solutions of the differential equation (11.1). Combining the expression for ε , obtained from (3.5a), with (11.4) and putting $\varepsilon = 0$, we get

$$\frac{d^2}{dr^2} q^{-\frac{1}{2}} + \frac{1}{4r^2} q^{-\frac{1}{2}} = 0.$$

The general solution of this differential equation is

$$q^{-\frac{1}{2}} = (C + D \ln r) r^{\frac{1}{2}}$$

where C and D are arbitrary complex constants subject only to the restriction of not being simultaneously equal to zero, since this would not give a finite function $q(r)$. Substituting the above expression for $q^{-\frac{1}{2}}$ into (11.4), we get

$$Q^2(r) = \left\{ \frac{1}{4} + (C + D \ln r)^{-4} \right\} r^{-2}. \quad (11.7)$$

If $Q^2(r)$ is given by an expression of this kind, the modification given by the second member of (11.4) thus gives modified JWKB-functions, which (in contrast to the unmodified JWKB-functions) satisfy the differential equation (11.1) exactly. As the function $Q^2(r) = A/r^2$ with $A \neq \frac{1}{4}$ is a special case of (11.7), the corresponding modified JWKB-functions are exact solutions of the differential equation (11.1). The exceptional case $Q^2 = (4r^2)^{-1}$ gives meaningless JWKB-functions since $q^2(r)$ then becomes equal to zero according to (11.4).

Finally we shall determine the functions $Q^2(r)$ for which the modified JWKB-functions based on the choice (11.5) of $q^2(r)$ are exact solutions of the differential equation (11.1). Proceeding analogously as above we substitute the expression for Q^2 obtained from (11.5) into (3.5a) and put $\varepsilon = 0$, getting

$$\frac{d^2}{dr^2} q^{-\frac{1}{2}} - \frac{l(l+1)}{r^2} q^{-\frac{1}{2}} = 0.$$

The general solution of this differential equation is

$$q^{-\frac{1}{2}} = C r^{l+1} + D r^{-l}$$

where C and D are arbitrary constants. This is actually the general solution only if $l \neq -\frac{1}{2}$. In the physical applications, however, l is the quantum number of the orbital angular momentum and is thus a non-negative integer. Substituting the above expression for $q^{-\frac{1}{2}}$ into (11.5), we get

$$Q^2(r) = (C r^{l+1} + D r^{-l})^{-4} - l(l+1) r^{-2}. \quad (11.8)$$

If $Q^2(r)$ is given by such an expression, the omission of the centrifugal barrier in the usual JWKB-functions thus gives modified JWKB-functions which satisfy the differential equation (11.1) exactly.

After having thus determined those differential equations (11.1) for which the JWKB-functions are exact solutions, we shall now turn our attention to more general functions $Q^2(r)$ and discuss in some detail the two modifications of the JWKB-method based on the choices (11.4) or (11.5) of $q^2(r)$.

11.1. The modification corresponding to the replacement of $l(l+1)$ by $(l+\frac{1}{2})^2$ in the JWKB-formulae

In this section we shall treat the modification of the JWKB-method based on the choice (11.4) for $q^2(r)$. The modified JWKB-functions are then obtained from the unmodified ones by the replacement of $l(l+1)$ by $(l+\frac{1}{2})^2$ which was originally suggested by KRAMERS in order to make the JWKB-functions useful also for the case where $V(r)$ is approximately a Coulomb potential in the neighbourhood of the origin (KRAMERS [1926]). This modification has later been discussed by KEMBLE [1937] and by LANGER [1937].

The modification of the JWKB-method considered here is useful at the origin if the function $Q^2(r)$ has there a pole of the first or second order such that

$$\lim_{r \rightarrow 0} r^2 Q^2(r) \neq \frac{1}{4}. \quad (11.9)$$

For the unmodified JWKB-method the function $\varepsilon(r)q(r)$ then tends to infinity so rapidly as r tends to zero that the μ -integral (4.2) along a path emerging from the origin is divergent. Therefore the unmodified JWKB-method does not give satisfactory results in the immediate neighbourhood of $r = 0$. This conclusion is confirmed by the fact that the unmodified JWKB-functions do not have similar dependence on r as the exact solutions

of the radial wave equation (11.1) in the neighbourhood of $r = 0$. For the modified JWKB-method, however, the function $\varepsilon(r)q(r)$ tends to a finite limit as r tends to zero, provided the condition (11.9) is fulfilled. The modified JWKB-method should then give satisfactory results in the neighbourhood of $r = 0$. This assertion is confirmed by the fact that for sufficiently small values of r the modified JWKB-functions depend on r similarly as the exact solutions of the radial wave equation (11.1), provided $Q^2(r)$ does have a pole of the second order at the origin. Otherwise the wave function that tends to a constant $\neq 0$, as r tends to zero, is an exception.

For the special case that $V(r)$ is a Coulomb potential LANGER [1937] has justified the replacement of $l(l+1)$ by $(l + \frac{1}{2})^2$ as follows. Instead of r and $\chi(r)$ he introduces new variables x and $u(x)$ by writing

$$r = \exp\{x\} \quad (11.10a)$$

$$\chi = u \exp\{\frac{1}{2}x\}. \quad (11.10b)$$

The differential equation (11.1) then becomes

$$\frac{d^2u}{dx^2} + \left\{ Q^2(r) - \frac{1}{4r^2} \right\} \exp\{2x\} u = 0 \quad (11.11)$$

where we have retained the variable r in the expression in the brackets in order to show clearly the structure of this expression. Langer solves the differential equation (11.11) approximately by means of the usual unmodified JWKB-method. When he writes the resulting approximate solution in terms of the original variables, he obtains the usual JWKB-functions of the original differential equation (11.1) but with $l(l+1)$ replaced by $(l + \frac{1}{2})^2$. We realize that Langers' transformation will work very well in all those cases where the unmodified μ -integral (4.2) from $r = 0$, i.e. $x = -\infty$, is divergent for the differential equation (11.1) but convergent for the differential equation (11.11). It is seldom pointed out in the literature that there is such a restriction on the usefulness of Langer's transformation, and it seems to have been forgotten that Langer used this transformation only for the special case of a Coulomb potential.

When reading papers where radial wave equations are solved approximately by means of the JWKB-method one very often gets the misleading impression that the replacement of $l(l+1)$ by $(l + \frac{1}{2})^2$ in JWKB-formulae should always improve these formulae. As mentioned above this replacement actually improves the JWKB-approximation considerably for small values

of r , if the function $Q^2(r)$ has a pole of the first or second order for $r = 0$ and fulfils the condition (11.9). For other potentials or for larger values of r , however, it may be preferable not to replace $l(l+1)$ by $(l+\frac{1}{2})^2$. In quantal applications the function $Q^2(r)$ is usually meromorphic and different from zero for $r = \infty$. For sufficiently large values of r the quantity $\varepsilon(r)q(r)$ is then smaller for the choice (11.3) of $q^2(r)$ than for the choice (11.4). In such quantal problems one should therefore in general not replace $l(l+1)$ by $(l+\frac{1}{2})^2$ for large values of r .

The absolute value of the ratio of the function $\varepsilon(r)q(r)$ for $q^2(r)$ chosen according to (11.3) and the corresponding function for $q^2(r)$ chosen according to (11.4) gives a criterion for whether a linear combination of the unmodified or a linear combination of the modified JWKB-functions gives the best fit to an exact solution of the differential equation (11.1) in the immediate neighbourhood of a point where this linear combination and its first derivative have been fitted exactly to the corresponding quantities for an exact solution of the differential equation (11.1). As long as r lies in an interval where this ratio does not pass through the value 1, it is reasonable to use the kind of JWKB-functions which corresponds to the smaller one of the two functions $|\varepsilon(r)q(r)|$ in the whole interval. As one passes through a point where the ratio passes through the value 1, it is reasonable to expect that the approximation is improved if one changes to the other type of JWKB-functions by fitting the two types of JWKB-functions and their derivatives at the point where the ratio is equal to 1. This would certainly be rigorously true if the exact solution and its derivative were exactly the same as the corresponding quantities for the linear combination of the JWKB-functions at the point where the above-mentioned ratio is equal to 1. Although this is in general not the case, the suggested procedure of changing from one type of JWKB-functions to the other type at a point where the ratio passes the value 1 seems to be sound, but another question is whether one gains so much in accuracy that it is worth the complication involved in the procedure.

