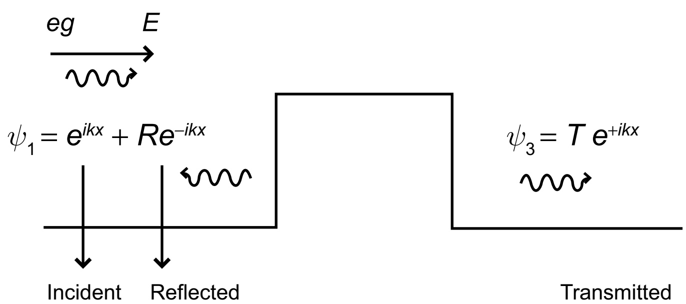
November 4, 2008

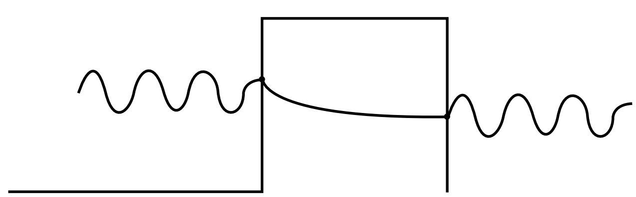
THE WKB (WENTZEL - KRAMERS - BRILLOUIN) APPROXIMATION

In the 2nd year (2nd year Quantum course at UCL) we solved simple examples of the TISE with piecewise constant potentials $V(x) \equiv V_0$ (over some region)



In the barrier region,

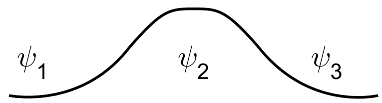
$$\psi_2(x) = Ce^{iqx} + De^{-iqx} \;\; if \;\; E > V_0$$
$$q = \sqrt{2m(E - V_0)}$$
$$\text{OR} \quad \psi(x) = Ce^{-qx} + De^{qx} \;\; if \;\; V_0 > E$$
$$q = \sqrt{2m(V_0 - E)}$$



Then, matching ψ_1, ψ_2, ψ_3, at boundaries, we could get transmitted currents from $J_T = \frac{\hbar k}{m}|T|^2$

$$J_T = \frac{\hbar}{2cm}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)$$

We may want a method to deal with smooth potentials and to match the wavefunctions in different regions



For potential barriers or also quantum wells.

THE WKB (WENTZEL - KARMERS - BRILLOUIN) APPROXIMATION

Take the TISE for the constant potential:

$$\begin{aligned} &\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0 \\ &= \frac{d^2\psi}{dx^2} + \frac{p^2}{\hbar^2}\psi = 0 \end{aligned} \tag{3.1}$$

These solution are plane waves

$$\psi(x) = Ae^{\pm i\frac{px}{\hbar}} \tag{3.2}$$

with a constant momentum

$$p = \hbar k = \frac{2\pi}{\lambda}\hbar = \frac{h}{\lambda}$$

Now, suppose $V(x)$ varies slowly with x

$$p \to p(x) = \sqrt{2m(E - V(x))}$$

we can still think of a 'local' wavelength $\lambda(x)$, ie,

$$\lambda(x) = \frac{h}{p(x)} \quad \text{provided} \tag{3.3}$$

the rate of change of wavelength with x is slow, is $\delta\lambda =$ the change in λ over one oscillation $= \lambda(x + \Delta x) - \lambda(x)$ is small. Then

$$\left|\frac{\delta\lambda}{\lambda(x)}\right| \simeq \left|\frac{\frac{\partial\lambda}{\partial x}\cdot\Delta x}{\lambda}\right| \simeq \underbrace{\left|\frac{\frac{\partial\lambda}{\partial x}\cdot\lambda}{\lambda}\right|}_{\text{since } \Delta x \sim \lambda} = \left|\frac{d\lambda}{dx}\right| \ll 1 \tag{3.4}$$

It reasonable to suppose that the phase accumulated by wavefunction (3.2) between two points x_0 and x

$$\psi(x) = \psi(x_0) e^{\pm \frac{i}{\hbar}} \int_{x_0}^{x} p(x')dx'$$

$$= Ae^{iS(x)/\hbar} \tag{3.5}$$

where $S' = \frac{\partial S}{\partial x}$. Substitute (3.5) into (3.1)to obtain:

$$-\left(\frac{S'}{\hbar}\right)^2 + \frac{iS''}{\hbar} + \frac{p^2(x)}{\hbar^2} = 0 \tag{3.6}$$

$S(x)$ is sometimes termed "the action" of a path from x to x_0.

