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Asymptotische Methoden in der Wellenmechanik

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Collection of Lecture Notes

Overview

This lecture has been given a few times in Potsdam with large variations in contents. The notes presented are by no means complete, and they contain material that has not been covered during the 18/19 winter term.

- WKB approximation: 'quantum flesh on classical bones'
  approximate solutions of one-dimensional Schrödinger equations
  connection formulas across a turning point
  matched asymptotic expansions (Langer's analysis with Airy functions)
  uniform asymptotics of Berry & Mount

- mathematical asymptotics: series expansions*
  approximate evaluation of integrals
  stationary phase method

- multiple-scale techniques*
  boundary layer theory
  examples from hydrodynamics

- the rainbow and other caustics

- quantum chaos

The items* marked with the asterix are a little more technical.

Presentation

This lecture is given with the aim to complement the undergraduate course in theoretical physics with a few approximation methods that are useful for calculations 'with pencil and paper'. The methods come under the name 'asymptotics' and allow to get approximate solutions to equations and integrals that one encounters in different fields of physics. The main idea is to identify small (or large) parameters and to make an expansion. This technique is a 'must' in physics, since exact solutions are the exception, not the rule. But approximations and expansions need also to be 'controlled' in the sense that one has to know how large are the errors one is making. Indeed, the difference between ordinary power series expansions (well-known in Taylor series, for example) and so-called asymptotic expansions is in the way errors and convergence are handled. We shall see that although the asymptotic series does not converge in the usual sense, it gives a better approximation than a conventional power series.

The general methods will be illustrated with examples from different fields of physics, with some emphasis on quantum mechanics. But similar techniques are also applied in hydrodynamics and optics.

From a historical perspective, asymptotic methods provide a way to recover a "simpler" description from a "more fundamental" one, for example classical mechanics from quantum mechanics. This point is quite paradigmatic for the structure of physical theories: e.g., we know that quantum mechanics is the more fundamental theory for the motion of material particles, but, nevertheless, classical mechanics is an excellent theory to describe the motion of planets, cars, or dust particles. It is thus a limiting case of the underlying quantum theory. In the same way, geometrical optics is a limiting case of wave optics, but accurate enough to engineer objects like telescopes, window panes, or contact lenses. It is not easy to give a precise formulation of the limiting conditions under which geometrical optics is valid. A generally accepted way of speaking is:

> 'The optical wavelength λ is small compared to the other dimensions of the problem.'[1]

For the mechanical theories, the formulation reads:

> 'The Planck constant $\hbar$ is small compared to the action of the corresponding classical system.'

These notes hopefully show in selected examples how these conditions acquire a sound mathematical sense. Asymptotic approaches have been quite important for the discovery of quantum mechanics in the 1920s. The relation between geometrical and wave optics is at the very heart of Schrdinger's papers on his equation (1926). In his interpretation, light rays and classical trajectories are identical concepts, and his equation is the strict analog of the wave equation of electrodynamics. In modern quantum mechanics courses, this intimate connection between classical and wave mechanics gets somewhat out of focus because the course also contains a lot of technical information about the algebraic formalism of quantum mechanics. This course tries to come back to the 'old-fashioned' wave mechanics and hopefully contributes to re-develop a small part of the intution people had when quantum mechanics was discovered. The focus will be on 'physics' and not on mathematical formalism. There is still work being done in the field. Some of the examples presented in the lecture or as problems are coming from research papers that appeared no longer than ten years ago. Much can be learnt still about a quantum system by investigating the behaviour of the trajectories followed by its classical counterpart. 'Semi-classical' (or, perhaps better, 'semi-quantum') approximations thus allow to study the recent field of quantum chaos. Another example is particle optics. Electron, neutron and, more recently, atom beams have been used to perform optical experiments like reflection, diffraction, and interference. It is often the case that the particles' wavelength (the de Broglie wavelength

[1] Throughout these notes, the 'reduced wavelength' $\lambda \equiv \lambda/2\pi$ is preferably used because the symbol looks so much like the (reduced) Planck constant $\hbar$.

$\lambda = \hbar/mv$) is 'small', and semiclassical concepts are a powerful tool to describe the observations made in these experiments. Atom optics may even be considered as a test ground for wave mechanics because a large range of wavelengths (of energies) is available and the potentials may often be taylored at will, without dissipation and without strong interactions between the particles. A substantial number of problems given in this lecture are related to current experiments in that field. It often happens that the answer is not yet known, but may be expected within reasonable reach of semiclassical techniques.

Overview

The material of this lecture is grouped in three chapters:

1. the (J)WKB method in wave mechanics
2. asymptotic series and multiple-scale techniques for solving differential equations
3. caustics and quantum chaos (in two and three dimensions)

The **first chapter** does not stop with the standard WKB approximation of quantum mechanics textbooks. We also present uniform approximations developed by Berry and co-workers since 1970, that allow to find globally regular semiclassical wave functions (Berry & Mount, 1972). A large number of examples give the occasion to compare semiclassical and exact solutions. This has the additional benefit of providing insight into the asymptotics of special mathematical functions, as listed in Abramowitz & Stegun (1972) and the Digital Library of Mathematical Functions. The chapter closes with a generalisation to two-component wave functions in one dimension: the Landau-Zener formula is derived.

The **second chapter** gives a more formal introduction into asymptotic series and how to identify singular points in differential equations. In this chapter, we illustrate the technique of 'matching' solutions to differential equations with small parameters that lead to a separation of length scales. This is known as the 'boundary layer problem' in hydrodynamics. It also provides a clean way to derive certain 'matching rules' that appear in the (J)WKB approximation.

In the **last chapter**, we move to more than one dimension and face the difficulty of generalizing the previous results. The opening example is the geometrical optics of the rainbow, and we go on to the fringe patterns that 'decorate' (Nye, 1999) the rainbow and other 'diffraction catastrophes' (Kravtsov & Orlov, 1998). The central paradigma developed is how to construct wave fronts with the help of light rays and what kind of interference phenomena happen near the 'natural focus' when this wave front is curved, also called a caustic. In the field of quantum chaos, classical rays or paths can be used to understand from a physical viewpoint the behaviour of the eigenfrequencies in a cavity or the energy spectrum in a box potential.

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Chapter 1

(J)WKB methods in one dimension

1.1 Motivation

We want to find an approximate solution to the stationary Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi + V(x)\,\psi = E\psi(x) \tag{1.1}$$

in the limit where the Planck constant $\hbar$ is 'small'. Observe that it is not very useful to put $\hbar = 0$ in this equation because then the wavefunction vanishes everywhere except at the classical turning points x_t where $V(x_t) = E$.

A better solution is found following Schrödinger (1926): we make the following ansatz to the wave function

$$\psi(x) = A(x)\,\exp\left(\frac{\mathrm{i}}{\hbar}S(x)\right) \tag{1.2}$$

where $A(x)$ and $S(x)$ are real functions; note that $S(x)$ has the dimension of an action. Putting (1.2) into the Schrödinger equation, we get

$$\begin{aligned} 0 \;=\; & \frac{1}{2m}\left(\frac{\mathrm{d}S}{\mathrm{d}x}\right)^2 + V(x) - E \\ & -\frac{\mathrm{i}\hbar}{2m}\left(2\frac{\mathrm{d}A}{\mathrm{d}x}\frac{\mathrm{d}^2S}{\mathrm{d}x^2} + A\frac{\mathrm{d}S}{\mathrm{d}x}\right) \\ & -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2A}{\mathrm{d}x^2} \end{aligned} \tag{1.3}$$

This equation already looks nicer when we put $\hbar = 0$. But we can do better and expand the action S in a power series

$$S = S^{(0)} + \hbar S^{(1)} + \dots \tag{1.4}$$

and similarly for the amplitude A. From (1.3), we clearly have the zeroth order solution

$$\begin{aligned} S_0(x) &= \pm \int^x \sqrt{2m\,(E - V(x'))}\,\mathrm{d}x' + \text{const.} & (1.5)\\ &= \pm \int^x p(x')\mathrm{d}x' + \text{const.} \\ p(x) &= \sqrt{2m\,(E - V(x))} & (1.6) \end{aligned}$$

where $p(x)$ is the classical momentum for a particle moving to the right in the potential $V(x)$. This solution only makes sense, of course, when $E > V(x)$.

The first order term of (1.3) can be re-written in the form

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(A^2(x)p(x)\right) = 0\,, \tag{1.7}$$

and this may be integrated to give

$$A(x) \sim \frac{1}{\sqrt{p(x)}} \tag{1.8}$$

Stopping the expansion at this point, we get the following approximation to the wave function

$$\psi(x) \approx \psi_{\mathrm{WKB}}(x) = \frac{C}{\sqrt{p(x)}} \exp\left(\pm\frac{\mathrm{i}}{\hbar}\int^x p(x')\mathrm{d}x'\right) \tag{1.9}$$

where the integration constants have been lumped into the global normalisation factor C. ψ_{WKB} is the wave function of the Wenzel Kramers Brillouin approximation (Messiah, 1995), obtained already in the 1920's.

Classically allowed region

In one dimension, it is easy to distinguish two types of regions in configuration space (see fig.1.1): the 'classically allowed region' I (where $E > V(x)$)

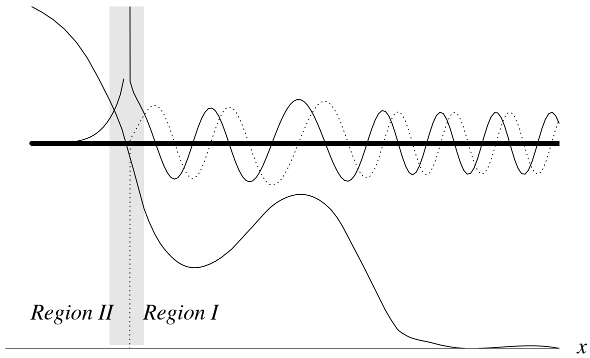

Figure 1.1: Classically allowed (I) and forbidden (II) regions for a particle of energy E in a potential $V(x)$. The thin solid and dotted lines show real and imaginary parts of the WKB wave function (1.9). The waves are not correctly matched at the transition point.

is accessible for a classical particle, while the region II ($E < V(x)$) is classically forbidden.