We shall now consider in more detail the modification (11.4) of the JWKB-approximation for the radial wave equation (11.1). First we shall draw certain conclusions from the requirement that the solution $\chi(r)$ shall tend to zero as the positive variable r tends to zero. Replacing in (3.25a) $\psi(z)$ by $\chi(r)$ and using (3.24a, b), we get

$$\chi(r) = \{a_1(r) + a_2(r) \exp\{-2i w(r)\}\} f_1(r).$$

If the μ -integral from the origin along a part of the positive real axis is convergent, and if the absolute value of $\exp\{i w(r)\}$ increases monotonically and tends to infinity as r tends to zero through positive values, we can apply the formulae (4.6a, b) according to which

$$\lim_{r \rightarrow +0} a_1(r) \text{ exists and is finite}$$

$$\lim_{r \rightarrow +0} a_2(r) \exp\{-2i w(r)\} = 0.$$

If the function $f_1(r)$ does not tend to zero as r tends to zero, the above formula for $\chi(r)$ therefore shows that in order that $\chi(+0) = 0$ the limit $a_1(+0)$ must be equal to zero. Using this result in the formula corresponding to (10.5) but with $+\infty$ replaced by $+0$, we can in a similar way as in chapter 10 show that the limit $a_2(+0)$ exists and that the a -coefficients are given by the formulae

$$a_1(z) = F_{12}(z, +0) a_2(+0) \quad (11.12a)$$

$$a_2(z) = F_{22}(z, +0) a_2(+0) \quad (11.12b)$$

which are analogous to (10.8a, b). One can then obtain formulae analogous to (10.9), (10.10), (10.11), and (10.12), but we shall not consider these formulae here. The conditions for the validity of (11.12a, b) are seen to be fulfilled in the physically important case when $q^2(z)$ is a meromorphic function with a pole of the second order for $z = 0$ such that

$$\lim_{r \rightarrow 0} r^2 q^2(r) \leq -\frac{1}{4} \quad (11.13)$$

provided the phase of $q(r)$ is defined conveniently.

From (3.20) and (3.22a) it follows that the matrix element $F_{22}(z, z_0)$ is an analytic function of z_0 which may have a branch point for $z_0 = 0$. Furthermore, the limit of $F_{22}(z, z_0)$ as z_0 tends to zero exists and is finite. We shall in the following use the fact that this limit is independent of how z_0 tends to zero.

Let us now study the case when the radial wave function $\chi(r)$ corresponds to a bound state. If the function $\exp\{i w(r)\}$ tends to infinity so rapidly as r tends to infinity that

$$\int_0^\infty |f_1(r)|^2 dr = \infty \quad (11.14)$$

and if the μ -integral along the positive real axis from a conveniently chosen point to infinity is convergent, we can take over the following formulae

directly from chapter 10

$$a_1(z) = F_{12}(z, +\infty) a_2(+\infty) \quad (11.15a)$$

$$a_2(z) = F_{22}(z, +\infty) a_2(+\infty) \quad (11.15b)$$

where $a_2(+\infty)$ must be different from zero in order that the wave function $\chi(r)$ shall not be identically zero. Letting z tend to zero through positive values in (11.15a, b), we get the formulae

$$a_1(+0) = F_{12}(+0, +\infty) a_2(+\infty) \quad (11.16a)$$

$$a_2(+0) = F_{22}(+0, +\infty) a_2(+\infty). \quad (11.16b)$$

We have previously found that $a_1(+0) = 0$ for bound states, and hence (11.16a) gives the quantization condition

$$F_{12}(+0, +\infty) = 0 \quad (11.17)$$

which is analogous to (10.13). From (11.12b), (11.15b), and (11.16b) one obtains the following more convenient quantization condition

$$F_{22}(+0, +\infty) = \frac{F_{22}(z, +\infty)}{F_{22}(z, +0)} \quad (11.18)$$

where z is an arbitrary point in the complex plane. This formula is analogous to (10.14a). If there is on the positive real axis only one region $r' < r < r''$ where $q^2(r) > 0$ as in fig. 10.1, the formulae (10.16) to (10.20) can be taken over here after the notations have been changed appropriately. Corresponding to (10.16) we have the estimate

$$|F_{22}(+0, +\infty) - 1| \leq \mu(0, \infty) + \text{higher powers of } \mu(0, \infty). \quad (11.19)$$

Corresponding to (10.20) we have the quantization condition

$$\int_{r'}^{r''} |q(r)| dr = (s + \frac{1}{2})\pi - \arg \frac{F_{22}(z, +\infty)}{F_{22}(z, +0)} \quad (11.20)$$

where s is an integer, and z is an arbitrary point in the complex plane. If $\mu(0, \infty) \ll 1$ the last term on the right-hand side of (11.20) is at the most of the order of magnitude $\mu(0, \infty)$. Neglecting this term, we get the approximate semi-classical quantization condition

$$\int_{r'}^{r''} |q(r)| dr \approx (s + \frac{1}{2})\pi. \quad (11.21)$$

To illustrate further the properties of the modification of the JWKB-approximation discussed in this section, we shall now consider a few special cases of radial wave equations which we shall discuss in some detail.

11.1.1. APPLICATION TO THE RADIAL WAVE EQUATION FOR HYDROGEN-LIKE IONS

For a hydrogen-like ion we have $V(r) = -Ze^2/r$, i.e.,

$$Q^2(r) = \frac{2m}{\hbar^2} \left[E + \frac{Ze^2}{r} \right] - \frac{l(l+1)}{r^2} \quad (11.22)$$

where e is the electronic charge and Z is the atomic number. The possible energy eigen-values are given by the formula

$$E = -\frac{me^4Z^2}{2\hbar^2n^2}$$

where n is the principal quantum number.

The above function $Q^2(r)$ has a pole of the first or second order at the origin, and it also fulfils the condition (11.9). Hence the unmodified JWKB-approximation is not good in the neighbourhood of the origin, whereas the modified JWKB-approximation corresponding to the replacement of $l(l+1)$ by $(l + \frac{1}{2})^2$ in the JWKB-functions is useful there.

For sufficiently large values of r we find that the function $\varepsilon(r)q(r)$ is of the order $O(r^{-3})$ for the unmodified JWKB-method but of the order $O(r^{-2})$ for the modified JWKB-method. Thus we expect that the unmodified JWKB-functions should be somewhat preferred to the modified ones for large values of r .

We shall now use our approach to the JWKB-method to prove the well-known fact that the semi-classical quantization condition with the function $q^2(r)$ chosen according to (11.4) gives the exact values of the energy levels for hydrogen-like ions. In the following mathematical treatment we shall allow the independent variable r to assume arbitrary values on the real axis (except for the origin and the zeros of q^2) and in the upper half of the complex plane, and therefore we find it convenient to denote this variable by z instead of r . The function $q^2(z)$ has two simple zeros, which never coincide. They lie on the real axis to the right of the origin and will be denoted by r' and $r'' (> r')$. These points as well as the origin are branch points for the functions $q(z)^{\frac{1}{2}}$ and $w(z)$. In fig. 11.1 we have indicated the phase of $q(z)^{\frac{1}{2}}$ on the different parts of the real axis (cf. fig. 10.1). The same

