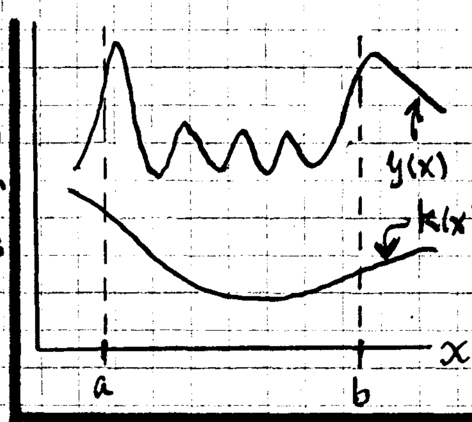
The WKB Method

1) Introduction

● The WKB method provides approximate solutions to 2^{nd} order linear differential equations of the form...

$$\boxed{y'' + k^2(x)\,y = 0}\ , \quad \text{w/ } y' = dy/dx, \text{ etc.} \qquad (1)$$

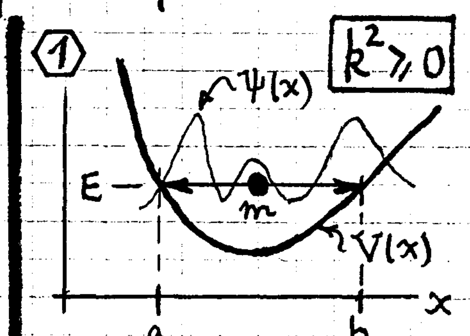


The fcn $k(x)$ can be real or imaginary; thus $k^2(x)$ can be >0 or <0. The method works best when $k(x)$ is a "slowly-varying" fcn of x over the solution interval; the method fails at points where $k(x) \rightarrow 0$. When $k^2(x) > 0$, solutions $y(x) \sim \sin$ & $\cos\left[\int k(x)\,dx\right]$ result, and when $k^2(x) = -\kappa^2(x) < 0$, one gets $y(x) \sim \sinh$ & $\cosh\left[\int \kappa(x)\,dx\right]$. Such solutions to Eq. (1) are familiar as those describing a simple harmonic oscillator with a variable spring constant $\propto k(x)$.

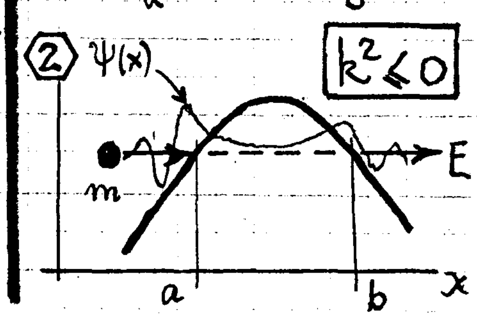
● Interest in the WKB method for QM follows from looking at the wave eqtn for a particle of mass m moving in 1D, with total energy E, in a potential $V = V(x)$ which depends on the particle position x...

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

$$\text{w/ } k(x) = \left\{\frac{2m}{\hbar^2}\left[E - V(x)\right]\right\}^{1/2}.$$



Here $k(x)$ is m's de Broglie wave #, and $\hbar k$ is its momentum. If $E \geqslant V(x)$, k is real, $k^2 \geqslant 0$, and we have the bound-state well problem shown in ①. If $E \leqslant V(x)$, k is imaginary, $k^2 \leqslant 0$, and we have the barrier-penetration problem shown in ②. Both



problems are important for understanding QM in 1D, and one would like to solve them for as general a class of potentials $V(x)$ as possible. So we have practical reasons for developing a solution to Eq. (1).

