The WKB Method

1 Introduction & Motivation

The WKB method (named after Wentzel, Kramers, and Brillouin) is a powerful technique for finding asymptotic approximations to solutions of linear differential equations, particularly where a small parameter multiplies the highest derivative.

- **Key Idea:** It assumes the solution's rapid variation is **exponential** in character. This is inspired by the exact exponential solutions of constant-coefficient equations.
- **Comparison to Other Methods:**
  - **Boundary Layers:** Solve for fast variation in specific spatial regions.
  - **Multiple Scales:** Introduce multiple temporal scales treated as independent variables.
  - **WKB:** Assume specific exponential dependence from the outset.

Historical Context

The method has multiple independent discoveries:

- **Carlini (1817):** Early use in planetary orbits.
- **Liouville & Green (1837):** Systematic formulation.
- **Quantum Mechanics (1920s):** Rediscovered for Schrödinger's equation.
- **Other Names:** Liouville-Green method, phase integral method, WKBJ method (Jeffreys), geometrical optics approximation.

Fundamental Difference from Multiple Scales

While both methods handle multiple scales of variation, they approach the problem differently:

- **Multiple Scales:** Treats different temporal scales as independent variables, determining the functional form through solvability conditions.
- **WKB:** Assumes an exponential ansatz from the beginning, then determines the phase and amplitude functions.
- **Multiple Scales:** More general but requires solving PDEs.
- **WKB:** More specific but often simpler for suitable problems.

2 Introductory Example

Consider the prototypical WKB problem:

$$\varepsilon^2 y'' - q(x)y = 0 \tag{2.1}$$

where the real-valued function $q(x)$ is smooth and nonzero, and $0 < \varepsilon \ll 1$.

2.1 Step 1: Assume WKB Ansatz

The WKB expansion is:

$$y \sim e^{\theta(x)/\varepsilon^\alpha}\left(y_0(x) + \varepsilon^\alpha y_1(x) + \varepsilon^{2\alpha} y_2(x) + \cdots\right). \tag{2.2}$$

This captures both rapid exponential variation and slower amplitude modulation.

2.2 Step 2: Compute Derivatives

From (2.2):

$$
\begin{aligned}
y' &\sim e^{\theta/\varepsilon^\alpha}\left(\varepsilon^{-\alpha}\theta' y_0 + y_0' + \theta' y_1 + \varepsilon^\alpha (y_1' + \theta' y_2) + \cdots\right) \\
y'' &\sim e^{\theta/\varepsilon^\alpha}\left(\varepsilon^{-2\alpha}(\theta')^2 y_0 + \varepsilon^{-\alpha}(\theta'' y_0 + 2\theta' y_0' + (\theta')^2 y_1) + (\theta'' y_1 + 2\theta' y_1' + (\theta')^2 y_2 + y_0'') + \cdots\right).
\end{aligned}
$$

2.3 Step 3: Substitute and Balance

Substituting into (2.1) and balancing dominant terms gives $\alpha = 1$. The resulting equations are:

$O(1)$ **- Eikonal Equation:**

$$
(\theta')^2 = q(x) \Rightarrow \theta(x) = \pm \int^x \sqrt{q(s)}ds. \tag{2.3}
$$

$O(\varepsilon)$ **- Transport Equation:**

$$
\theta'' y_0 + 2\theta' y_0' = 0 \Rightarrow y_0(x) = \frac{c}{\sqrt{\theta'}} = \frac{c}{q(x)^{1/4}}. \tag{2.4}
$$

2.4 Step 4: General Solution

Combining both exponential solutions:

$$
y(x) \sim q(x)^{-1/4}\left(a_0 e^{-\frac{1}{\varepsilon}\int^x \sqrt{q(s)}ds} + b_0 e^{\frac{1}{\varepsilon}\int^x \sqrt{q(s)}ds}\right). \tag{2.5}
$$

2.5 Verification and Applications From Holmes

- For $q(x) = -e^{2x}$, the WKB approximation matches the exact Bessel function solution remarkably well.
- Can approximate large eigenvalues efficiently.
- Provides physical insight into oscillatory vs. exponential behavior.