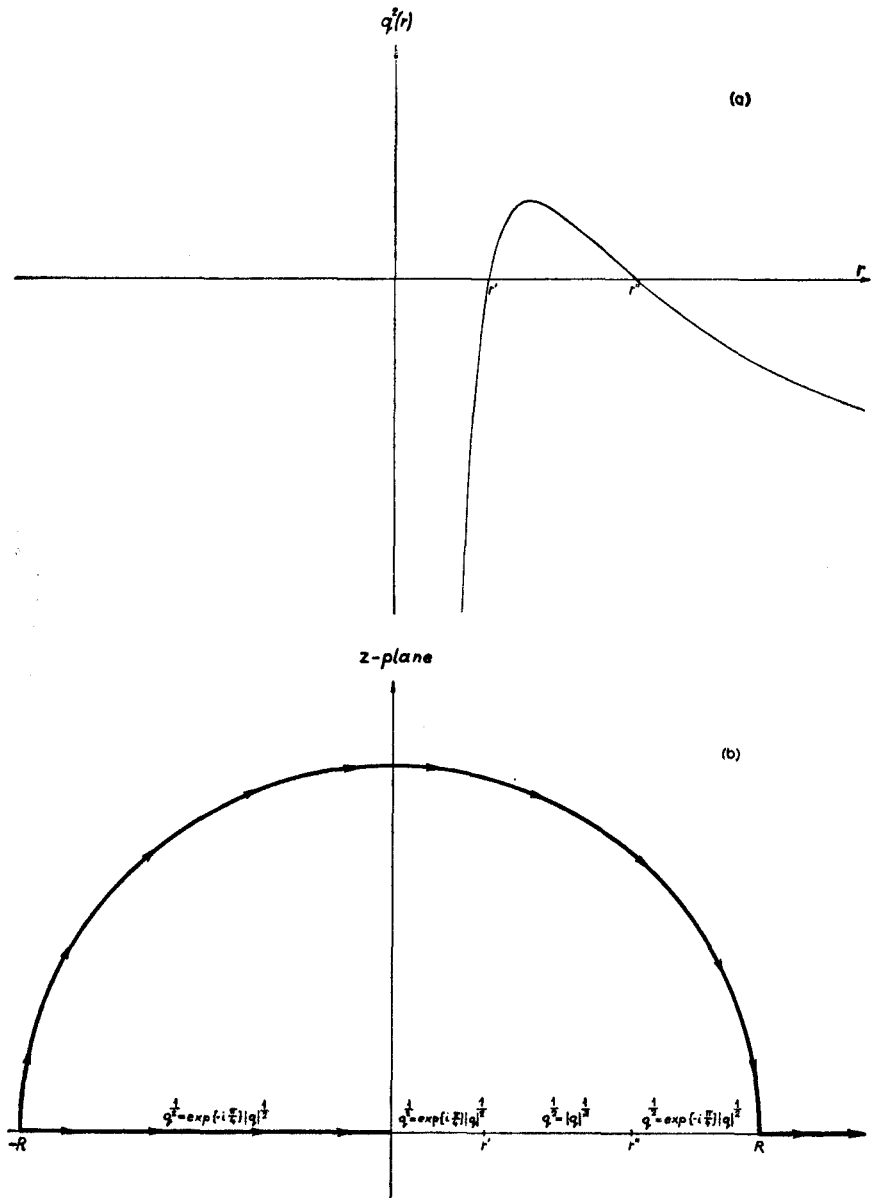


Fig. 11.1

figure also shows paths of integration which we shall use later. The directions in which the absolute value of $\exp\{i\omega\}$ increases monotonically along these paths have been indicated by arrows.

The conditions for the validity of (11.20) are fulfilled for all possible values of the quantum number l , and our aim presently will thus be to show that the quotient $F_{22}(z, +\infty)/F_{22}(z, +0)$ is real. As we have found previously, the limit in the denominator of this quotient is independent of how one approaches the origin, and we can therefore replace $F_{22}(z, +0)$ by $F_{22}(z, -0)$. Choosing z equal to a negative number $-R$, we then get a convenient form for the quotient considered, namely

$$\frac{F_{22}(z, +\infty)}{F_{22}(z, +0)} = \frac{F_{22}(-R, +\infty)}{F_{22}(-R, -0)}. \quad (11.23)$$

According to the symmetry relations (6.6) the elements of the matrix $F(-R, -0)$ are all real if the lower limit in the integral (3.3) defining $w(z)$ is chosen conveniently. Since the diagonal elements of the F -matrix are independent of this lower limit, it is in particular always true that

$$F_{22}(-R, -0) \quad \text{is real.} \quad (11.24)$$

Turning our attention to $F_{22}(-R, +\infty)$, we choose as the path of integration the semi-circle of radius $R (> r'')$ in the upper half-plane joining the points $-R$ and $+R$ completed by the real axis from $+R$ to $+\infty$. The absolute value of $\exp\{i\omega\}$ is then monotonically increasing along the whole path from $-R$ to $+\infty$, and according to (4.3a) and (3.20) we have

$$|F_{22}(-R, +\infty) - 1| \leq \frac{1}{2} [\exp\{\mu(-R, +\infty)\} - 1].$$

Noting that the right-hand side of this inequality tends to zero as R tends to ∞ , we then get

$$\lim_{R \rightarrow \infty} F_{22}(-R, +\infty) = 1. \quad (11.25)$$

From (11.20), (11.23), (11.24), and (11.25) it now follows that the semi-classical quantization condition

$$\int_{r'}^{r''} |q(r)| dr = (s + \frac{1}{2})\pi \quad (11.26)$$

where s is an integer, is exactly fulfilled. We emphasize that this conclusion is valid only for the modified function $q(r)$ obtained by replacing in the unmodified function $Q(r)$ the quantity $l(l+1)$ by $(l + \frac{1}{2})^2$.

We shall also say a few words about the radial wave function $\chi(r)$ in the

classically allowed region $r' < r < r''$. We choose $w(r') = 0$ and from (3.25a), (3.24a, b), (11.12a, b), (3.20), and (6.10a) we get

$$\chi(r) = 2 a_2(+0) \exp\left\{-\frac{1}{4}i\pi\right\} |F_{11}(0, r)| q(r)^{-\frac{1}{2}} \cos\left\{w(r) - \frac{1}{4}\pi - \arg F_{11}(0, r)\right\}. \quad (11.27)$$

If the principal quantum number n and the azimuthal quantum number l have such values that there is a convenient path similar to that in fig. 6.1b connecting 0 and r for which the μ -integral is small compared to 1, the formula (11.27) becomes

$$\chi(r) \approx 2 a_2(+0) \exp\left\{-\frac{1}{4}i\pi\right\} q(r)^{-\frac{1}{2}} \cos\left\{w(r) - \frac{1}{4}\pi\right\} \quad (11.28)$$

because of the estimate (6.13a). However, the μ -integral is of the order $(2l+1)^{-1}$ and is therefore not small compared to 1 unless l is large. In section 11.2 we shall consider another modification of the JWKB-method for which the μ -integral (now for the path in fig. 7.2a) is small compared to 1 if $l + \frac{1}{2} \ll \sqrt{n}$.

11.1.2. APPLICATION TO THE THREE-DIMENSIONAL HARMONIC OSCILLATOR

For the three-dimensional harmonic oscillator we have $V(r) = \frac{1}{2}m\omega^2 r^2$, i.e.,

$$Q^2(r) = \frac{2m}{\hbar^2} \left[E - \frac{1}{2}m\omega^2 r^2 \right] - \frac{l(l+1)}{r^2}. \quad (11.29)$$

The possible energy eigen-values are given by the formula

$$E = (n + l + \frac{1}{2})\hbar\omega$$

where n is an odd positive integer.

When $l = 0$ and r tends to zero, the function $\varepsilon(r)q(r)$ tends to a finite limit which is different from zero in the unmodified case but equal to zero in the modified case. The modified JWKB-functions are therefore expected to be better than the unmodified ones in the neighbourhood of the origin. Actually the unmodified JWKB-functions are not satisfactory, whereas the modified JWKB-functions are good, as is easily confirmed by comparing them with the exact solutions obtained as power series in the neighbourhood of the origin.

When $l > 0$ the function $Q^2(r)$ has a pole of the second order at the origin, and the condition (11.9) is fulfilled. The modified JWKB-functions are then

undoubtedly to be preferred to the unmodified ones in the neighbourhood of the origin. This is confirmed by the fact that the modified JWKB-functions have the right behaviour for small values of r in contrast to the unmodified ones.

As r tends to infinity, the functions $\varepsilon(r)q(r)$ for the unmodified and for the modified cases both tend to zero as r^{-3} , and the quotient of these two functions tends to $\frac{3}{4}$. For large values of r the unmodified JWKB-functions should therefore be slightly preferred to the modified ones.

