# The WKB approximation

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## 1 Derivation of the WKB approximation

### 1.1 Idea

Solving the Schrödinger equation is one of the essential problems in quantum mechanics. Since a non-linear second order ordinary differential equation(ODE) has, in general, no analytic solution, an approximation method is usually applied to tackle the problem. Instead of starting with a simplified potential and adding small terms, which leads to perturbation theory, the WKB approximation makes an assumption of a slowly varying potential. This method is named after physicists Wentzel, Kramers, and Brillouin, who all developed it in 1926[1][2]. Shortly before that, in 1923, a mathematician Harold Jeffreys had also developed a general method of approximating solutions to linear ODE[3], but the other three were unaware of his work. So today it is usually referred as WKB or WKBJ approximation.

To introduce the idea behind this approximation, we first consider the Schrödinger equation

$$\frac{d^2\psi}{dx^2} + k(x)^2\psi = 0 \tag{1}$$

with the abbreviations

$$\begin{aligned} k(x) &= (\frac{2m}{\hbar^2}(E - V))^{1/2} & \text{if} \quad \mathrm{E > V(x)} \\ k(x) &= i(\frac{2m}{\hbar^2}(V - E))^{1/2} = i\kappa(x) & \text{if} \quad \mathrm{E < V(x)} \end{aligned} \tag{2}$$

If $k(x) = \text{const}$, the function has the solution $\psi(x) = e^{\pm ikx}$. If $k$ is no longer constant, but varies at a slow rate, it is reasonable to try if this soluton, with $x$ dependent $k$

$$e^{\pm i\int k(t)dt} \tag{3}$$

still solves the equation. Substituting it in to the Schrödinger equation gives us

$$\frac{d^2\psi}{dx^2} + k(x)^2\psi = (\frac{d^2}{dx^2} + k^2)e^{\pm i\int k(t)dt} = \pm ik'(x)e^{\pm i\int k(t)dt} \tag{4}$$

Thus the solutions 3 solves the equation only when $k'(x)$ is equal to 0. However, this does not mean that our attempt was in vain, equation 4 suggests that 3 remains a good approximation, if $k'$ is negligible, or, more precisely, if

$$|k'| \ll k^2 \tag{5}$$

which is the condition we are going to use in the derivation of the WKM approximation.

## 1.2 Successive approximations method

Before we derive the WKB approximation, it is necessary to first introduce an approximation method for solving ODE, the successive approximations. Let's consider an ordinary differential equation:

$$\mathbf{y}' = f(x, \mathbf{y}) \tag{6}$$

Assume that the equation has a solution $y(x)$ satisfying the initial condition $y(x_0) = y_0$, then it must also satisfy the equation

$$\mathbf{y} = C + \int_{x_0}^{x} f(t, \mathbf{y}(t))dt \quad \text{with} \quad \mathrm{C} = \mathbf{y}(\mathrm{x}_0) \tag{7}$$

This can be treated mathematically as a fix point problem, with a series of function $y_n(x)$ converging to the true solution $y(x)$, if some specific conditions are satisfied such as Libschitz condition and boundary condition. Therefore we can define a succesive procedure:

$$\mathbf{y}_n = \mathbf{y}_0 + \int_{x_0}^{x} f(t, \mathbf{y}_{n-1}(t))dt \tag{8}$$

which will bring us vary close to the true solution after a large enough $n$.

## 1.3 Derivation of WKB

We assume that the solution to equation 1 is given by

$$\psi(x) = e^{iu(x)} \tag{9}$$

with $u(x)$ an unknown complex function. Substituting it in 1, we get the following equation of $u(x)$:

$$iu''(x) - u'(x)^2 + k(x)^2 = 0 \tag{10}$$

Now we sovle this ODE with the succesive approximation. We set the 0-th approximation to be our simple guess in section 1.1:

$$u_0 = \int_{x_0}^{x} k(t)dt \tag{11}$$

From equation 10 we can extract a succesive process:

$$u_n = \pm \int_{x_0}^{x} \sqrt{k^2(t) + iu''_{n-1}(t)}dt \tag{12}$$

In this way the first approximation can be written as:

$$\begin{aligned} u_1(x) &= \pm \int_{x_0}^{x} \sqrt{k^2(t) + iu''_0(t)}dt \\ &= \pm \int_{x_0}^{x} k^2(t)\sqrt{1 \pm i\frac{k'(t)}{k^2(t)}}dt \\ &\approx \int_{x_0}^{x} \pm k(t) + \frac{i}{2}\frac{k'(t)}{k(t)}dt \\ &= \int_{x_0}^{x} \pm k(t)dt + \frac{i}{2}\ln k(x) + C \end{aligned} \tag{13}$$

where at the second last step we used the condition $|k'| \ll k^2$. We can see from the second step that the first appximation is very close to the 0-th one, which indicate the validity of this first approximation. In this case, our first order approximation of the wave function is then given by

$$\begin{aligned}\psi_1(x) &= \exp[iu_1(x)] \\ &= \frac{1}{\sqrt{k(x)}} \exp\Big[\pm i \int_{x_0}^{x} k(t)\Big]\end{aligned} \tag{14}$$

The constant $C$ was neglected since it contributes only to the normalization. This approximation 14 is the so-called WKB apprximation.

# 2 Tunneling: Alpha decay

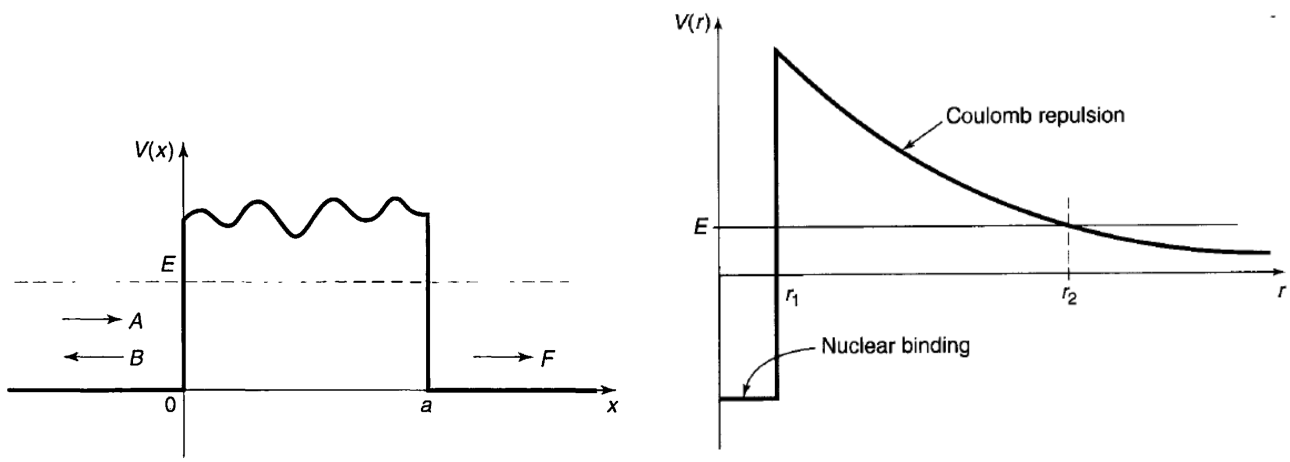


Abbildung 1: Potential barrier and Alpha decay [4]

Consider the potential shown in Fig 1 left, the WKB approximation gives the following solution:

$$\psi = Ae^{ikx} + Be^{-ikx} \qquad x < 0 \tag{15}$$

$$\psi \approx \frac{C}{\sqrt{\kappa(x)}} e^{\int_0^x \kappa(t)dt} + \frac{D}{\sqrt{\kappa(x)}} e^{-\int_0^x \kappa(t)dt} \qquad 0 \leq x \leq a \tag{16}$$

$$\psi = Fe^{ikx} \qquad x > a \tag{17}$$

Since we expect the wave function to decrease exponentially in respect of $x$ between $[0, a]$, the higher the potential, the smaller is the coefficient $C$. Due to the linearity of the wave function, we can estimate the transmission probability $T = |F|^2/|A|^2$ by the two boundary values of the wavefunction:

$$T \approx \frac{|F|^2}{|A|^2} = \exp\big[-2\int_0^x \kappa(t)dt\big] \tag{18}$$