3 Second Term and Error Analysis

To improve accuracy and estimate errors, at the $O(\varepsilon^2)$ we collect

$$
\theta'' y_1 + 2\theta' y_1' + (\theta')^2 y_2 + y_0'' - q y_2 = 0.
$$

By eikonal equation $(\theta')^2 = q$, the equation reduces to

$$
\theta'' y_1 + 2\theta' y_1' + y_0'' = 0.
$$

Setting $y_1 = y_0 w$ and using the transport equation, one finds that

$$
0 = \theta'' y_0 w + 2\theta' y_0' w + 2\theta' y_0 w' + y_0'' = 2\theta' y_0 w' + y_0''
$$

Integrating the equation, we find:

$$
w(x) = d + \frac{1}{8}\frac{q'}{q^{3/2}} + \frac{1}{32}\int^x \frac{(q')^2}{q^{5/2}} ds. \tag{3.1}
$$

The expansion remains well-ordered if $\varepsilon y_1(x) \ll y_0(x)$ or $\varepsilon w(x) \ll 1$ which holds provided that

$$
\varepsilon\left[|d| + \frac{1}{32}\left|\frac{q'}{q^{3/2}}\right|_\infty \left(4 + \int_{x_0}^{x_1}\left|\frac{q'}{q}\right| dx\right)\right] \ll 1. \tag{3.2}
$$

The expansion fails near **turning points** where $q(x) = 0$.

4 Rigorous Foundation via Fixed Point Theory

Setting $s = \frac{x}{\varepsilon}$ and $u(s) := y(x)$, we find that

$$u'' - q(\varepsilon s)u = 0,$$

where we note the coefficient function $q(\varepsilon s)$ is slowly varying. The second order ODE behaves mostly like a constant-coefficient one. Our objective is to construct a rigorous solution. We first rewrite it as a first order system

$$\begin{pmatrix} u \\ u' \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ q(\varepsilon s) & 0 \end{pmatrix} \begin{pmatrix} u \\ u' \end{pmatrix},$$

where we note the coefficient matrix can be diagonalized as

$$T \begin{pmatrix} 0 & 1 \\ q(\varepsilon s) & 0 \end{pmatrix} T^{-1} = \Lambda \quad \text{with} \quad T = \begin{pmatrix} -\sqrt{q(\varepsilon s)} & 1 \\ \sqrt{q(\varepsilon s)} & 1 \end{pmatrix} \quad \text{and} \quad \Lambda = \begin{pmatrix} -\sqrt{q(\varepsilon s)} & 0 \\ 0 & \sqrt{q(\varepsilon s)} \end{pmatrix}.$$

Performing a change of unknowns

$$W := T \begin{pmatrix} u \\ u' \end{pmatrix},$$

we find that W solves

$$W' = T \begin{pmatrix} u \\ u' \end{pmatrix}' + T' \begin{pmatrix} u \\ u' \end{pmatrix} = T \begin{pmatrix} 0 & 1 \\ q(\varepsilon s) & 0 \end{pmatrix} T^{-1}W + T'T^{-1}W = \Lambda W + \varepsilon p(\varepsilon s) \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} W,$$

where

$$p(x) := \frac{q'(x)}{4q(x)},$$

by the smoothness and non-vanishing assumptions made on $q(x)$, is well-defined and smooth.

Now define $\Phi := w_1/w_2$. We compute

$$\begin{aligned}
\Phi' &= \frac{w_1'w_2 - w_1w_2'}{w_2^2} \\
&= \frac{\left(-\sqrt{q(\varepsilon s)}w_1 + \varepsilon p(\varepsilon s)w_1 - \varepsilon p(\varepsilon s)w_2\right) w_2 - w_1 \left(\sqrt{q(\varepsilon s)}w_2 - \varepsilon p(\varepsilon s)w_1 + \varepsilon p(\varepsilon s)w_2\right)}{w_2^2} \\
&= -2\sqrt{q(\varepsilon s)}\Phi + \varepsilon p(\varepsilon s)\Phi^2 - \varepsilon p(\varepsilon s).
\end{aligned}$$