We shall now show that for the modified JWKB-method the semi-classical quantization condition gives the exact values of the energy levels for all possible values of the quantum number l . Instead of r we introduce the complex variable z . According to (11.4) and (11.29) the function $q^2(z)$ has all its four zeros on the real axis. We denote these zeros by $\pm r'$ and $\pm r''$ where r' and $r'' (> r')$ are positive quantities. In fig. 11.2 we have given the phase of $q(z)$ on the real and imaginary axes and indicated by arrows the directions in which the absolute value of $\exp\{i w\}$ increases on the paths shown in the figure. The conditions for the validity of the quantization condition (11.20) with the modified function $q^2(r)$ are fulfilled for all possible values of the quantum number l (including $l = 0$). Choosing $z = iR$, where R is a positive number, and replacing $F_{22}(z, +0)$ by $F_{22}(z, +i0)$, which is allowed as mentioned previously, we can write the quotient appearing in the last term on the right-hand side of (11.20) as follows

$$\frac{F_{22}(z, +\infty)}{F_{22}(z, +0)} = \frac{F_{22}(iR, +\infty)}{F_{22}(iR, +i0)}. \quad (11.30)$$

From formula (3.22d) we easily see that $F_{22}(iR, ir)$ is a real quantity if R and r are positive numbers. Thus the denominator in the right member of (11.30) is real. We shall next consider the numerator $F_{22}(iR, +\infty)$ in the right member of the same formula. From our knowledge of the behaviour of the function $\varepsilon(z)q(z)$ for large values of $|z|$ we easily find that the μ -integral (4.2) for the path from iR along the circular arc of radius $R (> r'')$ down to the positive real axis and then continuing to $+\infty$ along the real axis tends to zero as R tends to infinity. Using the inversion formula (3.20) and the basic estimate (4.3a), we therefore get

$$\lim_{R \rightarrow +\infty} F_{22}(iR, +\infty) = 1.$$

Since the argument of the quotient $F_{22}(iR, +\infty)/F_{22}(iR, +i0)$ is thus seen to be a multiple of π in the limit when $R = \infty$, we find from (11.20) and (11.30)

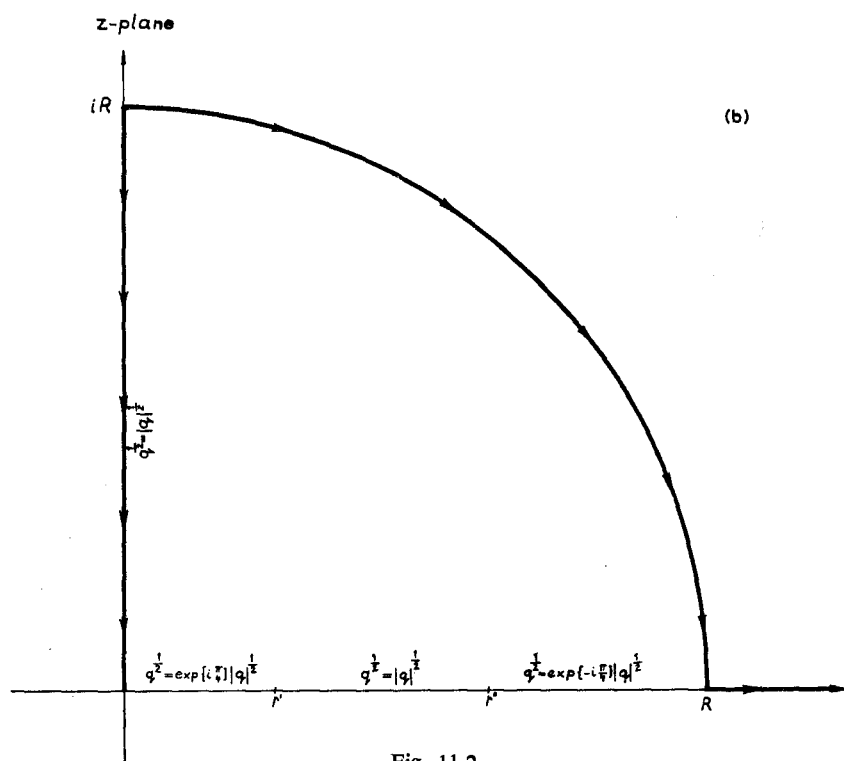
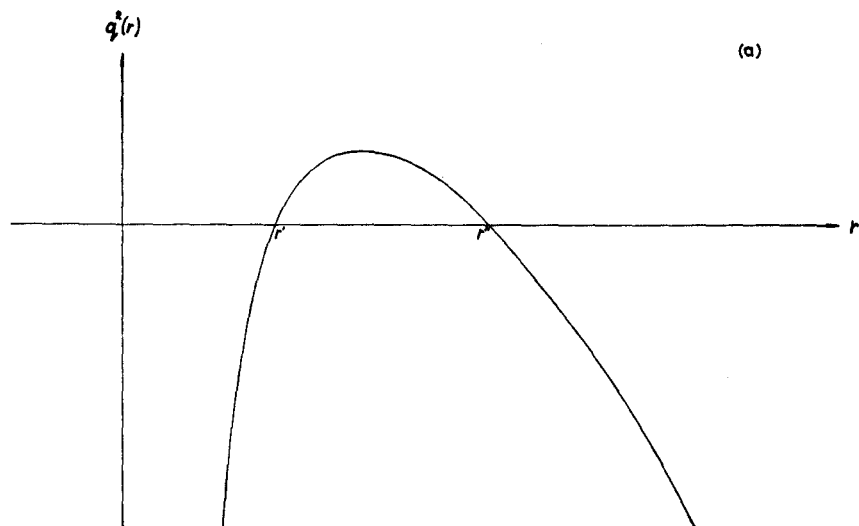


Fig. 11.2

that the semi-classical quantization condition

$$\int_{r'}^{r''} |q(r)| dr = (s + \frac{1}{2})\pi, \quad (11.31)$$

where s is an integer, is exactly fulfilled. Thus, the semi-classical quantization condition with the modified function $q(r)$ gives the exact energy eigen-values for all possible values of the quantum number l (including $l = 0$).

We shall next show that for $l = 0$ the exact values of the energy levels are given by the semi-classical quantization condition not only for the modified JWKB-method but also for the unmodified one. This can easily be realized by using the corresponding result for the linear harmonic oscillator and noting that, in contrast to the wave function $\psi(x)$ of the linear oscillator, the radial wave function $\chi(r)$ of the three-dimensional oscillator must be zero for $r = 0$. When $l = 0$ the radial wave functions $\chi(r)$ of the three-dimensional harmonic oscillator are therefore the same as those wave functions $\psi(x)$ of the linear harmonic oscillator for which the quantum number n in the formula $E = (n + \frac{1}{2})\hbar\omega$ for the energy levels assumes odd values. We find it, however, illuminating to show the exact validity of the semi-classical quantization condition for $l = 0$ and with the unmodified function $Q^2(r)$ also in a similar way as we have just shown its exact validity when the modified function $q^2(r)$ is used. The procedure used in that case cannot be taken over directly, since now $|\exp\{i\omega(r)\}|$ does not tend to infinity as $r \rightarrow +0$ and hence the conditions for the validity of (11.20) are not fulfilled. In the present case we proceed instead as follows. The zeros of the function $q^2(z) = Q^2(z)$ are $z = \pm r''$ where we let r'' denote the zero on the positive part of the real axis. A graphical representation of the function $q^2(r) = Q^2(r)$ is shown in fig. 11.3a. The phase of $q(z)^\dagger$ in the complex plane is chosen according to fig. 11.3b. This figure also shows the paths of integration to be used later on. The arrows on these paths show the directions in which the absolute value of $\exp\{i\omega(z)\}$ increases. From the formula $\chi(z) = f(z) a(z)$ and the definition (3.23) and (3.24a, b) of $f(z)$ we find that the condition that $\chi(+0)$ is equal to zero can be written as follows

$$a_1(+0) \exp\{i\omega(+0)\} + a_2(+0) \exp\{-i\omega(+0)\} = 0.$$

Introducing in this equation the expressions (11.16a, b) for $a_1(+0)$ and $a_2(+0)$, we get

$$F_{12}(+0, +\infty) = -\exp\{-2i\omega(+0)\} F_{22}(+0, +\infty). \quad (11.32)$$