As an example, we take the potential of a neuclei (Fig 1 right) and derive the alpha decay rate. The potential is given by

$$V(r) = \frac{Ze^2}{r} \quad r > r_1 \quad \text{and} \quad \mathrm{V(r) = 0} \quad \mathrm{r < r_1} \tag{19}$$

and $r_2$ denote the point where the energy equals the potential. The transmission probability Fun. 18 can be written as

$$T \approx \exp\left(\frac{-2}{\hbar}\int_{r_1}^{r_2}\sqrt{2m(\frac{Ze^2}{r}-E)}\right) \tag{20}$$

Substituting $E = Ze^2/r_2$, we get

$$T \approx \exp\left(\frac{-2\sqrt{2mE}}{\hbar}\int_{r_1}^{r_2}\sqrt{\frac{r_2}{r}-E}\right) \tag{21}$$

$$= \exp\left(\frac{-2\sqrt{2mE}}{\hbar}\left[r_2(\frac{\pi}{2}-sin^{-1}\sqrt{\frac{r_1}{r_2}})-\sqrt{r_1(r_2-r_1)}\right]\right) \tag{22}$$

$$\approx \exp\left(\frac{-2\sqrt{2mE}}{\hbar}\left[\frac{\pi}{2}r_2-2\sqrt{r_1r_2}\right]\right) \tag{23}$$

$$= \exp\left(-K_1\frac{Z}{\sqrt{E}}+K_2\sqrt{Zr_1}\right) \tag{24}$$

where $K1$, $K2$ are constant numbers. On the second last step we use the approximation $r_1 \ll r_2$. The transmission probability, on the other hand, represents the escape probability. Thus, from this result we can extract the relation between the lifetime and the energy

$$\ln\tau = \ln\frac{1}{T} \propto \frac{1}{\sqrt{E}} \tag{25}$$

This nice relation is verified by experiment result shown in Fig 2.

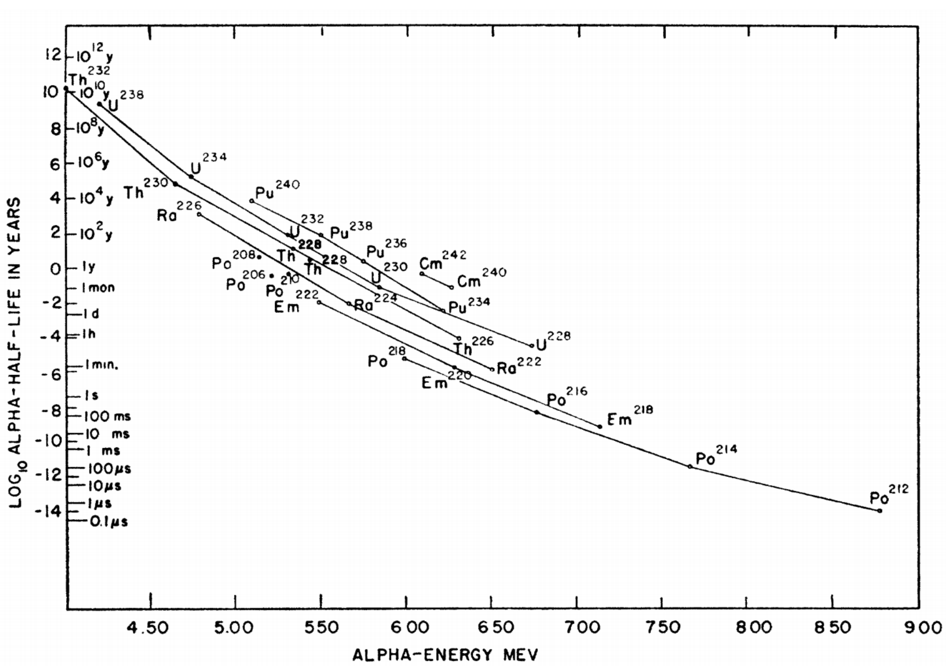


Abbildung 2: Graph of the logarithm of the lifetime versus Energy.[5]

