

Math 521 Lecture #25
§3.5: The WKB Approximation, Part I

The WKB method (named for Wentzel, Kramers, and Brillouin) is a perturbation method that applies to many problems, among which are the second-order linear ODEs,

$$\begin{aligned}\epsilon^2 y'' + q(x)y &= 0, \quad 0 < \epsilon \ll 1, \\ y'' + (\lambda^2 p(x) - q(x))y &= 0, \quad \lambda \gg 1, \\ y'' + q(\epsilon x)^2 y &= 0, \quad 0 < \epsilon \ll 1.\end{aligned}$$

What makes perturbation methods like the WKB method so important is that they provide uniformly valid approximations to solutions of second-order linear ODEs with variable coefficients (the functions $p(x)$ and $q(x)$) cannot be solved in explicit form in terms of elementary functions.

The history of the WKB method goes back to Liouville in the mid 1800's.

We set the stage for the WKB method in the context of a particle of mass m moving along the x -axis under the influence of a conservative force $F(x)$.

By Newton's second law, the motion of the particle is governed by

$$m \frac{d^2 x}{dt^2} = F(x).$$

This gives a deterministic system: for given initial conditions $x(0)$ and $x'(0)$ there is a unique solution of the IVP, so that the position of the particle is determined for all $t > 0$.

The dynamics of the particle can be easily analyzed with the help the conservation of energy law,

$$\frac{m(y')^2}{2} + V(x) = E,$$

where $y = x'$ and $V(x)$ is the potential energy that satisfies $V'(x) = -F(x)$.

In the phase plane, the orbits are given by

$$y = \pm \sqrt{\frac{2(E - V(x))}{m}}.$$

These orbits are only valid in the domain where $E > V(x)$, which is the classical (or permissible) region.

The particle can occupy the part of the domain where $E < V(x)$, which is the nonclassical (or forbidden) region.

Values of x where $E = V(x)$ are called **turning points**, because here the sign of x' switches sign.

In the early 1900's, this classical Newtonian model of particle motion under a conservative force was found to fail on the atomic scale.

Quantum mechanics was born out of this failure.

In quantum mechanics, the basic assumption is that a particle has no definite position or velocity.

The stipulation is that there is a probabilistic (as opposed to deterministic) interpretation of the state of the particle in terms of a complex-valued **wave function** $\Psi(x, t)$

The position of the particle is a continuous random variable X , and the probability that the particle occupies the interval $a < x \leq b$ at time t is

$$P(a < X \leq b) = \int_a^b |\Psi(x, t)|^2 dx.$$

So the real-valued nonnegative function $|\Psi(x, t)|^2$ is the probability density function of X at time t , which satisfies

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1.$$

Statistical information such as mean and variance of the particle's position are encoded in $|\Psi(x, t)|^2$.

The wave function is a solution of **Schrödinger's equation**,

$$i\hbar\Psi_t = -\frac{\hbar^2}{2m}\Psi_{xx} + V(x)\Psi,$$

where V is the potential energy of the particle, m is the mass of the particle, and $\hbar = h/2\pi$ where $h = 6.625 \times 10^{-34}$ kg m²/sec is Planck's constant.

Schrödinger's equation is a second-order linear PDE that is the quantum mechanical analogue of Newton's law for the classical mechanical system.

One way to solve Schrödinger's equation is the method of separation of variables.

We assume that a solution can be written in the product form $\Psi(x, t) = y(x)\phi(t)$.

For this guess we have

$$\begin{aligned}\Psi_t &= y(x)\phi'(t), \\ \Psi_{xx} &= y''(x)\phi(t).\end{aligned}$$

Substitution of the product guess into Schrödinger's equation gives

$$i\hbar y(x)\phi'(t) = -\frac{\hbar^2}{2m}y''(x)\phi(t) + V(x)y(x)\phi(t).$$

We factor out the common $\phi(t)$ on the right-hand side to get

$$i\hbar y(x)\phi'(t) = \left[-\frac{\hbar^2}{2m}y''(x) + V(x)y(x) \right] \phi(t).$$

Dividing both sides of equation by $y(x)\phi(t)$ gives

$$\frac{i\hbar\phi'(t)}{\phi(t)} = \frac{1}{y(x)} \left[-\frac{\hbar^2}{2m}y''(x) + V(x)y(x) \right].$$

We have literally separated the functions of t from the functions of x .

If we take the partial derivative of both sides with respect to t , the right-hand side equals 0, meaning that the t derivative of the right-hand side is 0, so that the right-hand side must be a constant.

On the other hand, if we take the partial derivative of both sides with respect to x , the left-hand side is zero, meaning that the x -derivative of the right-hand side is 0, so that the right-hand side must be a constant.

Since the left-hand side equals the right-hand side, both sides are equal to the same constant, call it E .

Thus we obtain two equations coupled only by the common value of E , a time equation and a spatial equation:

$$\begin{aligned} \frac{d\phi}{dt} &= -\frac{iE}{\hbar}\phi, \\ -\left(\frac{\hbar^2}{2m}\right)\frac{d^2y}{dx^2} + (V(x) - E)y &= 0. \end{aligned}$$

The time equation solves to give a complex-valued periodic function

$$\phi(t) = C \exp\left(-\frac{iEt}{\hbar}\right) = C \left[\cos\left(\frac{Et}{\hbar}\right) - i \sin\left(\frac{Et}{\hbar}\right) \right]$$

for an arbitrary constant C . [Here we used Euler's formula $e^{i\theta} = \cos\theta + i\sin\theta$.]

The spatial equation, giving the spatial part $y(x)$ of the wave function, is called the **time-independent Schrödinger equation**.

Because the wave function $\Psi(x, t)$ satisfies

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1$$

for all t , and because $|\phi(t)|^2 = C^2$ for all t , the physically relevant solutions $y(x)$ of the time-independent Schrödinger equation must satisfy

$$\int_{-\infty}^{\infty} |y(x)|^2 dx = \frac{1}{C^2}.$$

Because \hbar is extremely small, we set $\epsilon = \hbar/\sqrt{2m} \ll 1$ and set $q(x) = E - V(x)$ to obtain from the time-independent Schrödinger equation, the singularly perturbed second-order linear equation

$$\epsilon y'' + q(x)y = 0.$$

When $q(x) = E - V(x) > 0$ (the classical region) we expect to find rapidly varying oscillatory solutions, while when $q(x) = E - V(x) < 0$ (the non-classical region) we expect to find exponentially growing and decaying solutions.