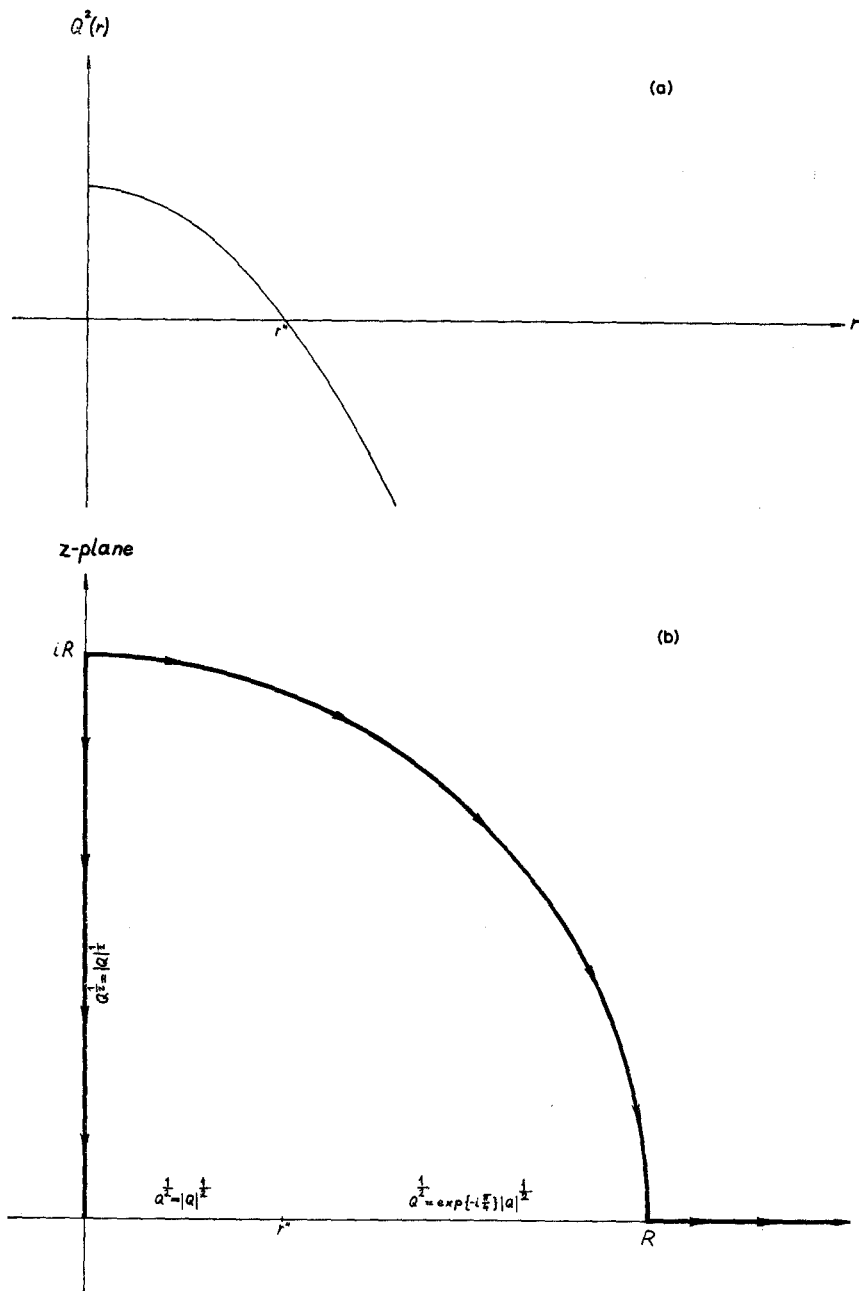


Fig. 11.3

Another relation between $F_{12}(+0, +\infty)$ and $F_{22}(+0, +\infty)$ is provided by the symmetry relations. If we choose the fixed lower limit in the integral (3.3) defining $w(z)$ to be r'' , we can apply the formulae (6.10a) and (3.20) to obtain

$$F_{12}(+0, +\infty) = i F_{22}^*(+0, +\infty). \quad (11.33)$$

From (11.32) and (11.33) we easily obtain the following exact quantization condition

$$\int_0^{r''} |Q(r)| dr = (s - \frac{1}{4})\pi - \arg F_{22}(+0, +\infty) \quad (11.34)$$

where s is an integer. We shall now show that the argument of the quantity $F_{22}(+0, +\infty)$ appearing in (11.34) is a multiple of π . In the 22-element of the matrix equation

$$F(z, +\infty) = F(z, +0) F(+0, +\infty)$$

we substitute the formula (11.32) for $F_{12}(+0, +\infty)$ and use the inversion formula (3.20), getting

$$F_{22}(+0, +\infty) = \frac{F_{11}(+\infty, z)}{F_{11}(+0, z) + \exp\{-2i w(+0)\} F_{21}(+0, z)}.$$

We now choose $z = iR$, where $R (> r'')$ is a positive number which shall later be made to tend to infinity. In the expression on the right-hand side of the above formula the numerator tends to 1 as $R \rightarrow \infty$ because of the estimate (4.3a), and the denominator is real because of the formula (3.42a) and the fact that according to (3.5) and fig. 11.3b the quantity ε is real on the imaginary axis. Thus the argument of the quantity $F_{22}(+0, +\infty)$ is a multiple of π . From (11.34) we therefore obtain exactly the semi-classical quantization condition

$$\int_0^{r''} |Q(r)| dr = (s - \frac{1}{4})\pi \quad (11.35)$$

where s is an integer.

11.1.3. APPLICATION TO THE DETERMINATION OF THE ASYMPTOTIC PHASES IN SCATTERING PROBLEMS

If the condition (11.13) is fulfilled, the boundary condition $\chi(0) = 0$ selects a solution $\chi(r)$ of the differential equation (11.1) which is unique except for an arbitrary constant factor. If, furthermore, the potential

$V(r)$ tends to zero faster than $1/r$ as r tends to infinity, the solution $\chi(r)$ is (except for a constant factor) for large values of r represented by the well-known asymptotic formula

$$\chi(r) \sim \sin(kr - \frac{1}{2}\pi l + \eta_l) \quad (11.36)$$

where k is a constant defined by

$$E = \frac{\hbar^2 k^2}{2m} \quad (11.37)$$

and η_l is a constant called the asymptotic phase corresponding to the quantum number l of the angular momentum. Assuming the above mentioned conditions for the validity of (11.36) to be fulfilled, we shall derive an expression for the asymptotic phase η_l in terms of the F -matrix connecting the points $+0$ and $+\infty$. Instead of r we introduce the complex variable z . Furthermore we cut the complex z -plane and define the phase of $q(z)^{\frac{1}{2}}$ such that $q(r) = |q(r)|$ for large positive values of r and that $q(r) = i|q(r)|$ for small positive values of r . In the integral (3.3) defining $w(z)$ we choose the fixed lower limit of integration such that $w(r)$ is real for large positive values of r . Substituting (3.24a, b) and (11.12a, b) into the formula (3.25a) and using (3.20), we get

$$\chi(r) = a_2(+0) q(r)^{-\frac{1}{2}} \{F_{11}(+0, r) \exp\{-i w(r)\} - F_{12}(+0, r) \exp\{i w(r)\}\}. \quad (11.38)$$

The symmetry relation (5.9a) shows that

$$|F_{12}(+0, r)| = |F_{11}(+0, r)|$$

if r lies in the classically allowed region extending to $+\infty$. For such values of r the formula (11.38) can therefore be written as follows

$$\begin{aligned} \chi(r) = & 2 a_2(+0) q(r)^{-\frac{1}{2}} F_{11}(+0, r) \exp\left\{i \left[\frac{1}{2} \arg \frac{F_{12}(+0, r)}{F_{11}(+0, r)} - \frac{\pi}{2} \right]\right\} \times \\ & \times \sin\left(w(r) + \frac{1}{2} \arg \frac{F_{12}(+0, r)}{F_{11}(+0, r)}\right). \quad (11.39a) \end{aligned}$$

Comparing this formula with (11.36), we get

$$\eta_l = \lim_{r \rightarrow \infty} [w(r) - kr] + \frac{1}{2}l\pi + \frac{1}{2} \arg \frac{F_{12}(+0, +\infty)}{F_{11}(+0, +\infty)}. \quad (11.39b)$$

Let us now consider the case shown in fig. 11.4a where the function $q^2(z)$ has one single zero r' on the positive part of the real axis, the region to the right of r' being classically allowed in the generalized sense, and the region between r' and the origin being classically forbidden in the generalized