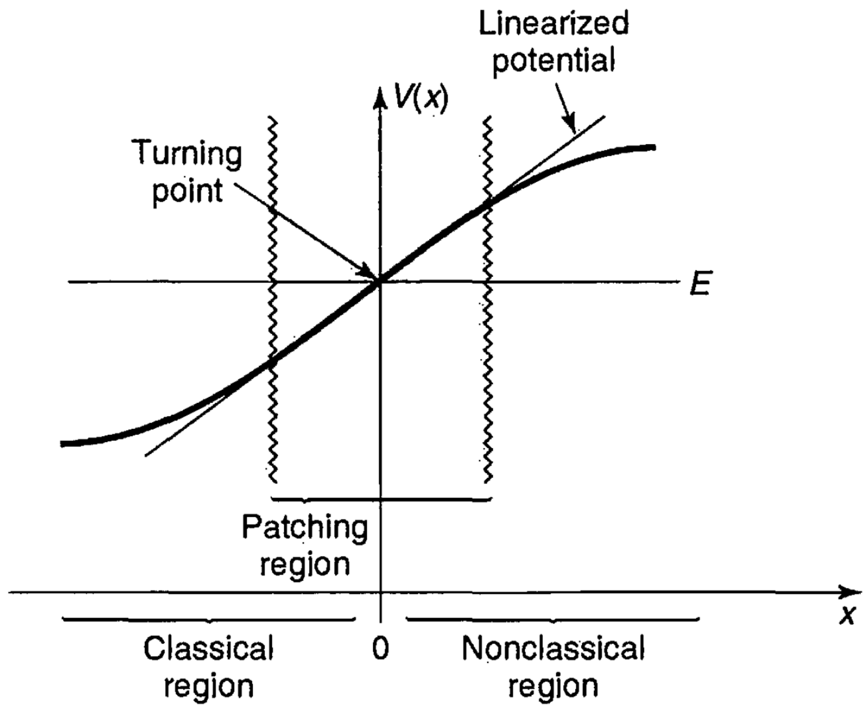


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Abbildung 3: Approximation at the turing points [4]

# 3 At the turning point: connection formulas

From the first section, we know that in each region, either $E > V$ or $E < V$, the WKB approximation 14 raises two different solutions, thus two coefficients remain to be determined by the boundary condition. Usually, we connect the coefficient of solutions from two regions by identifying their limitation at the turning points. However, it is easy to see that the WKB fails at the turning point, where $E = V$ and the solutions are all divergent. In order to build relation between the coefficients and obtain one single solution up to a normalization factor, we introduce the Airy functions. With help of the Airy functions, we can connect the four coefficients by comparing the approximated solution and the Airy functions, which yields the so-called connection formulas.

In Fig 3, we can see that at the turning point, the general solutions of the WKB approximation can be written as:

$$\psi(x) = \begin{cases} \frac{1}{\sqrt{k(x)}} B e^{i \int_x^0 k(t)dt} + \frac{1}{\sqrt{k(x)}} C e^{-i \int_x^0 k(t)dt} \\ \frac{1}{\sqrt{\kappa(x)}} D e^{-\int_0^x \kappa(t)dt} \end{cases} \tag{26}$$

with $t = 0$ as the turning point. The potential at $x = 0$ equals the energy and $k(x) \to 0$ or $\kappa(x) \to 0$ implys an unphysical divergence of $\psi(x)$. In this case, we expand $V(x) - E$ near the turning point and get

$$V(x) - E = V'(0)x + O(x^2) \tag{27}$$

From the Schrödinger equation we obtain again a simplified equation:

$$\frac{d^2\psi}{dz^2} - z\psi = 0 \tag{28}$$

with

$$z = \alpha x \quad \text{and} \quad \alpha = \left[\frac{2\text{m}}{\hbar^2}\text{V}'(0)\right]^{\frac{1}{3}} > 0 \tag{29}$$