Consider in more detail the region I in fig.1.1. The momentum (1.6) is real there, and the WKB wave function (1.9) is the natural generalisation of a plane wave $\exp(\pm \mathrm{i}px/\hbar)$ that would propagate towards the right (left) if the momentum p were spatially constant (we conventionally use the factor $\exp(-\mathrm{i}Et/\hbar)$ for the time-dependence of the wave function). The wave function (1.9) being complex, we show its real and imaginary parts. They are oscillating and behave as $\cos\phi(x)$ and $\sin\phi(x)$ (sinusoidal curves with a phase difference $\pi/2$). From the relative positions of the maxima in the real and imaginary part, we deduce that the phase $\phi(x)$ increases towards the right, the figure thus shows a wave propagating to the right. In agreement with de Broglie's formula $\lambda = \hbar/p$, the phase varies slowly (the wave length is large) when the classical momentum $p(x)$ is small (above the barrier in the figure), while it varies rapidly when $p(x)$ is larger.

As regards the envelope of the oscillations, it follows an opposite trend: the magnitude of the wave function $|\psi(x)| = C/\sqrt{p(x)}$ is larger when the particle moves more slowly. This is because the quantity $|\psi(x)|^2 \mathrm{d}x = \rho(x)\mathrm{d}x$ gives the probability to find the particle in the interval $x \ldots x + \mathrm{d}x$. Since for a stationary flow in one dimension, the equation of continuity gives

$\partial j/\partial x = -\partial\rho/\partial t = 0$, the particle current density $j(x) = \rho(x)p(x)/m$ is conserved. This gives $j(x) = \text{const.}$, and we have

$$|\psi(x)|^2 = \rho(x) = \frac{mj}{p(x)}. \tag{1.10}$$

Physically speaking, the probability $\rho(x)\mathrm{d}x = j\mathrm{d}t$ is proportional to the time $\mathrm{d}t$ the particle needs to move across the interval $x \ldots x + \mathrm{d}x$ at the local velocity $p(x)/m$. Note that we cannot predict at which particular time the particle will cross the position x because the flow (the wave function) is stationary by assumption. We do not know the time when the particle started, and therefore, only a probabilistic prediction may be given.

Finally, we note from (1.10) that the WKB wave function diverges at a 'classical turning point' where the velocity vanishes. This divergence, also called a 'catastrophe' in mathematics (Berry & Upstill, 1980; Kravtsov & Orlov, 1998) is clearly visible in Figs.1.1. But it is *unphysical* because it is not reproduced by the exact solution of the Schrödinger equation. We shall look into this later in the lecture.

Forbidden region

Turn now to region II in fig.1.1 that is classically forbidden because the potential is larger than the energy. The momentum

$$p(x) = \sqrt{2m(E - V(x))} = \mathrm{i}\sqrt{2m(V(x) - E)}$$

is then purely imaginary, and the wave function (1.9) shows a sort of exponential growth or decay. The local decay constant is approximately equal to $\pm|p(x)|$. The wave function shown in the figure decreases exponentially when the position x moves into the forbidden region. Whether this is physically acceptable depends on the overall behaviour of the potential.

Tunnelling through a barrier

The situation shown in fig.1.1 would be false if there were an additional potential well to the left, as shown in fig.1.2. Indeed, in this case, the particle is predominantly localised in the potential well, and (at least if the barrier is quite thick) the wave function must decrease when the position

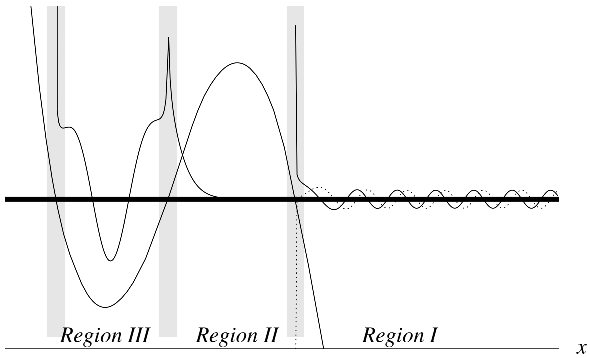

Figure 1.2: WKB wave functions leaking out of a potential well (region III) through a barrier (II) into an allowed region (I). Real (solid) and imaginary (dotted) parts are shown. The waves are not matched at the transition points. The wave in region I is not drawn to scale.

x moves towards the right into the forbidden region. On the other hand, once the barrier has been crossed, the waves 'leaks' out of the exponentially small tail towards the right. A wave propagating to the right in region I is therefore physically reasonable.[1] This process is the 'tunnel effect', and we shall derive a simple formula for the tunnelling rate below.

Reflection from a barrier

Figure 1.3 shows the case that the forbidden region II extends up to $x = -\infty$. The exponential decay towards the left (or increase towards the right) is then physically reasonable because otherwise the total probability of being in the forbidden region would be infinite. But now, the wave function in region I is not correct: classically, one would expect that there is also a flow of particles incident from the right and being reflected from the potential barrier. The wave function must therefore contain also a term proportional to $\exp\left(-\mathrm{i}\int^x p(x')\mathrm{d}x'/\hbar\right)$, describing a wave moving towards the left. We discuss below how in this case of barrier reflection the WKB solutions are matched across the turning point.

[1]Although one should ask the question: how can this be a stationary state if probability is continuously leaking out of the regions II and III? Answer: construct a wave function with a complex energy.

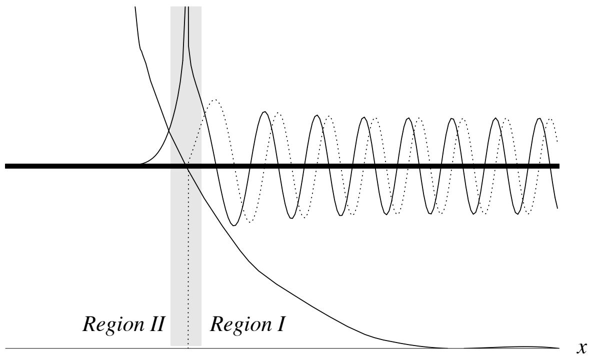

Figure 1.3: Reflection from a potential barrier. The waves are not correctly matched across the turning point, and the incident wave is missing in region I.

Open questions

The discussion presented so far leads us naturally to a number of questions. They are going to be analyzed in the following sections of this chapter.

- What is a precise criterion for the validity of the WKB approximation?
- How are the WKB wave functions to be matched across the boundary between the classically allowed and forbidden regions? We anticipate that this matching depends on the global behaviour of the potential for the chosen energy (particle trapped in a well or incident from infinity, e.g.).
- The WKB wave functions should also be able to yield approximations for, e.g., the quantised energy levels in a potential well or the tunnelling rate through a barrier. We would also like to know in what regime these approximations are valid.
- How is it possible to remove the divergence $\propto 1/\sqrt{p(x)}$ of the WKB wave functions at a turning point without losing precision far away from the turning point?
- How may the above treatment be generalized to multi-component ('spinor') wave functions that are no longer scalar complex functions? And what about spatial dimensions larger than one?

1.2 Validity criteria

Naive estimate

The quantum mechanics textbooks often quote the following condition of validity of the WKB approximation: in the Schrödinger equation (1.3), we neglect the term containing $\hbar$ compared to the others. This is reasonable if

$$\left|\frac{\hbar}{2m}\frac{\mathrm{d}^2 S}{\mathrm{d}x^2}\right| \ll \frac{1}{2m}\left(\frac{\mathrm{d}S}{\mathrm{d}x}\right)^2 \tag{1.11a}$$

where the right hand side is a particular term representing the 'large' terms in (1.3). This condition may be written in terms of the local classical momentum $p(x)$ or, equivalently, the local wavelength $\lambda(x) = \hbar/p(x)$, and we get

$$\left|\hbar\frac{\mathrm{d}p}{\mathrm{d}x}\right| \ll p^2(x) \qquad \text{or} \qquad \left|\frac{\mathrm{d}}{\mathrm{d}x}\frac{\hbar}{p(x)}\right| = \left|\frac{\mathrm{d}\lambda(x)}{\mathrm{d}x}\right| \ll 1. \tag{1.11b}$$

The WKB approximation is thus valid when *the local wavelength changes slowly*. As a rule of thumb, the gradient $\mathrm{d}/\mathrm{d}x$ in (1.11b) is of the order of $1/a$ where a is a classical length scale (that may depend on position and energy). We thus recover the intuitive idea that the de Broglie wave length must be small compared to the classical length scales of the problem.

It is a simple exercise to re-write the validity condition (1.11b) in terms of the classical force acting on the particle:

$$\hbar m|F(x)| \ll p^3(x) \tag{1.11c}$$

Note that both conditions (1.11b, 1.11c) predict a breakdown of the WKB approximation at classical turning points because of the vanishing momentum $p(x)$.

On the other hand, if the wave length is spatially constant, the WKB approximation is valid (it is even exact).