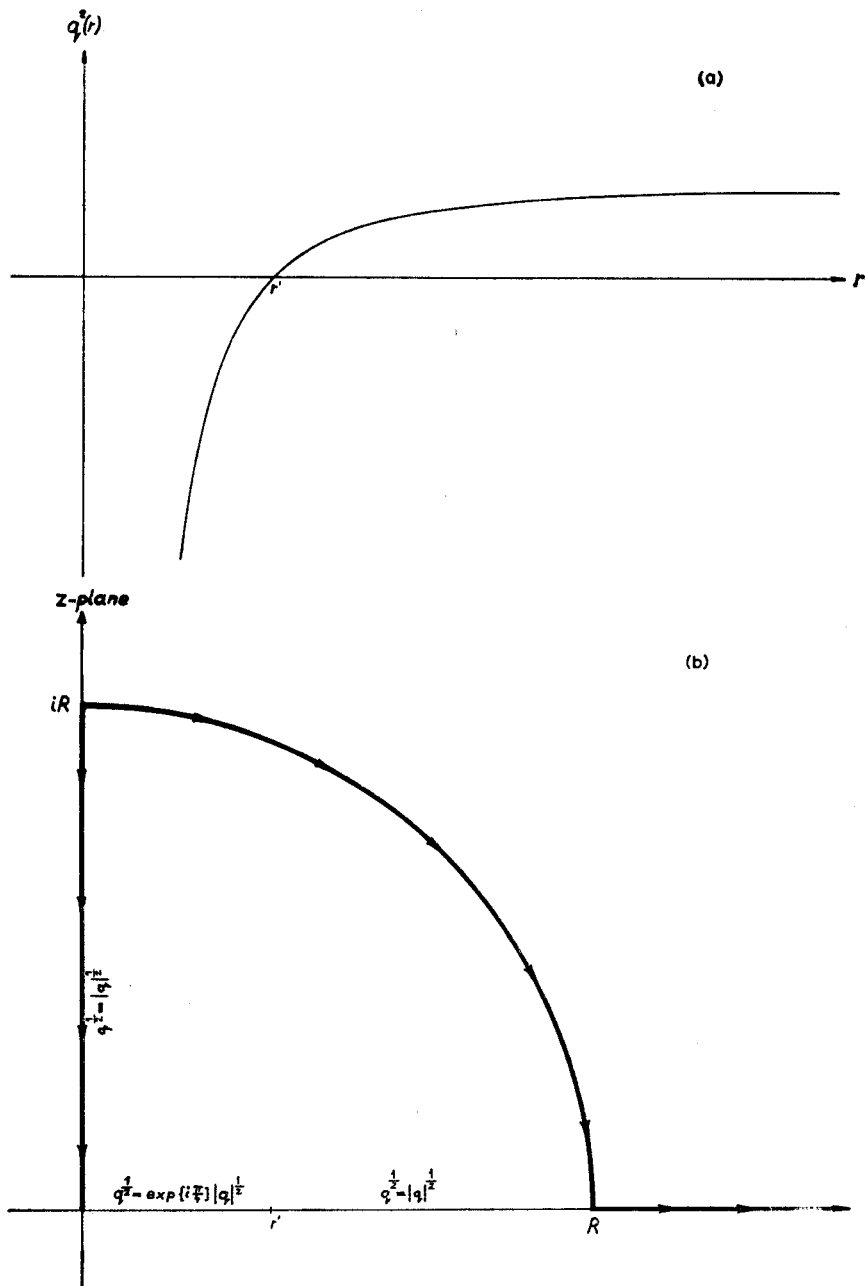


Fig. 11.4

sense. If the fixed lower limit in the integral (3.3) defining $w(z)$ is chosen to be equal to r' , we have according to (6.10a) the symmetry relation

$$F_{12}(+0, r) = i F_{11}^*(+0, r) \quad \text{for } r > r'$$

by means of which the formulae (11.39a, b) can be written as follows

$$\begin{aligned} \chi(r) = & 2a_2(+0) \exp\{-\frac{1}{4}\pi i\} |F_{11}(+0, r)| q(r)^{-\frac{1}{2}} \times \\ & \times \cos \left[\int_{r'}^r q(r) dr - \frac{1}{4}\pi - \arg F_{11}(+0, r) \right] \end{aligned} \quad (11.40a)$$

and

$$\eta_l = \int_{r'}^{\infty} [q(r) - k] dr - kr' + (l + \frac{1}{2}) \frac{1}{2}\pi - \arg F_{11}(+0, +\infty). \quad (11.40b)$$

If there exists a path as in fig. 6.1b for which $\mu = \mu(+0, +\infty)$ is small compared to 1, we have according to (6.13a) the estimate

$$|F_{11}(+0, +\infty) - 1| \leq \mu + \text{higher powers of } \mu$$

and hence

$$|\arg F_{11}(+0, +\infty)| \leq \mu + \text{higher powers of } \mu.$$

The error in the modified JWKB-approximation for the phase η_l , obtained by neglecting the term $\arg F_{11}(+0, +\infty)$ in (11.40b), is therefore at the most of the magnitude μ . Sometimes the absolute value of $\arg F_{11}(+0, +\infty)$ is much less than we can conclude from the above estimate, and the JWKB-approximation for η_l is then much better than one could expect from the value of the μ -integral. Thus there are cases where the absolute value of $\arg F_{11}(+0, +\infty)$ is small compared to 1, although the μ -integral is not small compared to 1. According to (11.40a) the right member of the connection formula (8.21) has then approximately the right phase, whereas the amplitude may differ considerably from the right value.

To illustrate the important fact that the absolute value of $\arg F_{11}(+0, +\infty)$ may sometimes be much smaller than the μ -integral, we consider the potential

$$V(r) = \beta \frac{\hbar^2}{2mr^2} \quad (11.41)$$

where β is a real constant. According to (11.2) and (11.37) we have

$$Q^2(r) = k^2 - \{\beta + l(l+1)\}r^{-2} \quad (11.42)$$

and hence

$$q^2(r) = k^2 - \{\beta + (l + \frac{1}{2})^2\} r^{-2}. \quad (11.43)$$

In order that the condition (11.13) be fulfilled for all possible values of the quantum number l , the constant β is assumed to be non-negative. The conditions for the validity of the formulae (11.40a, b) are then fulfilled for every possible value of the quantum number l . In fig. 11.4b we have given some useful information on the phase chosen for $q(z)^\dagger$ and indicated by arrows the directions in which the absolute value of $\exp\{i w\}$ increases along certain paths. We shall now apply the formula (6.12a) with $x_1 = +0$, $x_2 = +\infty$, and $z_0 = iR$. Using also the basic estimates (4.3) and letting R tend to infinity, we get

$$F_{11}(+0, +\infty) = F_{11}(+0, +i\infty).$$

Since the limit of $F_{11}(z, +\infty)$ as z tends to zero is independent of the path along which z tends to zero, the last formula can be written as follows

$$F_{11}(+0, +\infty) = F_{11}(+i0, +i\infty). \quad (11.44)$$

From (3.5), (11.42), and (11.43) it follows that the quantity ε is real on the imaginary axis. If in the formula (3.22a) we choose $w_0 = +i\infty$ and $w = +i0$ and use the path of integration along the imaginary axis of the z -plane, all terms in the series on the right-hand side of (3.22a) are real, and hence $F_{11}(+i0, +i\infty)$ is a real number. Using the basic estimate (4.3a) and the definition (4.2) of the μ -integral, we get the rough estimate

$$|F_{11}(+i0, +i\infty) - 1| < 1.$$

Hence $F_{11}(+i0, +i\infty)$ is not only real but also positive. According to (11.44) the matrix element $F_{11}(+0, +\infty)$ is also real and positive, and therefore $\arg F_{11}(+0, +\infty)$ is exactly zero. Hence it follows from (11.40b) that the modified JWKB-formula

$$\eta_l = \int_{r'}^{\infty} [q(r) - k] dr - kr' + (l + \frac{1}{2}) \frac{1}{2} \pi \quad (11.45)$$

gives the exact value of η_l in the special example considered above. Evaluating the integral in (11.45), we get

$$\eta_l = -\{\beta + (l + \frac{1}{2})^2\}^\dagger - (l + \frac{1}{2}) \frac{1}{2} \pi. \quad (11.46)$$

In the special case considered here the solution of the differential equation

(11.1) which vanishes at the origin is (except for an arbitrary constant factor) equal to \sqrt{r} times the Bessel function of the first kind and the order $[\beta + (l + \frac{1}{2})^2]^{\frac{1}{2}}$. The formula (11.46) can therefore also be obtained by using the asymptotic expansion of this Bessel function for large values of r .

We shall conclude this section by making some remarks about the scattering of a charged particle of velocity $v (= \hbar k/m)$ against a screened (attractive or repulsive) Coulomb potential $V(r) = \mp Ze^2/r$. For values of r that are not too large the screening can be neglected, and we have approximately

$$Q^2(r) = k^2 \pm \frac{2\eta k}{r} - \frac{l(l+1)}{r^2}$$

where

$$\eta = \frac{Ze^2}{\hbar v}.$$

The modified function $q^2(r)$ defined by (11.4) is

$$q^2(r) = Q^2(r) - \frac{1}{4r^2} = k^2 \pm \frac{2\eta k}{r} - \frac{(l + \frac{1}{2})^2}{r^2}.$$

Estimating the μ -integral along a convenient path from the origin to the point at infinity on the positive real axis, we find that the μ -integral is of the order of magnitude $(2l+1)^{-1}$ and is thus small compared to 1, only when l is large. At first sight it therefore seems dangerous to neglect the term $\arg F_{11}(+0, +\infty)$ in (11.40b) unless l is large. However, for any value of l , $\arg F_{11}(+0, +\infty)$ tends to zero as η tends to zero. Thus, for sufficiently small values of $|\eta|$ the approximate value of the scattering phase obtained by neglecting $\arg F_{11}(+0, +\infty)$ in (11.40b) is always good although the μ -integral is not small for small values of the quantum number l .

