Approximation Methods

WKB approximation is an important part of QM as such, and also a very useful technique in many other areas of physics. "W.K.B." stands for *Wentzel, Kramers* and *Brillouin* (1926) but the concept has been exploited, probably, since Liouville in 1837... In QM this method is often called "quasi- or semi-classical" approximation.

In general, this is one of several methods of treating the wide range of problems characterised by two simultaneous physical processes, each acting with their own scale. (One may contrast it with the method of matched asymptotic expansions, when two processes also have different scales, but act separately, in different regions). The WKB aims to obtain an asymptotic solution of

$$\psi'' + k^2(x)\psi = 0 \qquad (*)$$

It can be a Schrödinger equation, $k^2(x) = \frac{2m}{\hbar^2}[E - V(x)]$ (from $\frac{\hbar^2}{2m}\psi'' - V(x)\psi + E\psi = 0$). The approximation is in assuming the slowly varying potential — $V(x)$ changes appreciably over the characteristic distance l such that $kl \gg 1$.

We look for an approximate solution in the form $\psi = Ae^{iS}$, where $A(x)$ and $S(x)$ are real functions. Substituting this into our master equation $(*)$ we have $A'' + 2iA'S' + iS''A - S'^2A + k^2A = 0$. Since real and imaginary parts of a function are orthogonal, we have separately:

$$\begin{array}{lll} Re: & A'' - S'^2A + k^2A = 0 & \\ Im: & 2A'S' + S''A = 0 & \Rightarrow \dfrac{A'}{A} = -\dfrac{S''}{2S'} \quad \rightarrow \quad A = \dfrac{a}{\sqrt{S'}} \end{array}$$

From the Re-part we get $(S')^2 = k^2 + A''/A$. The approximation comes at this stage: we should assume that all functions stemming from our potential $V(x)$ vary on the same length scale $\sim l$ and, therefore, $A''/A \sim 1/l^2$ by the order of magnitude; hence $k^2 \gg A''/A$. So we take, as a first step, $(S')^2 = k^2$ and recover the corresponding $A = a/\sqrt{k}$ from the Im-part:

$$\begin{aligned} \psi(x) &= \frac{a_1}{\sqrt{k(x)}} \exp\left[i\int_{x_0}^{x} kdx\right] + \frac{a_2}{\sqrt{k(x)}} \exp\left[-i\int_{x_0}^{x} kdx\right], \qquad \text{for } E > V \ \text{ or } k^2 > 0 \\ \psi(x) &= \frac{a_1}{\sqrt{k(x)}} \exp\left[\int_{x_0}^{x} |k|dx\right] + \frac{a_2}{\sqrt{k(x)}} \exp\left[-\int_{x_0}^{x} |k|dx\right], \qquad \text{for } E < V \ , \ \text{ imaginary } k \end{aligned}$$

So, for $E > V$ the solutions ("wave functions") are oscillating and in the opposite case we obtain the increasing and decreasing exponentials. This result, $\psi \sim (k)^{-1/2}\exp[i\int kdx]$ is the first order approximation in powers of $1/(kl)^2$, one can obtain the next orders accordingly, the full solution represents the so-called *asymptotic series*.

Asymptotic Series. Let $s_n = \sum_{k=0}^{n} a_k(1/z^k)$ be the partial sum. Suppose that for a fixed z and $n \to \infty$ the quantity $s_n \to \infty$ (i.e. the sum does not converge), but for a fixed n and $z \to \infty$ the sum $s_n(z)$ gives an even better approximation of some function $f(z)$. In other words

$$\lim_{z\to\infty} z^n \left[s_n(z) - f(z)\right] = 0$$

Then we say that s_n is an asymptotic representation of $f(z)$ (this is not a usual series because there is no convergence!) Let us construct s_n:
$s_0 = a_0$ so that $a_0 = f(\infty)$;
$s_1 = a_0 + (a_1/z)$ so that we must have $\lim_{z\to\infty} z[a_0 + a_1/z - f(z)] = 0$,

i.e. $a_1 = \lim_{z\to\infty} z[f(z) - f(\infty)]$;
All the next coefficients may be found in the same way. However, it is not possible to "invert" this and reconstruct $f(z)$ from a given asymptotic seris s_n. For instance, for $f(z) = e^{-z}$ we can easily obtain that $a_0 = 0,\ a_1 = 0,\ ...\ a_n = 0$, i.e the asymptotic series for $f(z)$ and $f(z) + e^{-z}$ are identical...