This equation is known as Airy equation and possesses very nice exact solutions $Ai(x)$ and $Bi(x)$. We know that for this linearized potential and $x$ far from the approximation, the Airy functions must be identical with the WKB approximation. For $x > 0$, we obtain

$$\kappa(x) = \alpha^{\frac{3}{2}}\sqrt{x} \tag{30}$$

$$\psi(x)_{WKB} = \frac{D}{\alpha^{3/4}x^{1/4}}\exp\left[-\frac{2}{3}(\alpha x)^{\frac{3}{2}}\right] \tag{31}$$

and for $x < 0$

$$k(x) = \alpha^{\frac{3}{2}}\sqrt{-x} \tag{32}$$

$$\psi(x)_{WKB} = \frac{1}{\alpha^{3/4}(-x)^{1/4}}\left\{B\exp\left[i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}\right] + C\exp\left[-i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}\right]\right\} \tag{33}$$

The asymtotic behaviour of the Airy-function is given by

$$\psi(x)_{Airy} \approx \frac{a}{2\sqrt{\pi}(\alpha x)^{1/4}}\exp\left[-\frac{2}{3}(\alpha x)^{\frac{3}{2}}\right] + \frac{b}{2\sqrt{\pi}(\alpha x)^{1/4}}\exp\left[\frac{2}{3}(\alpha x)^{\frac{3}{2}}\right] \quad x \gg 0 \tag{34}$$

$$\psi(x)_{Airy} = \frac{a}{\sqrt{\pi}(-\alpha x)^{1/4}}\frac{1}{2i}\left\{\exp\left[i\frac{\pi}{4} + i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}\right] - \exp\left[-i\frac{\pi}{4} - i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}\right]\right\} \quad x \ll 0 \tag{35}$$

By comparison we can indentify the two functions by

$$\frac{D}{\sqrt{\alpha}} = \frac{a}{2\sqrt{\pi}} \tag{36}$$

$$\frac{B}{\sqrt{\alpha}} = \frac{a}{2i\sqrt{\pi}}e^{i\pi/4} \qquad \frac{C}{\sqrt{\alpha}} = -\frac{a}{2i\sqrt{\pi}}e^{-i\pi/4} \tag{37}$$

which lead to the solution

$$B = -ie^{i\pi/4}\cdot D \qquad C = -ie^{-i\pi/4}\cdot D \tag{38}$$

The term with $b$ is set to be 0 since we expect only an exponential decreasing wave function at $x > 0$. These relations illustrates the connection between the coefficients of the solution from WKB approximation on two sides of the turning point and are thus called connection formulas. Notice that so far the WKB is still divergent at the turning points, we merely adjust the phase so that they are compatible with each other. To get one continuous solution one has to replace the wave function near the turning points by Airy functions.

To justify our approximation, the comparison of the solutions of WKB and Airy functions is shown in Fig 4. Notice that the WKB approximation fails at the origin where the functions divergent and far from the turning point, the approximation works very well.