More careful estimate

Recall that the WKB approximation is based on the expansion (1.4) of the action function. This expansion is accurate if higher-order terms become successively smaller in the limit of small $\hbar$. In the following discussion, we combine the phase S and the amplitude A in Eq.(1.2) into a complex action S for which we assume an expansion in powers of $\hbar$. We thus obtain the condition

$$\ldots \ll \hbar^2 |S_2| \ll \hbar |S_1| \ll |S_0| \tag{1.12}$$

where we have also included the second order term S_2. This term may be explicitly calculated from the Schrödinger equation by working out higher-order terms. One gets the differential equation (primes denotes differentiation with respect to x):

$$\frac{\mathrm{d}S_2}{\mathrm{d}x} = \frac{1}{2\,\mathrm{d}S_0/\mathrm{d}x}\left[\mathrm{i}\frac{\mathrm{d}^2 S_1}{\mathrm{d}x^2} - \left(\frac{\mathrm{d}S_1}{\mathrm{d}x}\right)^2\right] \tag{1.13}$$

This expression allows to calculate condition (1.12) for a given problem. One has to be careful with the arbitrary constants that appear in the S_n. In practice, it seems a good choice to fix a reference point x_r and to evaluate condition (1.12) for the differences $\hbar^{n-1}\left[S_n(x) - S_n(x_r)\right]$.

There is an *additional condition* that is due to the fact that the action appears in the exponent of the wave function. We have to impose that the term $\hbar S_2$ is *small compared to unity* to assure that we make only a small error in the wave function:

$$\hbar |S_2| \ll 1 \tag{1.14}$$

If this is case, we may expand

$$\exp\left[\frac{\mathrm{i}}{\hbar}\left(S_0 + \hbar S_1 + \hbar^2 S_2\right)\right] \approx \psi_{\mathrm{WKB}}(x)\left[1 + \mathrm{i}\hbar S_2(x)\right]$$

and get a correction that is small relative to the WKB wave function. If $\hbar S_2 = 0.01$, say, then the WKB wave function is accurate to one percent. Of course, condition (1.14) has also to be calculated explicitly for a given problem.

Spatially constant wave length. This an example where it is easy to obtain the actions S_n explicitly. The momentum p is constant, and choosing $x_r = 0$ as reference point, we get

$$S_0(x) \;=\; px \tag{1.15}$$

$$S_1(x) - S_1(0) = \frac{\mathrm{i}}{2} \log \frac{p(x)}{p(0)} = 0 \tag{1.16}$$

$$S_2(x) - S_2(0) = 0 \tag{1.17}$$

Both inequalities in condition (1.12) are therefore fulfilled. Furthermore, since S_2 is constant, one is free to choose $S_2 = 0$, and thus satisfy condition (1.14).

More examples are given in the exercises. We finally note that a good check for the WKB approximation is the comparison with exactly solvable potentials and with numerical calculations. This will also be done in the lecture and in the problems.

1.3 Langer matching

In this section, we present a first solution that avoids the divergence of the WKB wave function at the classical turning point. As we have alluded to in the motivation, such a solution also provides us with the 'connection rules' for matching the wave function left and right of the turning point.

The idea is sketched in fig.1.4. We linearise the potential around the

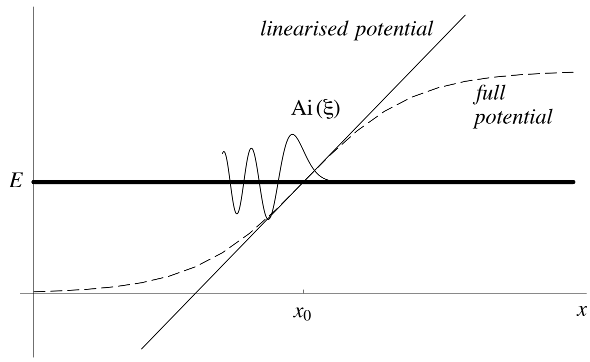

Figure 1.4: Linearisation of the potential around a turning point and local wave function $\mathrm{Ai}(\xi)$.

position x_0 of the turning point (note that this position depends on the energy) and solve the Schrödinger equation for the linearised potential. This full (and hopefully regular) solution is then matched to the WKB expressions in the regions 'far' from x_0.

Exact solution for a linear potential

For the linearised potential, the Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi + \left[E + F\left(x - x_0\right)\right]\,\psi = E\psi(x) \tag{1.18}$$

where $-F$ is the classical force evaluated at the turning point x_0. Let us assume that the potential increases to the right ($F > 0$) and introduce the characteristic length

$$w = \left(\frac{\hbar^2}{2mF}\right)^{1/3}. \tag{1.19}$$

(Note that this length scale explicitly depends on $\hbar$.) We then get

$$-w^2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi + \frac{x - x_0}{w}\,\psi = 0 \tag{1.20}$$

and see that $\xi = (x - x_0)/w$ is a good dimensionless variable for this problem. In terms of this variable, $\xi > 0$ ($\xi < 0$) corresponds to the classically forbidden (allowed) regions. In problem 1.4, it is shown that one solution of

$$-\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\psi + \xi\,\psi = 0 \tag{1.21}$$

is the *Airy function* $\mathrm{Ai}(\xi)$. This function is plotted in figs.1.4 and 1.5. The function $\mathrm{Ai}(\xi)$ is finite all over the real ξ-axis, has a turning point at $\xi = 0$ (as it must), and decays in an exponential manner in the classically forbidden region $\xi \to \infty$. For $\xi \to -\infty$, it displays an oscillating behaviour. These properties make the $\mathrm{Ai}(x)$ the physically acceptable solution when there is no other classically allowed region in the interval $x < x_0$.

Using the saddle point approximation, we get the following asymptotic behaviours of the Airy function (see problem 1.4)

$$\xi \ll -1 : \mathrm{Ai}(\xi) \;\approx\; \frac{1}{\sqrt{\pi}(-\xi)^{1/4}}\sin\left[\frac{2}{3}(-\xi)^{3/2} + \frac{\pi}{4}\right] \tag{1.22a}$$

$$\xi \gg 1 : \mathrm{Ai}(\xi) \;\approx\; \frac{1}{2\sqrt{\pi}\xi^{1/4}}\exp\left[-\frac{2}{3}\xi^{3/2}\right] \tag{1.22b}$$

These asymptotics are compared in Fig.1.5 to the Airy function. We see that already for $|\xi| \geq 1$, they are an excellent approximation.

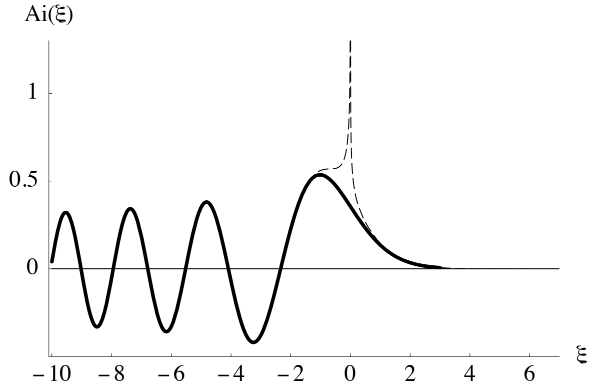

Figure 1.5: The Airy function $\mathrm{Ai}(x)$ (solid curve) and its asymptotic forms (dashed curves).

The matching rule at a reflecting turning point

We now match the WKB solutions with the Airy function 'far' from the turning point. Here, the calculation becomes tricky. We know that the WKB approximation breaks down close to the turning point. We suppose that it is valid 'sufficiently close' to x_0 where the linearisation of the potential is valid. In this spatial region (actually two regions on both sides of the turning point), two expansions are simultaneously possible: the expansion of the WKB solutions 'close' to the turning point and the asymptotic expansion of the Airy function solution 'far' from the turning point. If both expansions have the same functional behaviour (exponentials of certain powers, e.g.), we get the coefficients in front of these functions.

In a small region around the turning point, the classical momentum reads

$$p(x) = \begin{cases} \sqrt{2mF(x_0 - x)} & \text{for } x < x_0, \\ \mathrm{i}\sqrt{2mF(x - x_0)} & \text{for } x > x_0. \end{cases} \tag{1.23}$$

The action integral is easily performed and gives (we choose the turning point x_0 as second integration limit)

$$\int_x^{x_0} p(x)\mathrm{d}x = \frac{2}{3}\sqrt{2mF}\,(x_0 - x)^{3/2} = \frac{2\hbar}{3}(-\xi)^{3/2} \tag{1.24a}$$

$$\int_{x_0}^{x} p(x)\mathrm{d}x = \frac{2\mathrm{i}\hbar}{3}\xi^{3/2} \tag{1.24b}$$

In these formulae we already recognise the dimensionless variable ξ introduced before. In particular, in the classically forbidden region, the WKB wave function behaves as

$$x > x_0 : \psi_{\rm WKB}(x) = \frac{C \exp\left(-\frac{2}{3}\xi^{3/2}\right) + D \exp\left(\frac{2}{3}\xi^{3/2}\right)}{(2mFw)^{1/4}\xi^{1/4}} \tag{1.25a}$$

Comparing to the exponential decay (1.22a) of the Airy function in the limit $\xi \to \infty$, we read off that the coefficient D of the increasing wave must be exactly zero, and that the coefficient for the decaying wave has the value $C = (2mFw)^{1/4}/2\sqrt{\pi}$. In the classically allowed region close to the turning point, the WKB waves take the form

$$x < x_0 : \psi_{\rm WKB}(x) = \frac{A \exp\left(-\mathrm{i}\frac{2}{3}(-\xi)^{3/2}\right) + B \exp\left(\mathrm{i}\frac{2}{3}(-\xi)^{3/2}\right)}{(2mFw)^{1/4}(-\xi)^{1/4}} \tag{1.25b}$$

where the first term represents the wave moving to the right (its phase increases with x). Comparing with the behaviour (1.22a) of the Airy function, we get

$$A = C\,\mathrm{e}^{\mathrm{i}\pi/4} \tag{1.26a}$$

$$B = C\,\mathrm{e}^{-\mathrm{i}\pi/4} \tag{1.26b}$$

We thus get a particular linear combination of incident and reflected waves.