NOTE - There is a formulation of quantum theory (path - integral approach) due to *Feynman* where we propagate wave functions as a sum over different paths from $x_0 \to x$

$$< x|T(t,0)|x_0' >= \sum_j A_j e^{i\ S_j(x,x_0)/\hbar} \tag{3.7}$$

The *semiclassical* regime occurs where the typical action is large:

$$S_j/\hbar \gg 1 \tag{3.8}$$

Mathematically equivalent to $\hbar \to 0$ and we refer to this as the 'small $\hbar$' regime.

Neighbouring paths rapidly fall out of phase and interfere destructively ... EXCEPT where the action $\frac{\partial S}{\partial y} = 0$, is stationary (y is a small deviation from the $x_0 \to x$ path) . This corresponds to a *classical path.* Hence for $S/\hbar \gg 1$ contributions from classical paths dominate.

WKB is a simple 1-D version of this semiclassical theory.

NB if $\hbar \to 0$, the wavelength $\lambda = \frac{2\pi\hbar}{p} \to 0$

Semiclassical physics $\Rightarrow$ short wavelengths and is most valid at high kinetic energies eg highly excited electrons or high energy particles. For finite $\hbar$, non classical paths contribute to (3.8). Corrections from these non-classical paths (which yield diffractive or tunneling corrections) can be added but beyond a certain point, a full solution of the Schrodinger equation becomes necessary.

Since $\hbar$ is small, we expand:

$$S(x) = S_0(x) + \hbar S_1(x) + \hbar^2 S_2(x) \cdots \tag{3.7}$$

as a power series in $\hbar$. We subs. into (3.6).

If making the WKB approximation, we keep only the 1st two terms in (3.6). Grouping terms with the same $\hbar$ dependence,

$$\underbrace{\frac{-(S_0')^2 + p^2(x)}{\hbar^2}}_{\text{term(1)}} + \underbrace{\frac{i\ S_0'' - 2S_1'S_0'}{\hbar}}_{\text{term(2)}} + 0(\hbar^0) = 0 \tag{3.8}$$

Exercise 3.1
Obtain (3.8).
We want terms to vanish (order by order)

(1)
$$\begin{aligned} S_0' &= \pm p(x) \qquad (3.9) \\ S_0 &= \pm \int^x p(x')dx' \end{aligned}$$

(2)
$$\begin{aligned} iS_0'' &= 2S_1'S_0' \\ \frac{S_0''}{S_0'} &= -2iS_1' \qquad (3.10) \end{aligned}$$

$$\begin{aligned} \Rightarrow \ln S_0' &= -2iS_1 + C \\ S_1 &= \frac{-1}{2l}\ln S_0' + \frac{C}{2i} \\ S_1 &= i\ln\left(\frac{\partial S_0}{\partial x}\right)^{1/2} + \tilde{C} \end{aligned}$$

Note that $1/2\ln y = \ln y^{1/2}$. From (3.9),

$$\Rightarrow S_1 = i\ln\sqrt{\pm\, p(x)} + \tilde{C} \qquad (3.11)$$

Since from (3.5) & (3.7)

$$\begin{aligned} \psi(x) &\simeq \exp\frac{i}{\hbar}(S_0 + \hbar S_1) \\ &= \exp\pm\frac{i}{\hbar}\int^x p(x')dx' \cdot \exp\frac{i}{\hbar}\ \hbar[i\ln(\pm p^{1/2}) + \tilde{C}] \end{aligned} \qquad (3.12)$$