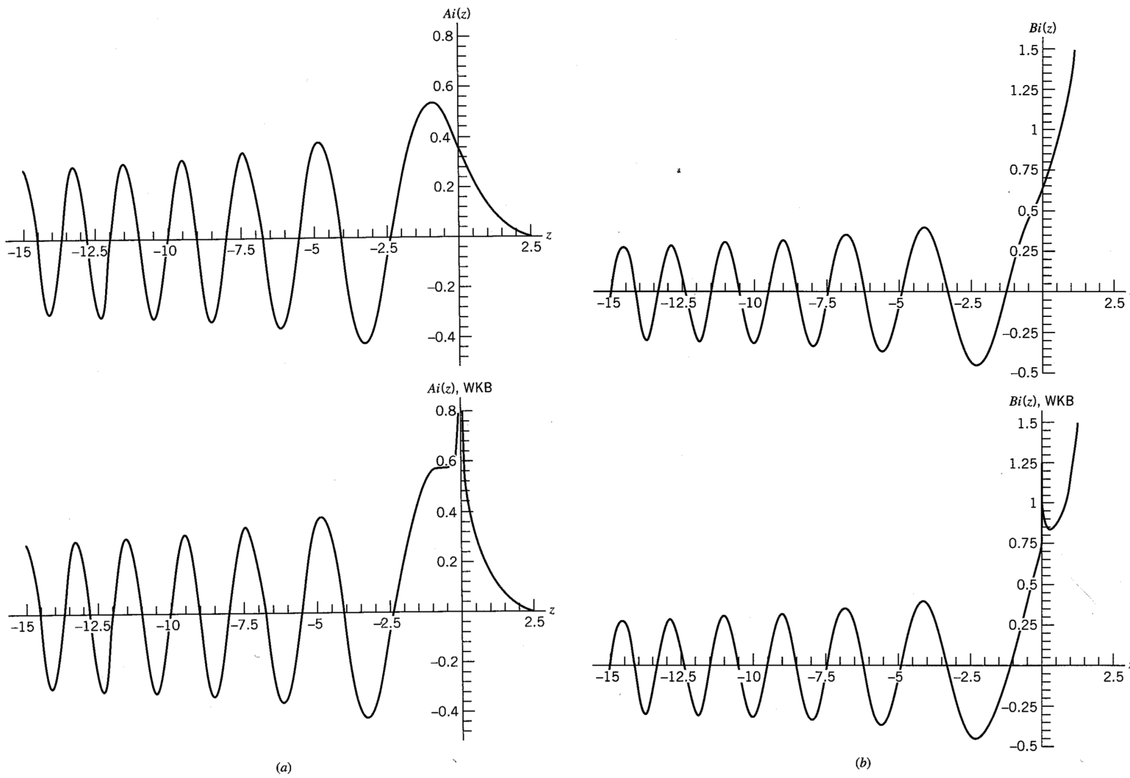


Abbildung 4: Comparison of the exact solution of the airy equation and the WKB approximated solution. [6] Left: $Ai(x)$; Right: $Bi(x)$

# 4 New development and applications

Although the WKB method was developed almost a hundred years ago, it is still a very useful tool in today's research. Many modern works use this method to solve their equations, like this one concerning early modified gravity[7]. However, here I'd like to show one example in detail, where the author does not only apply WKB to solve his problem, but also tries to estimate its limitation and make new improvements. This article concerns the cosmological particle production[8]. In this article, the author investigated the precision of the WKB approximation used in calculating the vacuum state of quantum field theory in an slowly expanding universe. He proved that the standard WKB approximation (even with high orders) cannot offer the expected precision to describe particle production and demonstrated an improvement to the WKB approximation.

The calculation of particle product can be reduced to solving the equation

$$\epsilon^2 \frac{d^2\psi}{dt^2} + \omega(t)^2\psi = 0 \tag{39}$$

where $\epsilon$ is a very small constant. Since the first order WKB is not sufficient to obtain the desired result the author turned first to the higher order WKB.

To get the higher order WKB, we first assume that the solution has the form

$$\psi(x) = \exp\Big[\pm i \int W(t) + iB(t)dt\Big] \tag{40}$$

with $W(t)$ and $B(t)$ real functions and $W(t) \approx \omega(t)$ by the assumption of slowly changing $\omega$. Substituting in equation 1 and separate the real and the imaginary part gives us two equations. By solving them, one can find the solution

$$\psi(x) = \frac{C}{\sqrt{W(x)}} \exp\Big[\pm i \int W(t)dt\Big] \tag{41}$$

with the condition

$$\frac{\ddot{W}}{2W} - \frac{3\dot{W}^2}{4W^2} = \omega^2 - W^2 \tag{42}$$

We would get our first approximation by setting $W(t) = \omega(t)$. Since $W$ is very close to $\omega$, we assume that it has the following expansion of $\epsilon$

$$W(t) = \omega(t) + \epsilon S_1(t) + \epsilon^2 S_2(t) + \cdots \tag{43}$$

By substituting this form in the previous equaiton and collecting terms with equal powers of $\epsilon$ like in the pertubation theory, one can calculate iteratively $S_n$. However, this series is in general divergent as $n \to \infty$, only the first few terms show a decreasing trend. The scaling of each Term is estimated by

$$|S_n| \propto \Big(\frac{\epsilon}{2\omega(t)}\Big)^{2n} \frac{(2n)!}{|t - t_1|^{2n+1}} \tag{44}$$