- The WKB method also applies to the solution of a rather general 2nd order linear differential eqtn. This follows from the fact that...

$$\rightarrow y'' + f(x)\,y' + g(x)\,y = 0, \tag{3}$$

with the substitution: $y(x) = \psi(x) \exp\left[-\frac{1}{2}\int f(x)dx\right]$, transforms to...

$$\rightarrow \psi'' + k^2(x)\,\psi = 0, \quad \text{w/}\; k(x) = \pm\sqrt{g(x) - \tfrac{1}{2}\left[f'(x) + \tfrac{1}{2}f^2(x)\right]}. \tag{4}$$

So, every eqtn like (3) has a WKB form (4) which can be solved approximately. The only restrictions on the method is that $k(x) \neq 0$ on the solution interval, and $k(x)$ is "slowly-varying" on the interval. In a moment, we will show that "slowly-varying" means...

$$\boxed{\left|\frac{dk}{dx}\Big/ k^2(x)\right| << 1}, \tag{5}$$

on the interval -- this condition must hold for the WKB method to give a "good" approx$^{\underline{n}}$, and it restricts the choices of $f(x)$ & $g(x)$ in (4).

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2) The WKB Solution: Summary

- We assume the reader is familiar with how the WKB calculation is done, and so here we shall just summarize results.¶ Our major interest is in applying these results to the QM problems connected with Eq. (2).

¶ Results are worked out in Φ566 notes. Or see Mathews & Walker "Math. Methods of Physics" (Benjamin, 1970), pp. 27-37; or A.S. Davydov "QM" (Pergamon, 2nd ed., 1991), Chap. III; or J. Sakurai "Modern QM" (Addison Wesley 1985), Sec. 2.4.

WKB Solution Summary

● When, in $y'' + k^2 y = 0$, $k \to k_0$ is a cnst, the eqtn is exactly solvable in terms of $y \propto \sin, \cos[\int k_0 dx]$; equivalently $y \propto \exp[\pm i \int k_0 dx]$. If $k \to k(x)$ has a weak x-dependence, then $y \sim \exp[\pm i \int k(x) dx]$ might be a reasonable approx$^{\underline{n}}$. So we do the following substitution...

$$\left[\begin{array}{l} \text{For: } y'' + k^2(x) y = 0, \text{ let: } y(x) = \exp[i\phi(x)]. \\ \text{Then: } \underline{\underline{(d\phi/dx)^2 = k^2(x) + i(d^2\phi/dx^2)}}. \end{array}\right. \tag{6}$$

Eq. (6) is an exact eqtn for $\phi(x)$. It is $2^{\underline{nd}}$ order and nonlinear, and it cannot be solved in closed form. However, a series solution for $\phi(x)$ can be generated, by iteration. We expect that the first iteration will give $\phi(x) \sim \int k(x) dx$. Indeed this is the case.

● The zeroth iteration to (6) follows by claiming that if $k(x)$ has a weak x-dependence, then so will $\phi(x)$, and the derivatives $\phi', \phi'', \ldots$ will become rapidly smaller. Then, in (6), we ignore ϕ'' on the RHS compared to $(\phi')^2$ on the LHS, so that $(\phi')^2 \simeq k^2$. As a consequence, we have: $d\phi/dx \simeq \pm k$, and so: $\underline{\phi(x) \simeq \int k(x) dx}$, immediately. Evidently, this works only if $\phi \simeq \int k dx$ in fact satisfies $(\phi')^2 \gg |\phi''|$, and this condition -- quoted in terms of k -- gives the "slowly-varying" restriction as cited in Eq. (5) above...

$$\rightarrow \phi \simeq \pm \int k dx, \;\; {}^{\text{and}}\!/\!/ \; (\phi')^2 \gg |\phi''| \Rightarrow \boxed{\left|\frac{1}{k^2}\left(\frac{dk}{dx}\right)\right| \ll 1.} \tag{7}$$

● The first iteration to (6) consists of <u>not</u> ignoring ϕ'' on the RHS, but replacing it (for $\phi \simeq \pm \int k dx$) with $\phi'' \simeq \pm dk/dx$. An improved solution for $\phi(x)$ then follows, and it yields...

$$\rightarrow \phi(x) \simeq \pm \int k(x) dx + \tfrac{1}{2} i \ln k(x) + \text{cnst}. \tag{8}$$

The iteration can be continued to produce additional correction terms to the series for $\phi(x)$, but the procedure is rarely carried past the point of Eq.(8). For the amplitude y in the original eqtn $y''+k^2y=0$, we have $y=e^{i\phi}$, and so the (approximate) ϕ solution of Eq.(8) produces,

$$\boxed{y(x)=\exp\left\{i\left[\pm\int k\,dx+\frac{i}{2}\ln k+\mathrm{cnst}\right]\right\}=\frac{\mathrm{cnst}}{\sqrt{k}}\,e^{\pm i\int k\,dx}}. \quad (9)$$

This y is the (approximate) WKB solution to $y''+k^2y=0$, w/ $k=k(x)$, and provided that: $\left|\frac{1}{k^2}(dk/dx)\right|\ll 1$.