Integrate with initial condition $\Phi(0) = 0$ (corresponding to the solution with initial conditions $w_1(0) = 0, w_2(0) = 1$):

$$\Phi(s) = \varepsilon \int_0^s e^{\int_t^s -2\sqrt{q(\varepsilon\tau)}d\tau} p(\varepsilon t)(\Phi^2(t) - 1)dt.$$

Define the operator on $C^b([0, L/\varepsilon], \mathbb{C})$:

$$(\mathcal{T}\Phi)(s) := \varepsilon \int_0^s K(s,t)(\Phi^2(t) - 1)dt,$$

where the kernel is:

$$K(s,t) = e^{\int_t^s -2\sqrt{q(\varepsilon\tau)}d\tau} p(\varepsilon t).$$

4.1 Contraction Mapping Argument

Step 1: Define the Banach Space

Let $X = C^b([0, S], \mathbb{C})$ with $S = L/\varepsilon$, equipped with the supremum norm:

$$\|\Phi\|_\infty = \sup_{s\in[0,S]} |\Phi(s)|.$$

Step 2: Estimate the Kernel

For real-valued, smooth, non-vanishing $q(\cdot)$, we have:

$$-\operatorname{Re}\sqrt{q(\varepsilon s)} \leq 0 \quad \text{and} \quad |K(s,t)| \leq |p(\varepsilon t)| \leq P(L)$$

where $P(L) = \sup_{x\in[0,L]} |p(x)|$.

Step 3: Invariance of $\mathcal{T}$ on a Ball

Let $B_R = \{\Phi \in X : \|\Phi\|_\infty \leq R\}$. For $\Phi \in B_R$:

$$|(\mathcal{T}\Phi)(s)| \leq \varepsilon \int_0^s P(L)(|\Phi(t)|^2+1)dt \leq \varepsilon P(L)(R^2+1)S = P(L)L(R^2+1).$$

To ensure $\mathcal{T} : B_R \to B_R$, we require:

$$P(L)L(R^2+1) \leq R. \tag{3.1}$$

Step 4: Contraction Property

For $\Phi, \Psi \in B_R$, we estimate that

$$|(\mathcal{T}\Phi)(s) - (\mathcal{T}\Psi)(s)| \leq \varepsilon \int_0^s |K(s,t)| \cdot |\Phi^2(t) - \Psi^2(t)|dt.$$

Since $|\Phi^2 - \Psi^2| = |\Phi - \Psi||\Phi + \Psi| \leq 2R\|\Phi - \Psi\|_\infty$, we get

$$|(\mathcal{T}\Phi)(s) - (\mathcal{T}\Psi)(s)| \leq \varepsilon \int_0^s P(L) \cdot 2R\|\Phi - \Psi\|_\infty dt = 2P(L)LR\|\Phi - \Psi\|_\infty.$$

Thus, $\mathcal{T}$ is a contraction if:

$$2P(L)LR < 1. \tag{3.2}$$

Step 5: Optimal Choices of R

We seek $R > 0$ satisfying both (3.1) and (3.2). The optimal choice is $R = 1$, which set $\frac{R}{R^2+1} = \frac{1}{2R}$. Now we obtain the condition for the choice of L:

$$\alpha(L) := 2LP(L) < 1,$$

which makes $\mathcal{T}$ is a contraction on B_1.

Theorem 4.1. *If $q(x)$ is real-valued, smooth, and nonzero on $[0, L]$, and if:*

$$L \sup_{x\in[0,L]} \left|\frac{q'(x)}{4q(x)}\right| < \frac{1}{2}$$

then there exists a unique fixed point $\Phi^* \in C^b([0, L/\varepsilon], \mathbb{R})$ with $\|\Phi^*\|_\infty \leq 1$ satisfying the WKB ratio equation. Moreover, the iterative scheme $\Phi_{n+1} = \mathcal{T}\Phi_n$ converges geometrically:

$$\|\Phi^* - \Phi_n\|_\infty \leq \frac{\alpha(L)^n}{1-\alpha(L)}\|\Phi_1 - \Phi_0\|_\infty.$$

4.2 Refined Order Analysis of Φ_1

Set $\Phi_0 \equiv 0$. We now demonstrate that the first iterate Φ_1 satisfies $\|\Phi_1\|_\infty = O(\varepsilon)$ in both the exponential ($q(x) > 0$) and oscillatory ($q(x) < 0$) cases.