LANGER [1937] has remarked that, when the potential is attractive and the quantum number l is small, as well as when the potential is repulsive and the energy is very large (i.e. η is very small), the classical turning point on the positive real axis lies so close to the origin that the use of the connection formulae (8.20) and (8.21) is questionable and is generally less satisfactory than otherwise. In this connection we also refer to our previous remark in this section on the connection formula (8.21).

If the potential is attractive and $l + \frac{1}{2} \ll \sqrt{\eta}$, one may use another modification of the JWKB-method, which will be treated in the following section of this chapter.

11.2. The modification corresponding to the omission of the centrifugal barrier in the JWKB-formulae

In this section we shall consider the modification of the JWKB-method corresponding to the choice (11.5) of $q^2(r)$. We shall treat the case that this function $q^2(r)$ has a pole of the first order at the origin. To begin with we also assume that $q^2(r)$ is positive in a certain region immediately to the right of the origin. Defining the function $q(r)$ to be positive in this region and choosing the lower limit in the integral (3.3) defining $w(r)$ to be the origin, we have in the above mentioned region where $q^2(r)$ is positive

$$w(r) = \int_0^r q(r) dr > 0. \quad (11.47)$$

From (7.28) we get

$$\chi(r) \approx (\pi c)^{-\frac{1}{2}} q(r)^{-\frac{1}{2}} \cos[w(r) - (l + \frac{3}{4})\pi] \quad (11.48)$$

where c is the residue of the function $[\chi(r)]^{-2}$ at the origin and is therefore determined by the power series expansion of $\chi(r)$ for small values of r . We recall that it is essential for the validity of the approximate formula (11.48) that there exists a curve circumscribing the origin as in fig. 7.2a on which the absolute value of the function $\exp\{i w\}$ has a single minimum and for which the μ -integral is small compared to 1. The formula (11.48) is a generalization of the first one of the two formulae (34) in LANGER'S [1937] paper, which Langer has derived for the special case of an attractive Coulomb potential.

Considering a hydrogen atom or a hydrogen-like ion with the atomic number Z in a state with the quantum numbers n and l , and using Bohr's radius as the unit of length, we have

$$Q^2(r) = -\frac{Z^2}{n^2} + \frac{2Z}{r} - \frac{l(l+1)}{r^2}.$$

According to (11.5) we choose

$$q^2(r) = Q^2(r) + \frac{l(l+1)}{r^2} = -\frac{Z^2}{n^2} + \frac{2Z}{r}$$

and note that the function $q^2(r)$ is positive in the region $0 < r < 2n^2/Z$. From the definition (11.47) we easily get

$$w(r) = 2n \left\{ \arcsin \left(\frac{Zr}{2n^2} \right)^{\frac{1}{2}} + \left[\frac{Zr}{2n^2} \left(1 - \frac{Zr}{2n^2} \right) \right]^{\frac{1}{2}} \right\}$$

and hence

$$w(r) \approx \sqrt{8Zr} \quad \text{if} \quad \frac{Zr}{2n^2} \ll 1.$$

If $l + \frac{1}{2} \ll \sqrt{n}$, the μ -integral for a circle of radius

$$r_0 \approx \pi^2 \left(\frac{l + \frac{1}{2}}{\sqrt{n}} \right)^2 \frac{2n^2}{Z}$$

around the origin is of the order of magnitude $(l + \frac{1}{2})/\sqrt{n}$ which according to our assumption is much smaller than 1. Furthermore, the condition for one minimum of the absolute value of $\exp\{i w\}$ on the above mentioned circle of radius r_0 is fulfilled. In the neighbourhood of the point r_0 on the real axis the solution $\chi(r)$ is therefore given by the approximate formula (11.48). The μ -integral along the real axis from r_0 towards larger values of r to a point lying well to the left of the turning point $r = 2n^2/Z$ is at the most of the order of magnitude $(l + \frac{1}{2})/\sqrt{n}$, and therefore the formula (11.48) is approximately valid also in the classically allowed region to the right of r_0 except in the immediate neighbourhood of the turning point $r = 2n^2/Z$. We remark that in a region where the above mentioned approximation $w(r) \approx \sqrt{8Zr}$ may be used, one obtains from (11.48) a formula which corresponds to the formulae (3.33) or (3.37) on p. 105 in the review article by BETHE and SALPETER [1957] on the quantum mechanics of one- and two-electron systems. However, the conditions given by these authors for the validity of their equations (3.33) and (3.37) are not sufficient, when not only n but also l is large.

Next we consider the scattering of a particle of velocity v against an attractive (screened) Coulomb potential $V(r) = -Ze^2/r$. Using $k^{-1} = \hbar/(mv)$ as the unit of length, we have

$$Q^2(r) = 1 + \frac{2\eta}{r} - \frac{l(l+1)}{r^2}$$

where as previously η is a positive quantity defined by

$$\eta = \frac{Ze^2}{\hbar v}.$$

According to (11.5) we choose

$$q^2(r) = Q^2(r) + \frac{l(l+1)}{r^2} = 1 + \frac{2\eta}{r}.$$

From the definition (11.47) we easily get

$$w(r) = 2\eta \left\{ \left[\frac{r}{2\eta} \left(1 + \frac{r}{2\eta} \right) \right]^{\frac{1}{2}} + \ln \left[\left(\frac{r}{2\eta} \right)^{\frac{1}{2}} + \left(1 + \frac{r}{2\eta} \right)^{\frac{1}{2}} \right] \right\}$$

and hence

$$w(r) \approx \sqrt{8\eta r} \quad \text{if} \quad \sqrt{\frac{r}{2\eta}} \ll 1.$$

On a circle of radius r_0 enclosing the origin the function $\exp\{iw\}$ has a single minimum as in fig. 7.2a if $r_0 < \eta$. Furthermore, if $l + \frac{1}{2} \ll \sqrt{\eta}$ and

$$r_0 \approx \pi^2 \left(\frac{l + \frac{1}{2}}{\sqrt{\eta}} \right)^2 2\eta$$

the μ -integral for the above mentioned circle is roughly $\mu \approx (l + \frac{1}{2})/\sqrt{\eta} \ll 1$. Similarly as in our previous treatment of the hydrogen-like ion we now find that if $l + \frac{1}{2} \ll \sqrt{\eta}$ the formula (11.48) is valid for $r \geq r_0 = 2\pi^2(1 + \frac{1}{2})^2$.

Langer asserts erroneously that the formulae (34) in his above mentioned paper (LANGER [1937]) are usable in intervals which (in our notations) extend across and include the first zero r' of the function $Q^2(r) - 1/(4r^2)$. The value of r' , which is given by

$$r' = \frac{n}{Z} \{n - [n^2 - (l + \frac{1}{2})^2]^{\frac{1}{2}}\} \approx \frac{1}{4n} \left(\frac{l + \frac{1}{2}}{\sqrt{n}} \right)^2 \frac{2n^2}{Z}$$

for a hydrogen-like ion in a bound state and by

$$r' = [\eta^2 + (l + \frac{1}{2})^2]^{\frac{1}{2}} - \eta \approx \frac{1}{2} \left(\frac{l + \frac{1}{2}}{\sqrt{\eta}} \right)^2$$

in the case of scattering against an attractive Coulomb potential, is much smaller than r_0 . The μ -integral for a circle of radius r' with its centre at the origin is of the order of magnitude $(2l + 1)\pi$, and the μ -integral along the real axis between the points r' and r_0 is of the order of magnitude $2l + 1$. Since neither of these two μ -integrals is small compared to 1, we cannot expect the formula (11.48) to be valid so close to the origin as in the neighbourhood of r' . LANGER [1937] arrived at the opposite conclusion by using an asymptotic approximation of $J_{2l+1}(w)$ for large values of w , but he did not notice that this asymptotic approximation cannot be used in the neighbourhood of r' since $w(r') \approx 2l + 1$. For the validity of the asymptotic formulae used by Langer it is actually required that $w(r) \gg \frac{1}{2}(2l + 1)^2$.