● $\boxed{\text{REMARKS}}$ on WKB solution, Eq.(9).

1. y_{WKB} of Eq.(9) doesn't quite satisfy $y''+k^2y=0$. Instead...

$$\begin{cases} y_{WKB}=\left(\dfrac{\mathrm{cnst}}{\sqrt{k}}\right)e^{\pm i\int k\,dx}, \text{ satisfies: } \underline{\underline{y''_{WKB}+(1-\epsilon)k^2\,y_{WKB}=0}}, \\ \text{where: } \epsilon=\dfrac{3}{4}(k'/k^2)^2-\dfrac{1}{2}(k''/k^3). \end{cases} \quad (10)$$

This sharpens the slowly-varying condition... it is $|\epsilon|\ll 1$ that ensures y_{WKB} is a good approx^n to the actual y. We can rewrite ϵ as...

$$\rightarrow \epsilon=(-)\left[\delta+\frac{1}{k}\left(\frac{d}{dx}\right)\right]\delta, \quad \text{w/ } \delta=\frac{1}{2k^2}(dk/dx). \quad (11)$$

For y_{WKB} to be a good approx^n, we see that not only do we need $|\delta|\ll 1$ (the slowly-varying condition in Eq.(7)), but also $|d\delta/dx|\ll 1$.

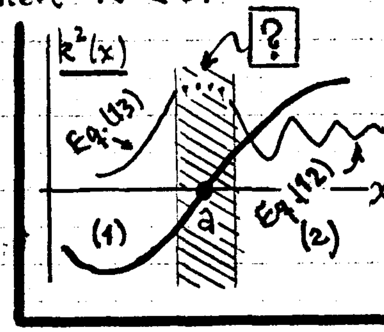
2. There are two indep^t integration cnsts in (9), one for each of $e^{\pm i\int k\,dx}$. So the full solution, for $k^2>0$, can be written...

$$\rightarrow \underline{\underline{y(x)=\frac{1}{\sqrt{k(x)}}\left[A\exp\left(+i\int k(x)\,dx\right)+B\exp\left(-i\int k(x)\,dx\right)\right],\ k^2>0.}} \quad (12)$$

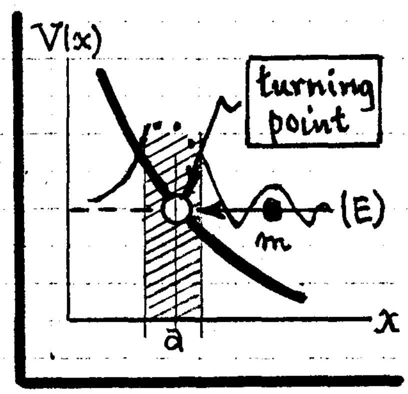
The cnsts A & B are free to fit initial conditions (e.g. prescribed values for $y(0)$ & $y'(0)$). The exponentials in (12) can be combined inside the [ ] to form the functional behavior $\sin,\cos\left(\int k(x)\,dx\right)$, and evidently y_{WKB} is oscillatory in regions where $k^2>0$. In those regions where $k^2=-\kappa^2<0$, i.e. $k=\pm i\kappa$, the exponents in (12) become real, and y_{WKB} takes the form:

$$\rightarrow y(x)=\frac{1}{\sqrt{\kappa(x)}}\left[C\exp\left(+\int\kappa(x)dx\right)+D\exp\left(-\int\kappa(x)dx\right)\right],\ k^2=(-)\kappa^2<0. \quad (13)$$

So y_{WKB} grows or declines exponentially in regions where $k^2<0$.