Case 1: $q(x) > 0$ **(Exponential Behavior)**

For the case $q(x) > 0$ on $[0, L]$, we have $-2\sqrt{q(\varepsilon\tau)} < -\theta < 0$ for $\tau \in [0, L/\varepsilon]$. Since

$$\Phi_1(s) = -\varepsilon \int_0^s e^{\int_t^s -2\sqrt{q(\varepsilon\tau)}d\tau} p(\varepsilon t)dt,$$

we estimate that for $s \in [0, L/\varepsilon]$

$$|\Phi_1(s)| \le \varepsilon \int_0^s e^{\int_t^s -2\theta d\tau} P(L)dt = \varepsilon P(L)\frac{1 - e^{-2s\theta}}{2\theta} \le \varepsilon\frac{P(L)}{2\theta}$$

whence $\|\Phi_1\|_\infty = O(\varepsilon)$.

Case 2: $q(x) < 0$ **(Oscillatory Behavior)**

For $q(x) < 0$ on $[0, L]$, let $q(x) = -r(x)$ with $r(x) > 0$. Then

$$\Phi_1(s) = -\varepsilon \int_0^s e^{\int_t^s -2i\sqrt{r(\varepsilon\tau)}d\tau} p(\varepsilon t)dt$$

Changing variables $x = \varepsilon s$, $u = \varepsilon t$, $\varepsilon\tau = v$ and denoting $\varphi(x, u) = -2\int_u^x \sqrt{r(v)}dv$, we obtain that

$$\Phi_1(\frac{x}{\varepsilon}) = -\int_0^x e^{i\varphi(x,u)/\varepsilon} p(u)du.$$

Now integrate by parts. We compute

$$\frac{d}{du}\left[e^{i\varphi(x,u)/\varepsilon}\right] = e^{i\varphi(x,u)/\varepsilon}\frac{i}{\varepsilon}\frac{\partial\varphi(x,u)}{\partial u} = e^{i\varphi(x,u)/\varepsilon}\frac{i}{\varepsilon}2\sqrt{r(u)},$$

whence

$$e^{i\varphi(x,u)/\varepsilon} = \frac{\varepsilon}{2i\sqrt{r(u)}}\frac{d}{du}\left[e^{i\varphi(x,u)/\varepsilon}\right]$$

Substitute into the integral:

$$\Phi_1(s) = -\int_0^x p(u) \cdot \frac{\varepsilon}{2i\sqrt{r(u)}}\frac{d}{du}\left[e^{i\varphi(x,u)/\varepsilon}\right]du$$

Now integrate by parts:

$$\Phi_1(s) = -\left[\frac{\varepsilon p(u)}{2i\sqrt{r(u)}}e^{i\varphi(x,u)/\varepsilon}\right]_0^x + \int_0^x \frac{d}{du}\left(\frac{\varepsilon p(u)}{2i\sqrt{r(u)}}\right)e^{i\varphi(x,u)/\varepsilon}du.$$

Then it is easy to see that $\|\Phi_1\|_\infty = O(\varepsilon)$.
In both cases, we have established that:

$$\|\Phi_1\|_\infty = O(\varepsilon).$$

4.3 Recovery of WKB Solutions

Step 1: Reconstruct W from Φ^*

The fixed point Φ^* gives the relationship between components:

$$w_1(s) = \Phi^*(s)w_2(s)$$

The w_2 equation becomes:

$$w_2'(s) = \sqrt{q(\varepsilon s)}w_2(s) - \varepsilon p(\varepsilon s)w_1(s) + \varepsilon p(\varepsilon s)w_2(s) = \sqrt{q(\varepsilon s)}w_2(s) + \varepsilon p(\varepsilon s)(1 - \Phi^*(s))w_2(s)$$

whose solution reads

$$w_2(s) = ce^{\int^s \left(\sqrt{q(\varepsilon\tau)}+\varepsilon p(\varepsilon\tau)(1-\Phi^*(\tau))\right)d\tau}.$$