Therefor, the highter orders can not be used beyond a certain oder of $n$. The author then performed another improvement by replacing the constant coefficients in the general solution by two functions

$$\psi(t) = p(t) * \psi_+(t) + q(t)\psi_-(t) \quad \text{with} \quad \psi_{\mp} = \frac{1}{\sqrt{\mathrm{k(t)}}} \exp\Big[\pm \mathrm{i} \int_{\mathrm{t_0}}^{\mathrm{t}} \mathrm{k(t)}\Big] \tag{45}$$

Since we included two degrees of freedom $p$ and $q$, another constraint can be added

$$\frac{d\psi(t)}{dt} = i\omega(t)\Big[ - p(t)\psi_+(t) + q(t)\psi_-(t)\Big] \tag{46}$$

which indicate that by the first derivative, $p$, $q$ and $\omega$ all behave like constant. Solving the two functions $p(t)$ and $q(t)$ leads to the Bremmer series, which is known to be uniformly convergent in this case.

With this exact solution, the author then goes back to estimate the precision of WKB series. He expands the Bremer series in terms of $\epsilon$ and compares them with the truncated WKB series. In this way, he manages to give the optimal order and an estimation of the error of higher order WKB.

$$n_{max} = min_{t_i} | \int_{t_0}^{t_i} \omega(t)dt| \tag{47}$$

$$\text{Error} = \frac{1}{\sqrt{\mathrm{n_{max}}}} \exp(-2\mathrm{n_{max}}) \tag{48}$$

To test this estimation, the author provides several examples. Figur 5 shows one of them. It is the higher order WKB series to the quation with

$$\omega(t) = \omega_0\Big(1 + A \tanh \frac{t}{T}\Big) \tag{49}$$

One can see the divergence after a certain order $n$ and the estimation of error (cross symbol). Each curve corresponds to a different integral lower limit $t_0$.

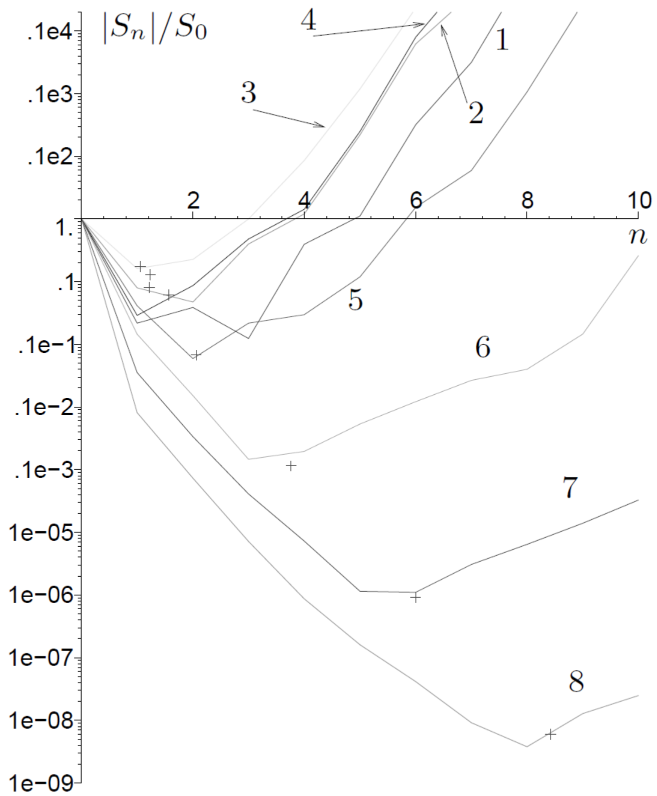


Abbildung 5: Magnitudes of first 10 terms $S_n$, $n = 1, 2, \cdots, 10$, of the WKB series for $\omega(t)$ and different values of $t_0$. Crosses indicate the error estimates.

# Literatur


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