3. If $k^2(x)$ goes through zero at some point, say $x=a$ as sketched at right, then (1) @ $x<a$, where $k^2<0$, the exponential sol^n of Eq. (13) applies, while (2) @ $x>0$, $k^2>0$, the oscillatory sol^n of Eq. (12) may be used. But in the neighborhood of $x=a$, where $k(x)\to 0$, we have trouble... the sol^{n}s in (12) & (13) both $\propto 1/\sqrt{k(x)}$, so they diverge... and it becomes impossible to satisfy the slowly-varying condition $|k'/k^2|\ll 1$. The WKB approx^n is no good in a neighborhood where $k^2\to 0$.



4. In QM, for the 1D motion of mass m in a potential $V(x)$, we have: $k^2=\frac{2m}{\hbar^2}[E-V(x)]\to 0$, whenever $E\to V(x)$, i.e. whenever m's total energy is purely potential energy and its kinetic energy $\to 0$. A classical particle would be reflected from the potential at such a point -- it would reverse its motion and turn around. Such points as $x=a$ in the sketch, where $E=V(a)$ and the QM $k^2(a)=0$ are therefore called "turning points". To do the QM problems outlined on p. W1, we clearly need to analyse what happens in the neighborhood of such turning points. In particular, we have to find out how the exponential WKB sol^n @ $x<a$ is related to the oscillatory WKB sol^n @ $x>a$.

WKB Solution Summary (cont'd)

- In passing, we note that the "slowly-varying" criterion $|k'/k^2| \ll 1$ [or its more precise version $|\epsilon| \ll 1$, in Eq. (11)] indicates qualitatively when a WKB sol$^{\underline{n}}$ is good, but the criterion does not give a quantitative measure of how closely y_{WKB} approximates the actual sol$^{\underline{n}}$ y to $y'' + k^2 y = 0$. We can gain information on $(y - y_{WKB})$ as follows.

Transform $y'' + k^2 y = 0$ by changing both indep$^{\underline{t}}$ & dep$^{\underline{t}}$ variables...

$$\left[\begin{array}{l} x \to s = \int_0^x k(\xi)\,d\xi\,; \\[6pt] y(s) \to u(s) = y(s)\big/\sqrt{k(s)}\,, \end{array}\right.$$

so// $d^2y/dx^2 + [k(x)]^2 y = 0$, becomes:

i.e.// $y(s) = u(s)/\sqrt{k(s)}$.

$$\boxed{\frac{d^2u}{ds^2} + [1 + b(s)]\,u = 0\,, \text{ where: } b(s) = \frac{1}{4k^2}\left(\frac{dk}{ds}\right)^2 - \frac{1}{2k}\left(\frac{d^2k}{ds^2}\right).} \tag{14}$$

$b(s)$ should be "small" for use of WKB, and when it can be neglected...

$$\to b(s) \to 0 \text{ implies: } \underline{u \to A e^{+is} + B e^{-is} = w(s)}. \tag{15}$$

This is the WKB sol$^{\underline{n}}$ to the problem, since $w(s)/\sqrt{k(s)} = y_{WKB}$ of Eq. (12). When $b(s)$ is not negligible, a sol$^{\underline{n}}$ to Eq. (14) will move away from $u_{WKB} = w$ by a bit, and toward the true u. We can explore this evolution by converting the u'' eqtn to an integral eqtn and solving it iteratively. The leading terms in the true sol$^{\underline{n}}$ for u are...

$$\to u(s) = w(s) + \int_0^s w(\sigma)\, b(\sigma) \sin(\sigma - s)\, d\sigma + \mathcal{O}(b^2). \tag{16}$$

The sol$^{\underline{n}}$s of interest are $y = u/\sqrt{k}$, so (16) prescribes the deviation...

$$\Big[\!\Big[\; y(s) - y_{WKB}(s) = \frac{1}{\sqrt{k(s)}} \int_0^s w(\sigma)\, b(\sigma) \sin(\sigma - s)\, d\sigma + \mathcal{O}(b^2). \tag{17}$$

between the true sol$^{\underline{n}}$ y and the approx$^{\underline{n}}$ y_{WKB}. The integral on RHS is calculable in principle, and it tracks the error $(y - y_{WKB})$.