Summarising, we have found the following 'connection formula' for the WKB waves at a single turning point:

$$\underset{\text{allowed region (I) } x < x_0}{\frac{2C}{\sqrt{p(x)}} \sin\left(\frac{\pi}{4} + \frac{1}{\hbar}\int_x^{x_0} p(x')\mathrm{d}x'\right)} \quad \longleftarrow \quad \underset{\text{forbidden region (II) } x > x_0}{\frac{C}{\sqrt{|p(x)|}} \exp\left(-\frac{1}{\hbar}\int_{x_0}^{x} |p(x')|\mathrm{d}x'\right)} \tag{1.27}$$

The arrow indicates that we got this formula by imposing a boundary condition in the forbidden region (the wave function must decrease).

The WKB wave function that results from the connection formula (1.27) is plotted in fig.1.6 and compared to the exact solution of the Schrödinger equation that was computed numerically.

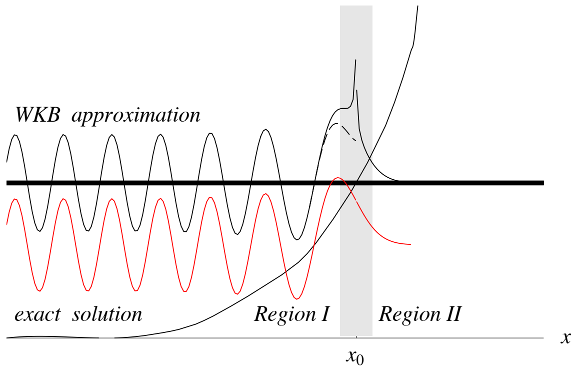

Figure 1.6: WKB wavefunction that is correctly matched at a turning point x_0. The red curve gives the (numerically computed) exact solution to the Schrödinger equation. It is shifted down because otherwise it would be indistinguishable from the WKB solution almost everywhere. The dashed curve continues the sine function in (1.27) without the $1/\sqrt{p(x)}$ divergence.

Comments

There is a simple 'short cut' to get the connection formula: just replace in the asymptotic behaviour (1.22) the quantities $\frac{2}{3}(\pm\xi)^{3/2}$ by the action integrals (1.24) and $(\pm\xi)^{1/4}$ by $\sqrt{|p(x)|}$. This gives a wave function with the same asymptotic behaviour as the Airy function.

If the allowed region is located to the right of the turning point (the potential has a negative slope), the connection formula becomes

$$\begin{array}{ccc} \dfrac{C}{\sqrt{|p(x)|}} \exp\left(-\dfrac{1}{\hbar}\displaystyle\int_x^{x_0} |p(x')| \mathrm{d}x'\right) & \longrightarrow & \dfrac{2C}{\sqrt{p(x)}} \sin\left(\dfrac{\pi}{4} + \dfrac{1}{\hbar}\displaystyle\int_{x_0}^{x} p(x') \mathrm{d}x'\right) \\ \text{forbidden region (II) } x < x_0 & & \text{allowed region (I) } x > x_0 \end{array} \qquad (1.28)$$

Short cut: simply write the integral in such a form that their values increase when x moves away from the turning point.

We observe in fig.1.6 that the sinusoidal oscillations in the allowed region are positioned in such a way that the sine wave is at 'half maximum' ($\sin\pi/4 = \sin 45° = \frac{1}{2}$) right at the turning point $x = x_0$ (although the amplitude of the WKB wave function still diverges). This is shown by the dashed curve in fig.1.6 where the sine function is plotted without the diverging prefactor $p(x)^{-1/2}$.

There is a phase jump of $\pi + \pi/2 \equiv -\pi/2$ between the incident and reflected wave. It is interesting that this phase jump is intermediate between the reflection at a 'fixed' end (phase shift π) and at a 'loose' end (zero phase shift) of a string. The reflection probability is unity.

More generally, a complex reflection coefficient R is defined by the following form of the wave function in the allowed region:

$$\psi(x) = C\left[\psi_{\text{inc}}(x) + R\,\psi_{\text{refl}}(x)\right] \tag{1.29}$$

If we choose incident and reflected waves in the WKB form (1.9),

$$\psi_{\text{inc, refl}}(x) = \frac{1}{\sqrt{p(x)}} \exp\left(\pm\frac{\mathrm{i}}{\hbar}\int_{x_0}^{x} p(x')\mathrm{d}x'\right)$$

we get from (1.27) a reflection coefficient

$$R = -\mathrm{i}$$

and hence a reflection probability $|R|^2 = 1$. On the other hand, there is zero transmission into the forbidden region. Both properties are related to the fact that the wave function is real over the entire x-axis. (Argue that this is a consequence of current conservation.)

The connection formula (1.27) is *unidirectional* in the sense that we have started from an asymptotic condition in the forbidden region (exponential decay of the wave function). The other direction of the connection formulas is needed when a tunnelling problem is studied: one then imposes that in the allowed region, there is only an outgoing and no incoming wave. This case gives rise to both exponentially decaying and increasing solutions in the forbidden region. We study it in more detail in the following subsection. There has been a long discussion about the directionality of the connection formula; see Berry & Mount (1972) for a review of this point.

We can derive a criterion for the validity of the above approach. We have to linearise the potential in an interval $x_0 - a \ldots x_0 + a$ whose length $2a$ must be at least a few $w = (\hbar^2/2mF)^{1/3}$. This is needed because otherwise we cannot use the asymptotic expansions of the Airy function towards the ends of the interval. We thus get the following condition:[2]

$$a^3 \gg w^3 = \frac{\hbar^2}{2mF} \tag{1.30}$$

This condition is of course valid if '$\hbar$ is sufficiently small'. On the other hand, it becomes violated if the classical length scale a gets too small. This length may be, for example, the distance to another turning point. If this second point comes closer than a few w's, it is in general no longer possible to treat them separately. In this case, one has to solve exactly a problem with two turning points and match the solution to the WKB wave functions that are valid at a larger distance. This topic is the subject of problem XX.

There is an alternative way to get a validity condition for the connection formula. Using the criteria of subsection 1.2, we can estimate how close the WKB method approach the turning point. This is studied in problem 1.3.

Landau's solution at a single turning point

Landau solves the connection problem by allowing the coordinate x to be complex. He uses only WKB wave functions and argues that these are valid for complex x provided the distance $|x - x_0|$ from the turning point is sufficiently large.

It seems that Landau starts from a wave incident upon the turning point, continues it analytically in a definite manner into the complex plane in order to describe both the exponentially damped (transmitted) wave and to find the correct amplitude for the reflected wave.

We shall try to elucidate his argument here for the example of a linear potential with a turning point at $x_0 = 0$. To define properly the momentum $p(x)$, we have to introduce a cut in the complex plane. We choose a cut in the classically allowed region, from $-\infty$ to 0 (see thick dashed line fig.1.7). In the cut plane, a complex position is parametrized as

$$x = r\,\mathrm{e}^{\mathrm{i}\varphi}, \qquad -\pi < \varphi < \pi$$

[2]It is interesting that we can get (1.30) from the previously derived condition (1.11b) by estimating $p \simeq \hbar/a$. This is the momentum of a particle in the ground state of a box with length a.

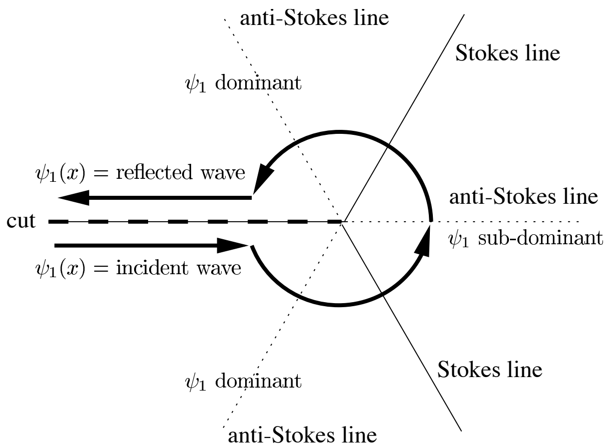

Figure 1.7: Cut, Stokes, and anti-Stokes lines close to a simple turning point. Landau continues analytically the incident wave along the path shown.

and we can write the momentum as

$$p(x) = \mathrm{i}\sqrt{2mFx} = \mathrm{i}\sqrt{2mFr}\,\mathrm{e}^{\mathrm{i}\varphi/2}. \tag{1.31}$$

The action integral finally becomes

$$S(x) = \frac{2\mathrm{i}\hbar}{3}\sqrt{2mF}\,x^{3/2} = \frac{2\mathrm{i}\hbar}{3}\sqrt{2mF}\,r^{3/2}\mathrm{e}^{3\mathrm{i}\varphi/2} \tag{1.32}$$

In the following, we shall use units with

$$S(x)/\hbar = \mathrm{i}x^{3/2}$$

to simplify the notation.

Consider now the following two WKB wave functions

$$\psi_1(x) = \frac{1}{x^{1/4}}\mathrm{e}^{-x^{3/2}}, \tag{1.33}$$

$$\psi_2(x) = \frac{1}{x^{1/4}}\mathrm{e}^{+x^{3/2}}. \tag{1.34}$$

Since x is real and positive in the forbidden region, $\psi_1(x)$ decays there and is the physically acceptable wave function. On the other hand, $\psi_2(x)$ is exponentially large in this region. We say that it is the dominant function there:

$$x > 0 : \quad \begin{cases} \psi_1(x) \text{ sub-dominant} \\ \psi_2(x) \text{ dominant} \end{cases}$$

This relationship ceases to be valid, however, when x moves into the complex plane. In particular, the functions $\psi_{1,2}(x)$ become of comparable magnitude when the quantity $x^{3/2}$ is purely imaginary. This happens when

$$0 = \mathrm{Re}\, x^{3/2} = r^{3/2} \cos(3\varphi/2) \quad \text{or} \quad \varphi = \pm\pi/3,\ \pm\pi \tag{1.35}$$

These lines are plotted as solid lines in fig.1.7. They are conventionally called Stokes lines.[3] When x crosses a Stokes line, the relative magnitudes of the wave functions $\psi_{1,2}(x)$ turn over. In particular, the function $\psi_1(x)$ becomes dominant when $|\varphi| > \pi/3$.