Thus WKB solution is a series $\psi = \sum_{\mu=0}^{n} a_\mu(x) 1/(kl)^{2\mu}$ (the parameter $z \equiv (kl)^2$ here). As we have just seen, this asymptotic series cannot account for exponentially small effects $\sim e^{-(kl)^2}$ at large (kl). Suppose $z = (kl)^2$ is fixed; then (because at $n \to \infty$ the sum diverges) there is an optimal number of terms, $n(z)$, which represent best the exact solution $\psi(x)$. Further approximations do not improve the solution, rather make it much worse! (What we have done in the first order is to neglect the term $(A''/k^2A) \sim 1/(kl)^2$ and there is no apriori guarantee that the next order is even worth looking at). [1].

This method of approximating in powers of the ratio of the two scales involved applies to many other areas of physics and types of equations. For instance, the wave equation $\ddot{x} + \omega^2(t)x = 0$ when the frequency varies slowly enough, $\dot{\omega}/\omega^2 \ll 1$. More complex equations are transformed to the form $(*)$ by an appropriate substitution, for example

$$y'' + a(x)y' + b(x)y = 0 \qquad \text{requires} \quad y \Rightarrow \psi(x) \exp\left[-\frac{1}{2}\int_0^x a(\xi)d\xi\right] .$$

Integral representation, Saddle-point. Consider an integral:

$$J(z) = \int_C e^{zf(x)}dx \qquad \approx e^{i\mathrm{Im}[zf(x)]} \int e^{\mathrm{Re}[zf(x)]}dx$$

The contour of integration must be chosen such that $\mathrm{Im}[zf(x)]$ is constant over the region where $\mathrm{Re}[zf(x)]$ is Maximal (otherwise – the integrand will have oscillations and no saddle-point). Near this maximum the exponent is given by $f(x) = f(x_0) - \frac{1}{2}f''(x_0)(x - x_0)^2 + ...$ Now

$$J(z) \approx \text{Const.}e^{zf(x_0)} \int_C e^{-\frac{1}{2}zf''(x_0)(x-x_0)^2}dx$$

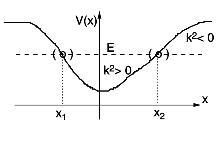
As $z \to \infty$ the less of C is relevant and eventually we obtain the main saddle-point result: $J(z) \approx e^{zf(x_0)}\sqrt{2\pi/zf''(x_0)}$. This, in fact, is the leading term of asymptotic series. Let us look at the next terms:
Instead of expansion of $f(x)$ we shall use the exact substitution $f(x) = f(x_0) - w^2$ (note that w is a real function by virtue of choice $\mathrm{Im}[f(x)]$ =const: $\mathrm{Im}[f(x)]$ =$\mathrm{Im}[f(x_0)]$). Then

$$J(z) = e^{zf(x_0)}\int e^{-zw^2}dx \quad = e^{zf(x_0)}\int e^{-zw^2}\left(\frac{dx}{dw}\right)dw .$$

Now we should invert the definition of $w = w(x)$ to obtain (dx/dw) as a function of w and exploit the Gaussian integral. The explicit result depends on the specific $f(x)$, but suppose we obtain $(dx/dw) = \sum_{n=0}^{\infty} a_n w^n$ (near the maximum of f this is what one'd expect). Only even powers w^n contribute to the Gaussian integral (we remember that $\int e^{-zw^2}w^{2n}dw = (-1)^n\partial^n/\partial z^n(\sqrt{\pi/z})$) and we obtain the asymptotic series

$$J(z) = e^{zf(x_0)}\sqrt{\frac{\pi}{z}}\sum_{n=0}^{\infty}\frac{(2n-1)!!}{2^n}a_n\left(\frac{1}{z}\right)^n$$

where a_0 gives the previous zero-order result.