Changing back to the original coordinate, we find

$$\begin{aligned}
w_2(x/\varepsilon) &= ce^{\frac{1}{\varepsilon}\int^x \sqrt{q(x')}dx' + \int^x p(x')(1-\Phi^*(x'/\varepsilon))dx'} \\
&= ce^{\frac{1}{\varepsilon}\int^x \sqrt{q(x')}dx'} e^{\int^x p(x')dx'} e^{\int^x p(x')\Phi^*(x'/\varepsilon))dx'} \\
&= ce^{\frac{1}{\varepsilon}\int^x \sqrt{q(x')}dx'} e^{\int^x \frac{q'(x)}{4q(x)}dx'} e^{\int^x p(x')\Phi^*(x'/\varepsilon))dx'} \\
&= ce^{\frac{1}{\varepsilon}\int^x \sqrt{q(x')}dx'} q(x)^{\frac{1}{4}} e^{\int^x p(x')\Phi^*(x'/\varepsilon))dx'} \\
&= ce^{\frac{1}{\varepsilon}\int^x \sqrt{q(x')}dx'} q(x)^{\frac{1}{4}} e^{O(\varepsilon)} \\
&= ce^{\frac{1}{\varepsilon}\int^x \sqrt{q(x')}dx'} q(x)^{\frac{1}{4}} (1+O(\varepsilon))
\end{aligned}$$

where the $O(\varepsilon))$ term is measured in the Banach space $C^b([0,L],\mathbb{C})$ equipped with L^∞-norm. We pause to remark that the observation $\|\Phi^*\|_{L^\infty} = O(\varepsilon)$ follows from

$$\|\Phi^*\|_{L^\infty} = \|\Phi^* - \Phi_0\|_{L^\infty} \leq \|\Phi^* - \Phi_1\|_{L^\infty} + \|\Phi_1 - \Phi_0\|_{L^\infty} \leq \alpha(L)\|\Phi^* - \Phi_0\|_{L^\infty} + \|\Phi_1\|_{L^\infty}.$$

Step 2: Return to Original Variables

Since

$$\begin{pmatrix} u \\ u' \end{pmatrix} = T^{-1}W = \frac{1}{2}\begin{pmatrix} -\frac{1}{\sqrt{q}} & \frac{1}{\sqrt{q}} \\ 1 & 1 \end{pmatrix}\begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} -\frac{1}{\sqrt{q}} & \frac{1}{\sqrt{q}} \\ 1 & 1 \end{pmatrix}\begin{pmatrix} \Phi^* \\ 1 \end{pmatrix} w_2$$

we rigorously justify the validity of the solution of form

$$a_0 q(x)^{-1/4} e^{\frac{1}{\varepsilon}\int^x \sqrt{q(s)}ds}\left(1+O(\varepsilon)\right).$$

The other part can be obtained by working with $\tilde{\Phi} := w_2/w_1$. We also note that in this case we shall integrate in the backward direction when defining the contraction mapping to gain smallness from the exponential part in the case $q > 0$. Such solution is independent from the foregoing one because at $x = 0$ $|w_2(0)/w_1(0)| < \infty$ while the ratio of the foregoing one is infinite.

Question: How to justify for higher order expansions?

5 Summary

The WKB method is characterized by:

- **Exponential ansatz** for rapid variation
- **Eikonal equation** determines phase (nonlinear)
- **Transport equation** determines amplitude (linear)
- **Turning points** require Airy function matching (Next class)
- **Wide applicability** in quantum mechanics, wave propagation, and eigenvalue problems
- **Historical significance** with multiple independent discoveries across disciplines

The method remains a cornerstone of asymptotic analysis for linear wave-type problems with slowly varying coefficients.