What becomes of $\psi_1(x)$ when we reach the negative real axis? This is also a Stokes line, and $\psi_1(x)$ is essentially a complex phase factor. But we find that the result depends on whether we pass through the upper or lower half-plane, and find:

$$\begin{aligned} \varphi \to \pi: \quad \psi_1(x) &= \frac{\mathrm{e}^{-\mathrm{i}\pi/4}}{r^{1/4}} \mathrm{e}^{\mathrm{i}r^{3/2}} = \text{reflected wave} \\ \varphi \to -\pi: \quad \psi_1(x) &= \frac{\mathrm{e}^{\mathrm{i}\pi/4}}{r^{1/4}} \mathrm{e}^{-\mathrm{i}r^{3/2}} = \text{incident wave} \end{aligned}$$

Depending on the path, we thus recover either the incident or the reflected wave (and never a combination of both).

On the other hand, the wave function $\psi_2(x)$ becomes subdominant as we cross the Stokes lines at $\varphi = \pm\pi/3$. It reaches the following values when continued to the negative real axis:

$$\varphi \to \pi: \quad \psi_2(x) = \frac{\mathrm{e}^{-\mathrm{i}\pi/4}}{r^{1/4}} \mathrm{e}^{-\mathrm{i}r^{3/2}} = \text{incident wave} \tag{1.37}$$

$$\varphi \to -\pi: \quad \psi_2(x) = \frac{\mathrm{e}^{\mathrm{i}\pi/4}}{r^{1/4}} \mathrm{e}^{\mathrm{i}r^{3/2}} = \text{reflected wave} \tag{1.38}$$

We observe a similar phenomenon as for $\psi_1(x)$, save that the role of incident and reflected waves are reversed.

We can now re-phrase Landau's argument:

(1) We want to find the phase relation between the incident and reflected waves, using analytic continuation in the complex plane.

[3] We use the notation of Bender & Orszag (1978). Berry & Mount (1972), e.g., choose the inverse convention and call the lines (1.35) 'anti-Stokes lines'.

(2) We write the wave in the allowed region as incident plus reflected wave,

$$x < 0 : \quad \psi(x) = \psi_{\rm inc}(x) + \psi_{\rm refl}(x).$$

In order to represent the incident wave in terms of the $\psi_{1,2}(x)$, we have two choices depending on whether we are on the upper or lower side of the cut:

$$\psi_{\rm inc}(x) = \begin{cases} \psi_2(x) & \text{upper side} \\ \psi_1(x) & \text{lower side} \end{cases} \tag{1.39}$$

where the functions $\psi_{1,2}(x)$ are single-valued on the cut plane. Landau's choice is to take that side of the cut where the function becomes dominant when one moves into complex x. This is the lower side.

(3) We now continue analytically this function $\psi_1(x)$ along the path shown in fig.1.7 to the positive half of the real axis. Note that it does not stay dominant (although Landau says so in the german translation!) through the entire lower half plane. On the contrary, it becomes the subdominant exponential once the Stokes line at $\varphi = -\pi/3$ is crossed. In particular, it is subdominant in the forbidden region (on the anti-Stokes line $\varphi = 0$).

(4) Continuing the function $\psi_1(x)$ through the upper half plane back to the negative real axis, Landau finds the reflected wave, but with a definite phase relation to the incident wave. He then writes the wave function for $x < 0$ as the sum of both limits (1.36) on the upper and lower sides of the cut:

$$\begin{aligned} x < 0 : \quad \psi(x) &= \frac{\mathrm{e}^{-\mathrm{i}\pi/4}}{r^{1/4}} \mathrm{e}^{-\mathrm{i}r^{3/2}} + \frac{\mathrm{e}^{\mathrm{i}\pi/4}}{r^{1/4}} \mathrm{e}^{\mathrm{i}r^{3/2}} \\ &= \frac{2}{(-x)^{1/4}} \sin\left(\frac{\pi}{4} + (-x)^{3/2}\right) \end{aligned} \tag{1.40}$$

Why does he take the sum of both functions? Probably because if we continue the sum to the upper or lower side of the cut, only one term will become dominant (the incident wave on the lower side, the reflected wave on the upper side). And these two dominant terms are smoothly joined by the single function $\psi_1(x)$ in the cut plane.

(5) How can be sure that Landau' choice of path through the complex x plane will always yield an exponentially damped solution in the forbidden

region? The Stokes line pattern of fig.1.7 gives a hint: this procedure works well when one has to cross a Stokes line to get to the forbidden region. Across the Stokes line, the function that was dominant close to the allowed region becomes subdominant, and is therefore the physically acceptable solution. Landau' procedure should therefore work when there is an odd number of Stokes lines between the allowed and forbidden regions. It is not clear how to use it with multiple turning points, for example. It would be interesting to check whether we can get the connection formula for the unphysical solution with Landau's method. We quote the warning of Berry & Mount (1972):

> 'This method certainly gives the correct results in simple cases, but there appears to be no valid derivation of it which does not rest ultimately on arguments similar to ours [. . .].'

(See below for Berry's approach.)

(6) Finally, we would like to mention a different perspective of Landau's procedure. We can start in the forbidden region and single out the subdominant function $\psi_1(x)$ as acceptable solution there. This function is then analytically continued on both sides of the complex plane to the negative real axis. One then observes that the incident and reflected waves appear on the respective sides of the cut. The wave function in the allowed region is then postulated to be the sum of these two waves. From this perspective, the starting point is located in the forbidden region, as for Langer's connection formula (1.27).

There exists more sophisticated techniques to continue a wave function through the complex plane (Fröman & Fröman, 1965; Berry & Mount, 1972). At the heart of them is a system of differential equations for the coefficients $b_{1,\,2}(x)$ of the wave function

$$\psi(x) = b_1(x)\psi_1(x) + b_2(x)\psi_2(x).$$

The main difference to Landau's argument is that now the linear combination of WKB functions changes. The advantage of the method is that the coefficients $b_{1,\,2}$ only change when the path in the complex plane crosses a Stokes line, and that they change in a definite manner. This allows to fix the form of the 'transfer matrix' relating the b's at different positions in the complex plane. Armed with this knowledge, one can derive Langer's connection formula (1.27) by exploiting the fact that the wave function is real.

1.4 Bohr–Sommerfeld quantisation

As an important application of Langer's connection formula, we discuss here the semiclassical quantisation rule in an isolated potential well and the quantum-mechanical tunnelling through a potential barrier.

1.4.1 WKB quantisation rules

The quantisation of energy in a potential well is a second important application of Langer's connection formula. In fig.1.8, the results that may be obtained for a generic potential are sketched. We suppose that the 'walls' of

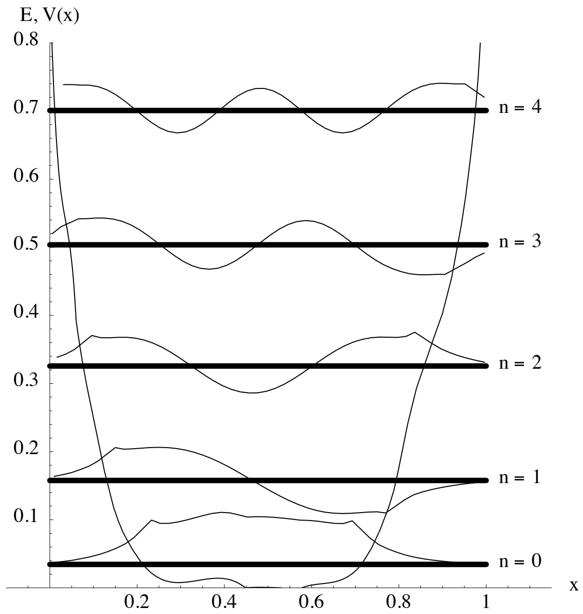

Figure 1.8: Potential well with quantised states, obtained with the semi-classical approximation.

the well are impenetrable and neglect tunnelling. The physically acceptable wave function must therefore decay exponentially in the forbidden regions $x < x_1$, $x > x_2$ (where $x_{1,2}$ denote again the turning points). If the turning points are sufficiently far apart, we may use the connection formula twice to find the wave function in the allowed region $x_1 < x < x_2$. The key point is that for a generic choice of energy, we get two expressions for the wave function that do not match. To be explicit, we get from (1.28) the wave function for $x > x_1$:

$$\psi_1(x) = \frac{C}{\sqrt{p(x)}} \sin\left(\frac{\pi}{4} + \frac{1}{\hbar}\int_{x_1}^{x} p(x')\mathrm{d}x'\right), \tag{1.41}$$

while the connection formula (1.27) at the turning point x_2 gives

$$\psi_2(x) = \frac{C'}{\sqrt{p(x)}} \sin\left(\frac{\pi}{4} + \frac{1}{\hbar}\int_{x}^{x_2} p(x')\mathrm{d}x'\right). \tag{1.42}$$

To compare these two functions, we write

$$\begin{aligned} \int_{x}^{x_2} p(x')\mathrm{d}x' &= \int_{x_1}^{x_2} p(x')\mathrm{d}x' - \int_{x_1}^{x} p(x')\mathrm{d}x' \\ &= S(x_1, x_2) - \int_{x_1}^{x} p(x')\mathrm{d}x' \end{aligned}$$

where $S(x_1, x_2)$ is the classical action integral for half an oscillation period in the well:

$$S(x_1, x_2) = \int_{x_1}^{x_2} \sqrt{2m\left(E - V(x)\right)}\,\mathrm{d}x. \tag{1.43}$$

We thus get

$$\psi_2(x) = \frac{C'}{\sqrt{p(x)}} \sin\left(\frac{S(x_1, x_2)}{\hbar} + \frac{\pi}{2} - \frac{\pi}{4} - \frac{1}{\hbar}\int_{x_1}^{x} p(x')\mathrm{d}x'\right)$$

This function is identical to (1.41) when the first two terms in the argument of the sine are an integer multiple of π. We may then choose the constant C' equal to C up to a sign. This is the WKB quantisation rule: *the classical action must be a half-integer multiple of the Planck constant:*[4]

$$\begin{aligned} S(x_1, x_2) &= \left(n + \tfrac{1}{2}\right)\pi\hbar, \qquad n = 0,\, 1,\, 2,\, \ldots \\ C' &= (-1)^n C, \end{aligned} \tag{1.44}$$

[4]The integer n must be non-negative because the action integral (1.43) is positive.