WKB quantisation.

$$\psi'' + k^2(x)\psi = 0 \qquad \text{with} \quad k^2 = \frac{2m}{\hbar^2}[E - V(x)]$$

However slow the variation of $V(x)$ might be, there is a region where WKB fails, at $E \sim V$ (turning points x_1 and x_2 on the picture). Two methods are usually used:
(1) Assume that near the turning point $E - V(x) \approx \alpha x$, a linear function [this is always so except for a few specific cases, like a vertical wall, or the point of $max(V)$]. The the equation in this region is just $\psi'' + x\psi = 0$, having solutions known as Airy functions. One then needs to match the coefficients with

[1] Read a corresponding chapter in Landau & Lifshits v.III (Quantum Mechanics) to see how this approximation is directly related to the quantum-mechanical $\hbar$

two families of WKB solutions for $k^2 > 0$ and $k^2 < 0$ of both sides.
(2) One can avoid using special functions by bringing the two areas, $k^2 > 0$ and $k^2 < 0$ into a direct contact on the complex plane $\{x \to z\}$. When we travel around a turning point via the complex plane at sufficient distance, the WKB condition that $|E - V(x)|$ is big enough is valid all the time. (Caution as the integration contour crosses the "Stokes lines" - branch cuts - where the analytic continuation breaks down).

Essentially, near each turning point we have a decreasing exponential $\sim |k|^{-1/2} \exp[-\int |k| dx]$ in the classically prohibited region $k^2 < 0$ and a real combination of:

$$\psi_{E>V} = \frac{c_1}{\sqrt{k(x)}} \exp\left[i \int_{x_1}^{x} k dx\right] + \frac{c_2}{\sqrt{k(x)}} \exp\left[-i \int_{x_1}^{x} k dx\right],$$

on the other, classically allowed side. In the cases when the potential $V(x)$ has linear behaviour near x_1 the matching gives

$$\frac{c}{2\sqrt{|k|}} \exp\left[-\int_{x}^{x_1} |k| dx\right] \quad \Rightarrow \quad \frac{c}{\sqrt{k}} \cos\left[-\int_{x_1}^{x} k dx - \frac{\pi}{4}\right]$$

(note the integration direction). If the classically accessible area $k^2 > 0$ is bounded by an infinitely high potential wall, then the boundary condition is just $\psi|_{wall} = 0$. The WKB approximation is valid up to the point of contact and the solution is $\psi = (c/\sqrt{k}) \sin[\int_x^{x_1} k dx]$.

If we have a potential well, i.e the classically accessible region is bounded by two turning points, $x_1 < x < x_2$, then we obtain from the matching near each point a separate solution:

$$\psi_1 = \frac{a_1}{\sqrt{k}} \cos\left[-\int_{x_1}^{x} k dx - c_1\pi\right] \qquad \text{and} \qquad \psi_2 = \frac{a_2}{\sqrt{k}} \cos\left[-\int_{x}^{x_2} k dx - c_2\pi\right]$$

(with the phases c_1, c_2 determined by the turning point details). The requirement that these two functions should be identical gives the quantisation condition

$$\int_{x_1}^{x_2} k dx = (n + c_1 + c_2)\pi$$

(with $a_1 = (-1)^n a_2$). The cosine goes through zero n times as x varies from x_1 to x_2, so that n is just the the number of nodes of $\psi(x)$ in this interval. For the most common case with linear $V(x)$ near both turning points the phase factors $c_1 = \frac{1}{4}$ and $c_2 = \frac{1}{4}$, so that the r.h.s. is $(n + \frac{1}{2})\pi$.

Estimates of Integrals. The following examples illustrate the approach:

$$\text{Case 1.} \qquad J(x) = \int_0^x e^{t^2} \frac{dt}{\sqrt{x^2 - t^2}}$$

If $x << 1$, then the exponential in the integrand is of order 1. Consequently

$$J(x) \approx \int_0^x \frac{dt}{\sqrt{x^2 - t^2}} = \int_0^1 \frac{dz}{\sqrt{1 - z^2}}$$