We shall finally make some remarks about the scattering of a particle of velocity v against a repulsive (screened) Coulomb potential $V(r) = Ze^2/r$. Using the same unit of length as above and defining also the positive

quantity η as previously, we have

$$Q^2(r) = 1 - \frac{2\eta}{r} - \frac{l(l+1)}{r^2}.$$

According to (11.5) we choose

$$q^2(r) = Q^2(r) + \frac{l(l+1)}{r^2} = 1 - \frac{2\eta}{r}.$$

The function $q^2(r)$ is negative in the region $0 < r < 2\eta$ and positive in the region $r > 2\eta$. Instead of r we introduce the complex variable z , and we cut the complex plane along the negative part of the real axis. We choose $q(z)$ to be positive on the lower lip of the cut and $w(z)$ to be zero at the origin. The two lips of the cut form two anti-Stokes' lines. On the lower one of these anti-Stokes' lines the coefficients a_1 and a_2 can be determined approximately according to (7.27a, b) if $l + \frac{1}{2} \ll \sqrt{\eta}$. By means of the basic estimates (4.3) or the estimates (4.4) we can then obtain the a -coefficients and hence the wave function $\chi(r)$ in the region $r_0 \ll r < 2\eta$ of the positive real axis. The result is (except for the sign)

$$\chi(r) \approx \frac{1}{2}(-\pi c)^{-\frac{1}{2}} |q(r)|^{-\frac{1}{2}} \exp\{|w(r)\} \quad \text{for } r_0 \ll r < 2\eta.$$

This formula should be compared with the first one of LANGER's [1937] formulae (36). To obtain the function $\chi(r)$ in the region $r > 2\eta$ we can use the usual connection formula, getting

$$\chi(r) \approx \exp\{|w(2\eta)\} (-\pi c)^{-\frac{1}{2}} |q(r)|^{-\frac{1}{2}} \cos[|w(r) - w(2\eta)| - \frac{1}{4}\pi] \quad \text{for } r > 2\eta.$$

Of course neither of the above two formulae for $\chi(r)$ is valid in the neighbourhood of the turning point $r = 2\eta$.

References

- Bethe, H.A. and E.E. Salpeter, 1957, Quantum mechanics of one- and two-electron systems. *Handbuch der Physik*, edited by Flügge, Band 35 (Springer-Verlag, Berlin).
- Birkhoff, G.D., 1933, *Bull. Am. Math. Soc.* 39, 681.
- Bohm, D., 1961, *Quantum theory* (Prentice-Hall, Inc.).
- Heading, J., 1962, *An introduction to phase-integral methods* (Methuen's Monographs on Physical Subjects, London and New York).
- Hecht, C.E. and J.E. Mayer, 1957, *Phys. Rev.* 106, 1156.
- Ince, E.L., 1926, *Ordinary differential equations* (republished in U.S.A. by Dover Publications, Inc., New York).
- Jeffreys, B.S., 1961, The asymptotic approximation method. Review article in : *Quantum theory I*, edited by D.R. Bates (Academic Press, New York and London).
- Jeffreys, H., 1956, *Proc. Cambr. Phil. Soc.* 52, 61.
- Kemble, E.C., 1935, *Phys. Rev.* 48, 549.
- Kemble, E.C., 1937, *The fundamental principles of quantum mechanics* (republished in U.S.A. by Dover Publications, Inc., New York).
- Kramers, H.A., 1926, *Z.f. Physik* 39, 828.
- Langer, R.E., 1934, *Bull. Am. Math. Soc.* 40, 545.
- Langer, R.E., 1937, *Phys. Rev.* 51, 669.
- Merzbacher, E., 1961, *Quantum mechanics* (John Wiley and Sons, Inc., New York).
- Messiah, A., 1959, *Mécanique quantique*, Tome 1 (Dunod, Paris). *Quantum mechanics*, Vol. 1 (North-Holland Publ. Co., Amsterdam, 1961).
- Miller, S.C., Jr., and R.H. Good, Jr., 1953, *Phys. Rev.* 91, 174.
- Morse, P.M. and H. Feshbach, 1953, *Methods of theoretical physics*, Part II (McGraw-Hill Book Company, Inc., New York and London).
- Olver, F.W.J., 1961, *Proc. Cambr. Phil. Soc.* 57, 790.
- Pauli, W., 1958, *Die allgemeinen Prinzipien der Wellenmechanik*. *Handbuch der Physik*, edited by Flügge, Band 5, Teil 1 (Springer-Verlag, Berlin).
- Schiff, L.I., 1949, *Quantum mechanics* (McGraw-Hill Book Company, Inc., New York and London).
- Seifert, H., 1942/43, *Mathematische Zeitschrift* 48, 173.
- Soop, M., 1965, to be published in *Arkiv för Fysik*.
- Zwaan, A., 1929, *Intensitäten im Ca-Funkenspektrum*. *Academisch Proefschrift* (Joh. Enschedé en Zonen, Haarlem).

INDEX

- a*-coefficients, *see also a*-vector,
definition of, 15
differential equations for, 15
limiting properties of, 29, 92, 103-105,
115-116
- anti-Stokes' line, 60
- asymptotic approximation method, 1
- asymptotic phase, 125-130
exact expressions for, 126, 128
- a*-vector, *see also a*-coefficients,
definition of, 16
differential equation for, 16
integral equation for, 16
- basic estimates, 26-27
- Bethe, 132
- Birkhoff, 3, 4
- Bohm, 7, 97
- Brillouin, 1
- Carlini, 1
- classically allowed region, 34
in the generalized sense, 34, 80
- classically forbidden region, 34
in the generalized sense, 34, 80
- classical turning point, 34
in the generalized sense, 34, 80
- connection formulae, 1-3, 6-8, 83-89, 97
derivation of, 83-86
one-directional (one-sided) nature of, 2,
6-8, 40, 46, 86-89, 97
- current density, 7, 91
- epsilon, ϵ ,
definition of, 13
- estimates of the *F*-matrix, chapters 4, 6, 7
- Feshbach, 7
- f*-functions,
definition of, 20
- F*-matrix,
basic estimates of, 26-27
definition of, 16
determinant of, 17-18
differential equation for, 17
estimates of, *see* estimates of the *F*-matrix
integral equation for, 17
inversion of, 18
limiting properties of, 27-29, 92, 103
multiplication rule for, 21
series for, 16, 18-20
symmetry properties of, 30-33
- f*-vector,
definition of, 20
- Gans, 1
- generalized classical turning point, 34, 80
- Good, 94
- Green, 1
- harmonic oscillator,
linear, 109
three-dimensional, 120-125
- Heading, 1, 3, 4, 7, 88, 97
- Hecht, 14
- hydrogen-like ion, 117-120, 131-132
- Jeffreys, B.S., 1, 94
- Jeffreys, H., 1, 2, 7, 88, 97
- JWKB-approximation, 1-2
first order, 11
second order, 10
modified, 4, 110
- JWKB-method, *see* JWKB-approximation
- Kemble, 3-5, 8, 15, 86, 90, 91, 94, 112
- Kramers, 1, 112
- Langer, 2, 6, 86, 88, 97, 112, 113, 130, 131,
133, 134

- Liouville, 1
 Liouville-Green approximation, 1
 Löwdin, 14
- Mayer, 14
 Merzbacher, 7, 51, 97
 Messiah, 86
 Miller, 94
 Morse, 7
 mu-integral, μ -integral,
 definition of, 26
- O-symbol, 2-3, 45-46
 Olver, 3, 23-25, 27, 35
- Pauli, 7
 phase-integral method, 1
 potential barrier,
 overdense, 34, 43-51
 underdense, 34, 51-59
 parabolic, 51, 59, 91, 94, 99
 potential well, 102
 probability current, 91
- quantization condition, 105-109, 115-116
 exact, 106, 108, 116
 semi-classical, 4, 9, 108-109, 116, 117-
 119, 121-125
- reflection coefficient,
 exact expressions for, 93, 99-100
 approximate expressions for, 94, 101
- Salpeter, 132
 Schiff, 86
 Schwarzian derivative, 14
 Seifert, 2
 semi-classical quantization condition, see
 quantization condition
 Stokes' constants, 4
 Stokes' line, 60
 Stokes' phenomenon, 5, 6, 12, 23, 74
 symmetry relations, 5, 30-33
- transition point, 34
 transmission coefficient,
 exact expressions for, 93, 99-100
 approximate expressions for, 90-91, 94,
 101
 turning point, see classical turning point
- $w(z)$,
 definition of, 13
 wave function,
 exact expression for, 20
 Wentzel, 1
 WKB-method, 1
 Zwaan, 3