Observe that depending on the parity of the quantum number, the eigenfunctions decay with the same sign or with different signs in the forbidden regions (see fig.1.8). This is reminiscent of the well-defined parity of the eigenfunctions in an even potential well.

The accuracy of the semiclassical approximation can be checked from the validity criteria given before: one has to compare the distance between the turning points to the length scales $w_{1,2}$ that appear in the WKB matching procedure at the turning points. The ground state wave function $n = 0$ shown in fig.1.8, e.g., is certainly inaccurate because it shows inflexion points in a region where both the potential and the wave function do not vanish.

It is not too easy to determine eigenvalues numerically, and for this reason the semiclassical formula (1.44) is useful, too. Typically one uses the 'shooting method': first, a trial value for E close to the semiclassical eigenvalue is chosen; then the Schrödinger equation is solved starting from a point deep in the forbidden region $x < x_1$. This solution typically diverges exponentially in the forbidden region $x > x_2$. Then the energy is changed until the sign of this divergence changes. One can then use successive bisections to find the energy where the wave function becomes smaller than a preset accuracy. It also helps to study the semiclassical wave functions when choosing the initial and final points in the forbidden regions.

Examples

For a *harmonic* potential, the WKB quantisation procedure reproduces the exact eigenvalues. Although this happens by accident (check it from the WKB validity criteria), it is nevertheless a simple nontrivial example. The action integral is

$$\sqrt{2m} \int_{x_1}^{x_2} \sqrt{E - \tfrac{m}{2}\omega^2 x^2}\, \mathrm{d}x = m\omega \frac{\pi x_2^2}{2} = \frac{\pi E}{\omega}$$

and the quantisation rule (1.44) gives $E = E_n = \left(n + \frac{1}{2}\right)\hbar\omega$.

For a *linear* potential well that is closed by an infinite potential barrier (Wallis & al., 1992), the WKB quantisation rule applies with a slight modification: there is no phase jump $\pi/4$ at the infinite barrier. We thus get

$$\sqrt{2m}\int_0^{x_2}\sqrt{E-Fx}\,\mathrm{d}x = \sqrt{2mF}\frac{2(E/F)^{3/2}}{3} \stackrel{!}{=} \left(n+\tfrac{1}{4}\right)\pi\hbar$$

$$\Longrightarrow \quad E_n = \left[\frac{3\pi}{2}\left(n+\tfrac{1}{4}\right)\right]^{2/3} Fw \tag{1.45}$$

where w is the length scale for the linear potential introduced in (1.19). Note the different power law $E \propto n^{2/3}$ as compared to the harmonic potential.

Since we know the exact wave function for the linear potential, we can evaluate the accuracy of the WKB approximation. The exact wave function is given by a displaced Airy function $\mathrm{Ai}((x-x_2)/w)$, where $x_2 = E/F$ is the right turning point. The boundary condition at $x_1 = 0$ imposes the quantisation of energy:

$$\mathrm{Ai}(-E/Fw) = 0$$

The energy eigenvalues are thus proportional to the zeros of the Airy function, with the quantity Fw giving the energy scale. Figure 1.9 compares this result with the semiclassical prediction. One sees that for $n \geq 10$ the agreement is already quite good.

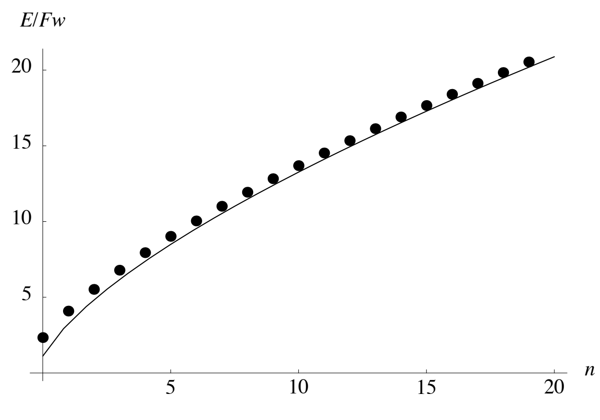

Figure 1.9: Quantised energy values in a linear potential well. Dots: exact zeroes of the Airy function; line: semiclassical prediction (1.45).

Other examples are the Eckart or Morse wells

$$V(x) = \frac{V_0}{\cosh^2(\kappa x)},$$

$$V(x) \quad = \quad V_0 \left(\mathrm{e}^{-\kappa x} - 1 \right)^2$$

where exact eigenfunctions and eigenvalues may be obtained. These potentials are studied as problems.

1.4.2 Barrier tunnelling

Consider a wave that is scattered by a potential barrier, as shown in fig.1.10. We shall suppose that the particle is incident from $x \to -\infty$ where the potential is small, and that its energy is below the barrier top. We have two turning points $x_{1,2}$ and the following asymptotic behaviours:

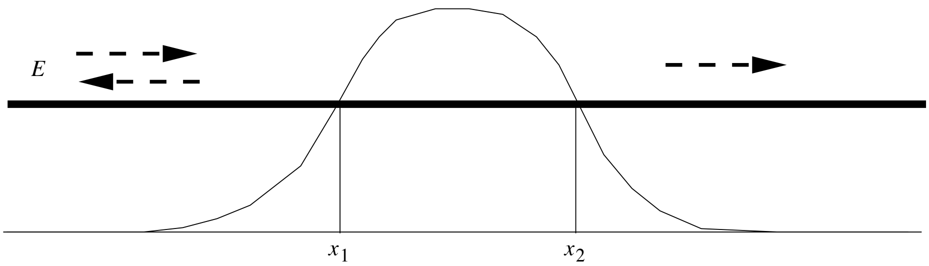

Figure 1.10: Reflection and transmission of a wave from a potential barrier.

$$\begin{aligned} x \to -\infty : & \quad \psi(x) = \text{incident wave} + R\,\text{reflected wave} \\ x \to +\infty : & \quad \psi(x) = T\,\text{transmitted wave} \end{aligned}$$

Note that to the right of the barrier, there is only a single transmitted and no incident wave. As a consequence, the wave function will be complex. We shall construct a suitable superposition of real wave functions, and for this purpose, we need a second wave function that solves the turning point problem.

Matching with an exponentially growing wave at a turning point. In the previous section, we constructed a physically acceptable wave function at a reflecting turning point. We consider here the opposite case, namely a wave function that diverges in the forbidden region. This divergence is not a real problem because for the barrier shown in fig.1.10, the forbidden region has a finite extension.

The calculation is quite parallel to the one in the previous section. We choose again the dimensionless variable ξ with $\xi > 0$ being the forbidden region. The Airy equation (1.21) has the second solution $\mathrm{Bi}(\xi)$ that is sketched in fig.1.11. It shows an exponential growth in the forbidden

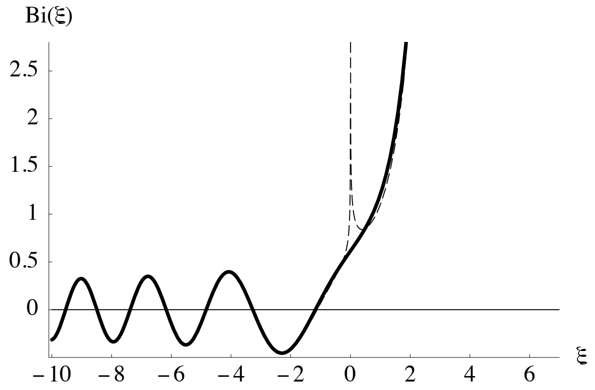

Figure 1.11: The Airy function $\mathrm{Bi}(x)$ (solid curve) and its asymptotic forms (dashed curves).

region. The asymptotic behaviours are (see problem 1.4)

$$\xi \ll -1 : \mathrm{Bi}(\xi) \approx \frac{1}{\sqrt{\pi}(-\xi)^{1/4}} \cos\left[\frac{2}{3}(-\xi)^{3/2} + \frac{\pi}{4}\right] \tag{1.46a}$$

$$\xi \gg 1 : \mathrm{Bi}(\xi) \approx \frac{1}{\sqrt{\pi}\xi^{1/4}} \exp\left[\frac{2}{3}\xi^{3/2}\right] \tag{1.46b}$$

Note the factor of 2 that is missing in (1.46b) and the cos instead of the sin in (1.46a). When we compare these formula to the WKB wave functions in the vicinity of the turning point, we arrive at the following connection formula

$$\begin{array}{ccc} \dfrac{D}{\sqrt{p(x)}} \cos\left(\dfrac{\pi}{4} + \dfrac{1}{\hbar}\displaystyle\int_x^{x_0} p(x')\mathrm{d}x'\right) & \longrightarrow & \dfrac{D}{\sqrt{|p(x)|}} \exp\left(\dfrac{1}{\hbar}\displaystyle\int_{x_0}^{x} |p(x')|\mathrm{d}x'\right) \\ \text{allowed region (I) } x < x_0 & & \text{forbidden region (II) } x > x_0 \end{array} \tag{1.47}$$

Berry & Mount (1972) quote the warning of Fröman & Fröman (1965) that this connection formula has to be taken with much care. Indeed, eq.(1.47) may only be understood as a relation between the asymptotic behaviour of this (unphysical) wave function. In numerical work, it is impossible to be sure that the decaying exponential has a nonzero coefficient – this does not change the numerical results just because the coefficient is multiplied by a small number. But a nonzero coefficient inevitably gives an admixture of a sine function in the allowed region and changes the phase of the standing wave. The derivation used here shows that (1.47) simply gives the asymptotic form of the other linearly independent solution to the Schrödinger equation.