Since this integral contains no parameters, we have $J(x) \sim 1$ for $x << 1$ [Actual calculation gives $J(x) \approx \pi/2$]
If $x >> 1$, then because of the exponential factor the principal contribution to the integral comes from the region near $t \sim x$. Let us expand around this point: $\xi = x - t$, so that

$$J(x) = \int_0^x e^{x^2 - 2\xi x + \xi^2} \frac{d\xi}{\sqrt{2\xi x - \xi^2}} \approx e^{x^2} \int_0^x e^{-2\xi x} \frac{d\xi}{\sqrt{2\xi x}} \approx \frac{e^{x^2}}{2x} \int_0^\infty e^{-z} \frac{dz}{\sqrt{z}} = \frac{e^{x^2}}{2x} \sqrt{\pi}$$

At $x \sim 1$ both expressions are of the same order of unity, as of course they must be.

$$\text{Case 2.} \qquad J(a) = \int_0^\infty e^{-x^2} \sin^2 ax dx$$

In all cases the important region is only $0 < x < 1$ because of the exponential. If $a >> 1$ then the sine oscillates many times over this region and can be replaced by its average, $\frac{1}{2}$. Then

$$J(a >> 1) \approx \int_0^\infty \frac{1}{2} e^{-x^2} dx = \text{const} \qquad \left[\text{actually } \frac{\sqrt{\pi}}{4}\right].$$

If $a << 1$ then the argument of sine is always small and we can expand it:

$$J(a << 1) \approx a^2 \int_0^\infty e^{-x^2} x^2 dx = a^2 \,\mathrm{const} \qquad \left[\text{actually } \frac{\sqrt{\pi}}{4} a^2\right] .$$

These two limits match at $a \sim 1$ and form a good description of $J(a)$ over the whole region of the variable a [an exact calculation, possible here, gives $J = \frac{\sqrt{\pi}}{4}(1 - e^{-a^2})$].

$$\text{Case 3.} \qquad J(\alpha) = \int_0^\infty \frac{e^{-\alpha z}}{z+1} dz$$

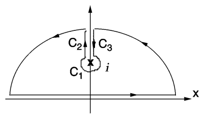
(important region is only $0 < z < 1/\alpha$. If $\alpha >> 1$ then z is always small and $J(\alpha) \approx \int_0^\infty e^{-\alpha z} dz = 1/\alpha$ (which is the same as simply taking $\int_0^{1/\alpha} dz$). If $\alpha << 1$ then in the most of relevant region $z >> 1$ and we can neglect 1:

$$J(\alpha << 1) \approx \int_0^\infty \frac{e^{-\alpha z}}{z} dz \approx \int_0^{1/\alpha} \frac{1}{z} dz = \ln(1/\alpha) .$$

Integrals of oscillating functions; high terms in Fourier series expansion.

$$\text{Case 4.} \qquad J(\omega) = \int_{-\infty}^{\infty} \frac{e^{i\omega t} dt}{\sqrt{1+t^2}} , \qquad \omega \to \infty$$

The singularities of the integrand occur on the imaginary axis, $t = \pm i$. We can deform the contour into the upper half-plane. The contributions from ∞ vanish, the small contour around the branch point tends to zero: $t = i + \rho e^{i\phi}$



$$\int_{C_1} \sim \int_0^{2\pi} \frac{\rho e^{i\phi} d\phi}{\sqrt{\rho} e^{i\phi/2}} \sim \sqrt{\rho} \to 0$$

Because the integrand ($\sqrt{1+t^2}$) has a different sign on the two sides of the branch cut, the integrals along C_2 and C_3 are equal. Changing the variable $t = i(1+\xi)$ we have

$$J(\omega) = 2e^{-\omega} \int_0^\infty e^{-\omega\xi} \frac{d\xi}{\sqrt{2\xi}} = \sqrt{\frac{2\pi}{\omega}} e^{-\omega}$$

For large ω the integral is exponentially small. This is a special case of a more general theorem: the high Fourier components of any function that has no singularities on the real axis are exponentially small. If x_1 is the "characteristic length" of $f(x)$ (i.e. roughly, the distance of the nearest singularities from the real axis is of order x_1), then

$$f_\omega \equiv \int_{-\infty}^{\infty} f(x) e^{i\omega x} dx \sim e^{-\omega x_1} \qquad \text{for } \omega x_1 \gg 1$$