The turning point x_2. The status of the connection formula (1.47) thus clarified, we can write it down for the turning point x_2 in fig.1.10. In this case, the forbidden region is located to the left of x_2, and the connection formula becomes

$$\underset{\text{forbidden region (II) } x < x_0}{\frac{D}{\sqrt{|p(x)|}} \exp\left(\frac{1}{\hbar}\int_x^{x_0} |p(x')| \mathrm{d}x'\right)} \quad \longleftarrow \quad \underset{\text{allowed region (I) } x > x_0}{\frac{D}{\sqrt{p(x)}} \cos\left(\frac{\pi}{4} + \frac{1}{\hbar}\int_{x_0}^{x} p(x') \mathrm{d}x'\right)} \qquad (1.48)$$

If we want to get a transmitted wave propagating to the right

$$x > x_2 : \quad \psi(x) = \frac{N}{\sqrt{p(x)}} \exp\left(\frac{\mathrm{i}}{\hbar}\int_{x_2}^{x} p(x') \mathrm{d}x' + \frac{\mathrm{i}\pi}{4}\right),$$

we thus have to superpose the wave functions (1.28, 1.48) with the coefficients

$$2C = \mathrm{i}N, \qquad D = N$$

where N is a global normalisation constant. 'Under the potential barrier' (in the forbidden region), the wave function is a superposition of exponentially growing and decreasing waves with weights given by $C,\ D$. We now match this superposition to incident and reflected waves at the first turning point x_1. To simplify the comparison, we write

$$\begin{aligned} \int_x^{x_2} |p(x')| \mathrm{d}x' &= \int_{x_1}^{x_2} |p(x')| \mathrm{d}x' - \int_{x_1}^{x} |p(x')| \mathrm{d}x' \\ &= \hbar W - \int_{x_1}^{x} |p(x')| \mathrm{d}x' \end{aligned}$$

where W is a positive number that depends on the energy and the behaviour of the potential in the forbidden region

$$W = \frac{\sqrt{2m}}{\hbar} \int_{x_1}^{x_2} \sqrt{V(x') - E}\, \mathrm{d}x' \qquad (1.49)$$

The turning point x_1. The wave function that arrives from the right at the turning point x_1 is thus of the form

$$\begin{aligned} x > x_1: \quad \psi(x) &= \frac{N}{\sqrt{|p(x)|}} \left[\mathrm{e}^{W} \exp\left(-\frac{1}{\hbar} \int_{x_1}^{x} |p(x')| \mathrm{d}x' \right) + \right. \\ & \left. + \frac{\mathrm{i}}{2} \mathrm{e}^{-W} \exp\left(\frac{1}{\hbar} \int_{x_1}^{x} |p(x')| \mathrm{d}x' \right) \right] \end{aligned} \tag{1.50}$$

The first term decreases when x moves into the forbidden region and therefore connects to the regular solution of formula (1.27). For the second, increasing term we need again the connection formula (1.47) for the 'unphysical' solution. We finally get, in the allowed region $x < x_1$, the following superposition of incident and reflected waves

$$\begin{aligned} x < x_1: \quad \psi(x) &= \frac{N}{\sqrt{p(x)}} \left[\alpha_{\text{inc}} \exp\left(\frac{\mathrm{i}}{\hbar} \int_{x_1}^{x} p(x') \mathrm{d}x' \right) + \right. \\ & \left. + \alpha_{\text{refl}} \exp\left(-\frac{\mathrm{i}}{\hbar} \int_{x_1}^{x} p(x') \mathrm{d}x' \right) \right] \end{aligned}$$

where the coefficients are given by

$$\alpha_{\text{inc}} = \mathrm{e}^{W + \mathrm{i}\pi/4} \left(1 + \tfrac{1}{4} \mathrm{e}^{-2W} \right), \tag{1.51}$$

$$\alpha_{\text{refl}} = \mathrm{e}^{W - \mathrm{i}\pi/4} \left(1 - \tfrac{1}{4} \mathrm{e}^{-2W} \right). \tag{1.52}$$

Using the fact that the WKB wave functions have unit flux, we thus get the following reflection and transmission coefficients:

$$R = -\mathrm{i} \frac{1 - \frac{1}{4} \mathrm{e}^{-2W}}{1 + \frac{1}{4} \mathrm{e}^{-2W}}, \qquad |R|^2 \approx 1 - \mathrm{e}^{-2W} \tag{1.53a}$$

$$T = \frac{\mathrm{e}^{-W}}{1 + \frac{1}{4} \mathrm{e}^{-2W}}, \qquad |T|^2 \approx \mathrm{e}^{-2W} \tag{1.53b}$$

where the approximations are valid when $W \gg 1$ (semiclassical regime: 'action integral' (1.49) large compared to $\hbar$). We observe that in this regime, the transmission through the barrier is extremely small: the current is transported to the second turning point x_2 only via the 'tail' of the exponentially decaying wave that enters the forbidden region at x_1.

Comments. One may verify from (1.53) that current conservation, $|R|^2 + |T|^2 = 1$, is also valid if W is not large. In this limit, however, the turning points $x_{1,2}$ approach each other too closely to allow for a separate application of the single turning point connection formula, and the results (1.53) cease to be valid. In problem xx, you are invited to derive an approximation that covers this regime. One result of this approximation is that when the incident energy coincides with the barrier top, both reflection and transmission probabilities $|R|^2$ and $|T|^2$ are equal to $\frac{1}{2}$. For energies below the barrier, the transmission decreases rapidly to exponentially small values. But even when the energy is larger than the barrier top, there is a nonzero probability of reflection. It becomes very small, too, when the energy is much larger than the barrier top.

We can get a simple estimate for the width in energy of the transition zone where the transmission goes over from close to zero to close to unity. Close to the barrier top, we approximate the potential by an inverted parabola with second derivative $V'' = -m\omega^2$. For an energy ΔE below the barrier top, two turning points exists and are spaced

$$a = \sqrt{\frac{8\Delta E}{m\omega^2}}$$

apart. In the estimate (1.30) for the validity of the single turning point connection formula, we have to require $a \gg w$ where w depends on the potential slope at the turning points. Using the definition (1.19) of the width w, we find that our result is valid provided $\Delta E \gg \hbar\omega/8$, i.e., the energy is sufficiently below the barrier top. This condition implies in turn that the transmission through the barrier is very small since we have (using again a parabolic shape for the barrier top) $W \approx \pi\Delta E/\hbar\omega \gg \pi/8 \approx 0.393$.

Remark. Langer was not the first to use the patching procedure with the Airy function at a turning point. This method was already employed by Jeffreys (1923) and Kramers (1926). The other two people in what is sometimes called the JWKB approximation are Wenzel and Brillouin.

1.5 Uniform asymptotic approximations

1.5.1 The basic idea

LANGER's connection formula tells us how to glue the WKB wave functions together on both sides of a turning point. But we still have a wave function that is made up of two or three different expressions, depending on whether the AIRY function is used close to the turning point or not. It would be great if we had a single formula that is valid throughout the transition region. Such a kind of formula exists, and in fact LANGER already wrote it in his papers.

? was able to derive a *uniform asymptotic* approximation to the wave function at a single turning point. His results were subsequently generalised, and are based on the following idea (Berry & Mount, 1972). We want an approximate solution of the Schrödinger equation[5]

$$-\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + W(x)\psi = 0, \tag{1.54a}$$

and we know the exact solution $\phi(y)$ to a 'similar', but simpler potential $U(y)$,

$$-\frac{\mathrm{d}^2\phi}{\mathrm{d}y^2} + U(y)\phi = 0. \tag{1.54b}$$

This equation is called the 'comparison equation'. We conjecture that the wave function $\phi(y)$ will be similar to $\psi(x)$ and may be obtained by 'streching or contracting it a little and changing the amplitude a little' (Berry & Mount, 1972, p.343). We thus make the *ansatz*

$$\psi(x) = f(x)\phi(y(x)) \tag{1.55}$$

where $f(x)$ and $y(x)$ are functions to be determined. Insert this into the SCHRÖDINGER equation (1.54a) and find, using (1.54b):

$$-\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\phi - \frac{\mathrm{d}\phi}{\mathrm{d}y}\left(2\frac{\mathrm{d}f}{\mathrm{d}x}\frac{\mathrm{d}y}{\mathrm{d}x} + f\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}\right) - f\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2 U\,\phi + f\,W\,\phi = 0. \tag{1.56}$$

[5] To simplify the notation, we write the potential in the form $W(x) = (2m/\hbar^2)\,[V(x) - E]$.

We can get rid of the first derivative $\mathrm{d}\phi/\mathrm{d}y$ by choosing

$$f = \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^{-1/2} \tag{1.57}$$

Then we may divide by $f\,\phi$ and find an equation for the 'coordinate mapping' $y(x)$:

$$-\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^{1/2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^{-1/2} - \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^{2} U(y(x)) + W(x) = 0 \tag{1.58}$$

We now make an approximation that is motivated by our idea that the coordinates x and y differ only by small strechtings. We can then expect that the second derivative in (1.58) to be 'small', and may neglect it.[6] We then get the first-order differential equation

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \pm\left(\frac{W(x)}{U(y(x))}\right)^{1/2} \tag{1.59}$$

With the initial condition $y(x_0) = y_0$, we find the following implicit solution

$$\int_{x_0}^{x} \sqrt{W(x')}\,\mathrm{d}x' \quad = \quad \pm\int_{y_0}^{y} \sqrt{U(y')}\,\mathrm{d}y' \tag{1.60a}$$

$$\int_{x}^{x_0} \sqrt{-W(x')}\,\mathrm{d}x' \quad = \quad \pm\int_{y}^{y_0} \sqrt{-U(y')}\,\mathrm{d}y' \tag{1.60b}$$

where the choice depends on the sign of $W(x)$, i.e., whether x is in an allowed ($W(x) < 0$) or forbidden ($W(x) > 0$) region (see footnote 5 on p. 35).

Once we have computed $y(x)$ by inverting these equations, we have the following approximation for the wave function

$$\psi(x) \approx \left[\frac{U(y(x))}{W(x)}\right]^{1/4} \phi(y(x)) \tag{1.61}$$

We shall see that this solution is valid for the whole range of x, even close to turning points.

This method works only when the coordinate mapping $x \mapsto y(x)$ is bijective, i.e., when the derivative $\mathrm{d}y/\mathrm{d}x$ is nowhere zero nor infinite. Looking

[6] This procedure is similar to what we did at the start to get the WKB approximation.

at (1.59), we observe that this implies that the zeros of the potentials $W(x)$ and $U(y)$ are mapped onto each other. In particular, both potentials must have the same number of turning points. 'We thus have what is potentially a very powerful principle: in the semiclassical limit all problems are equivalent which have the same *classical turning-point structure*' (Berry & Mount, 1972, p.344).

1.5.2 Examples

Recover the standard WKB waves. The first example is a *classically allowed region without turning points*. The function $W(x) = -p^2(x)/\hbar^2$ then vanishes nowhere, and we may take $U(y) \equiv -1$. The comparison equation reads

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}y^2} + \phi = 0$$

and its solutions are plane waves $\phi = \exp(\pm \mathrm{i}y)$. The coordinate mapping is obtained from the solution of

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \pm\frac{p(x)}{\hbar}. \tag{1.62}$$

The amplitude function (1.57) is thus equal to $f(x) = (\hbar/p(x))^{1/2}$, and we get the propagating WKB waves

$$\psi(x) \approx \frac{C}{\sqrt{p(x)}} \exp\left(\pm\frac{\mathrm{i}}{\hbar}\int_{x_0}^{x} p(x')\,\mathrm{d}x'\right).$$

These expressions are no longer valid at turning points because the mapping $x \mapsto y$ then becomes singular [see (1.62)]. Similarly, we can derive the WKB solutions in classically forbidden regions by choosing $U(y) \equiv 1$.

A single turning point. If the potential $W(x) = -p^2(x)/\hbar^2$ has a simple turning point at, say, x_0, we are advised to take a comparison potential with a simple zero, say, $U(y) = y$. This gives the Airy equation

$$-\frac{\mathrm{d}^2\phi}{\mathrm{d}y^2} + y\phi = 0$$

with the general solution $\phi(y) = \alpha\mathrm{Ai}(y) + \beta\mathrm{Bi}(y)$. To compute the coordinate mapping, we observe from (1.59) that the classically allowed region

$W(x) < 0$ must be mapped onto $y < 0$, and vice versa. This fixes the sign of the derivative $\mathrm{d}y/\mathrm{d}x$. Suppose for definiteness that the allowed region is $x < x_0$. We thus get from the implicit coordinate mapping (1.60)

$$\frac{2}{3}(-y)^{3/2} = \frac{1}{\hbar}\int_x^{x_0} p(x')\,\mathrm{d}x',\; x \in \text{allowed},\; y < 0 \tag{1.63a}$$

$$\frac{2}{3}y^{3/2} = \frac{1}{\hbar}\int_x^{x_0} |p(x')|\,\mathrm{d}x',\; x \in \text{forbidden},\; y > 0 \tag{1.63b}$$

If the allowed and forbidden regions are located the other way round, one simply has to change the order of the integration limits. The mapping (1.63) thus makes those points x, y correspond for which the classical action integral (divided by $\hbar$) has the same value. Recalling the expansion of the action in the vicinity of the turning point, we also conclude that the mapping $x \mapsto y = (\operatorname{sign} V'(x_0))(x - x_0)/w$ is approximately linear there. This justifies *a posteriori* the neglect of the second derivative in (1.58) around the turning point (the function $\mathrm{d}y/\mathrm{d}x$ is approximately constant).

Finally, we get the following uniform approximation for the wave function for a potential with a single turning point:

$$\psi(x) = C\left(\frac{y(x)}{p^2(x)}\right)^{1/4}\Big(\alpha\mathrm{Ai}(y(x)) + \beta\mathrm{Bi}(y(x))\Big) \tag{1.64}$$

It is a simple exercise to check that far from the turning point, this expression goes over into both connection formulas (1.27, 1.47): the argument $y(x)$ is then large in magnitude, and we may use the asymptotic expansions of the Airy functions. Because of the form (1.63) of the coordinate mapping, we then recover exponentials or trigonometric functions whose arguments are classical action integrals.

Explicit example: exponential barrier. Solve the Schrödinger equation for the potential

$$V(z) = V_0\,\mathrm{e}^{-2\kappa z} \tag{1.65}$$

An exact solution is available and involves modified Bessel functions $K_{\mathrm{i}k}(\mathrm{e}^{-\kappa(z-z_0)})$ that depends on the scaled momentum parameter $k = p/\hbar\kappa$ where p is the momentum for $z \gg 1/\kappa$, far from the barrier. The uniform asymptotic expansion using the AIRY function can be computed analytically to quite some extent. Details are provided in a paper draft that is in preparation.

Explicit example: uniform expansion for the BESSEL functions. To illustrate the power of the uniform expansion, we shall derive a uniform expansion of the BESSEL functions. One can define the BESSEL function $J_n(kr)$ as the physically acceptable solution to the radial SCHRÖDINGER equation

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2}J_n - \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}J_n + \frac{n^2}{r^2}J_n = k^2 J_n$$

where r is the radius in (two-dimensional) polar coordinates. To simplify the following calculations, we measure r in units of $1/k$ and put $k = 1$. We get rid of the first derivative in the BESSEL equation by putting

$$J_n(r) = \frac{1}{\sqrt{r}}j(r)$$

The physical boundary condition at the origin is now that $j(r)$ is of order $r^{n+1/2}$ there. The centrifugal potential then changes to

$$\frac{n^2}{r^2} \mapsto \frac{n^2 - \frac{3}{4}}{r^2} \equiv \frac{L^2}{r^2},$$

and we find the following potential

$$W(r) = \frac{L^2}{r^2} - 1$$

This potential has a single turning point at $r_0 = L$ (note that this zero does not exist when $n = 0$, we exclude this case). We map the forbidden region $0 < r < r_0$ onto the half-axis $y > 0$ of the AIRY equation using (1.63) and get

$$\begin{aligned} \frac{2}{3}y^{3/2} &= \int_r^{r_0} \sqrt{W(r')}\,\mathrm{d}r' = \int_r^{r_0} \sqrt{L^2 - r'^2}\frac{\mathrm{d}r'}{r'} \\ &= L\log\left(\frac{L + \sqrt{L^2 - r^2}}{r}\right) - \sqrt{L^2 - r^2} \end{aligned}$$

Similarly, the allowed region $r_0 < r < \infty$ is mapped onto $y < 0$ using

$$\begin{aligned} \frac{2}{3}(-y)^{3/2} &= \int_{r_0}^{r} \sqrt{r'^2 - L^2}\frac{\mathrm{d}r'}{r'} \\ &= L\arcsin\frac{L}{r} + \sqrt{r^2 - L^2} - L\frac{\pi}{2}. \end{aligned}$$

The prefactor of the wave function is given by $(y(x)/W(x))^{1/4}$. The coordinate mapping is illustrated in Fig.1.12(left) for different values of L. Note how $y(r)$ is smooth at $r = L = r_0$.

Using the boundary condition that the BESSEL functions $J_n(kr)$ vanish at the origin (for $n \geq 1$), we finally get the following asymptotic expression

$$J_n(kr) = C \left(\frac{y(kr)}{n^2 - \frac{3}{4} - k^2 r^2} \right)^{1/4} \mathrm{Ai}(y(kr)) \tag{1.66}$$

The uniform approximation cannot determine the global prefactor C. but comparing with the standard asymptotic form of the BESSEL functions for large argument $kr \gg n$, we find $C = \sqrt{2}$. Comparing to the standard asymptotics, one also finds that the uniform expansion is valid if the effective angular momentum L is large compared to unity.

In fig.1.12(right), we compare the uniform expansion (1.66) to the exact BESSEL functions $J_n(kr)$ for several values of n. We observe that the

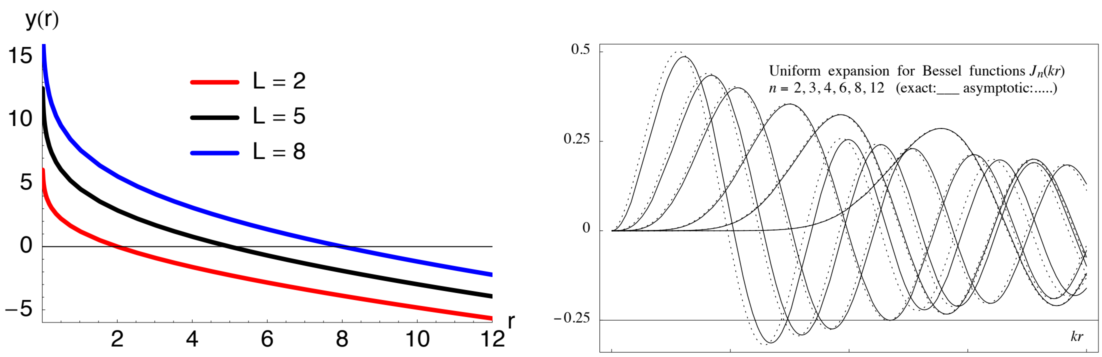

Figure 1.12: Uniform asymptotic expansion (1.66) for the BESSEL functions.

agreement is quite good over the entire range of the argument kr and becomes much better when the order n (and hence the effective angular momentum L) increases.

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