Note that last factor is just $e^{-\ln(\pm\, p^{1/2})+i\tilde{C}}$ now, $e^{\ln x} = x$

$$e^{-\ln \pm p^{1/2}} = \frac{1}{\sqrt{\pm p(x)}}; \quad e^{i\tilde{C}} = A \qquad (3.13)$$

so, finally,

$$\psi(x) \simeq \frac{A}{\sqrt{p(x)}}\exp\pm\frac{i}{\hbar}\int^x p(x')dx' \qquad (3.14)$$

(we include an i in A to allow for the $\pm p(x)$ if needed; A is just a constant amplitude).

Or, using $p = \hbar k$, we write solution, in most general form

$$\psi(x) \simeq \frac{A}{\sqrt{k(x)}}e^{i\int k(x)dx} + \frac{B}{\sqrt{k(x)}}e^{-i\int k(x)dx} \qquad (3.15)$$

Hence, the probability density $|\psi(x)|^2 \propto \frac{1}{k(x)} \propto \frac{1}{v}$ where v is the velocity $\hbar k/m$. This is not unreasonable since the time spent in a region between x and $x + dx$, classically, $\propto \frac{1}{v}$.

Below we will fix A, B for a given potential Eg for standing waves $A = B$.

RETURNING TO WKB SOLUTION: in *classically forbidden* region $E < V(x)$.

The WKB wavefunction is

$$\psi(x) \simeq \frac{1}{\sqrt{q(x)}} e^{\pm \int^x q(x')dx'}$$

with $q(x) = [\frac{2m}{\hbar^2}(V(x) - E)]^{1/2} > 0$

$$\Rightarrow \psi(x) = \frac{1}{\sqrt{q(x)}} \left\{ Ce^{+\int q(x)dx} + De^{-\int q(x)dx} \right\} \tag{3.16}$$

The WKB approximation breaks down if $k(x) = 0$ or $q(x) = 0$.

ie $k(x)$ vanishes at the turning points, where $E = V(x)$. The prefactor $1/\sqrt{k(x)}$ blows up. We need the 'CONNECTION FORMULAE' (next section) which serve to like up WKB solutions across turning points.

CONNECTION FORMULAE

We want to join together solutions of the form

$$\frac{1}{\sqrt{k}}[A \sin \phi(x) + B \cos \phi(x)] \qquad \text{(in allowed regions)}$$

and

$$\frac{1}{\sqrt{q}}[Ce^{+\phi(x)} + De^{-\phi(x)}] \qquad \text{(in forbidden regions)}$$

but these WKB approximate forms blow-up at the turning point $x = a$. We know, however, that the true solutions of the T.I.S.E. would be smooth at $x = a$.

We linearise $V(x)$ around $x = a$. We write:

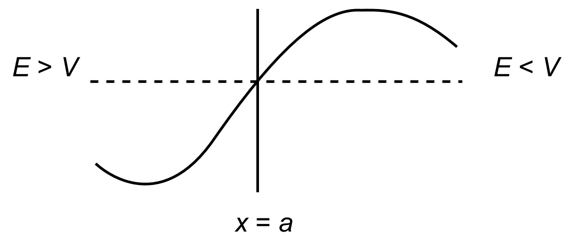
$$V(x) - E = g(x - a) \tag{3.17}$$

$g = \frac{dv}{dx} > 0$. The TISE is:

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{dx^2} + g(x - a)\psi = 0$$

Changing variables to

$$z = \left(\frac{2mg}{\hbar^2}\right)^{1/3} (x - a) \tag{3.18}$$



we get

$$\frac{d^2\psi}{dz^2} - z\psi = 0 \tag{3.19}$$

The solutions of (3.19) are *Airy FUNCTIONS*, $Ai(z)$ and $Bi(z)$, which have the required properties to interpolate across $x = a$: at z large and positive (in the 'forbidden' region)

$$Ai(z) \sim e^{-\phi(x)} \tag{3.20a}$$

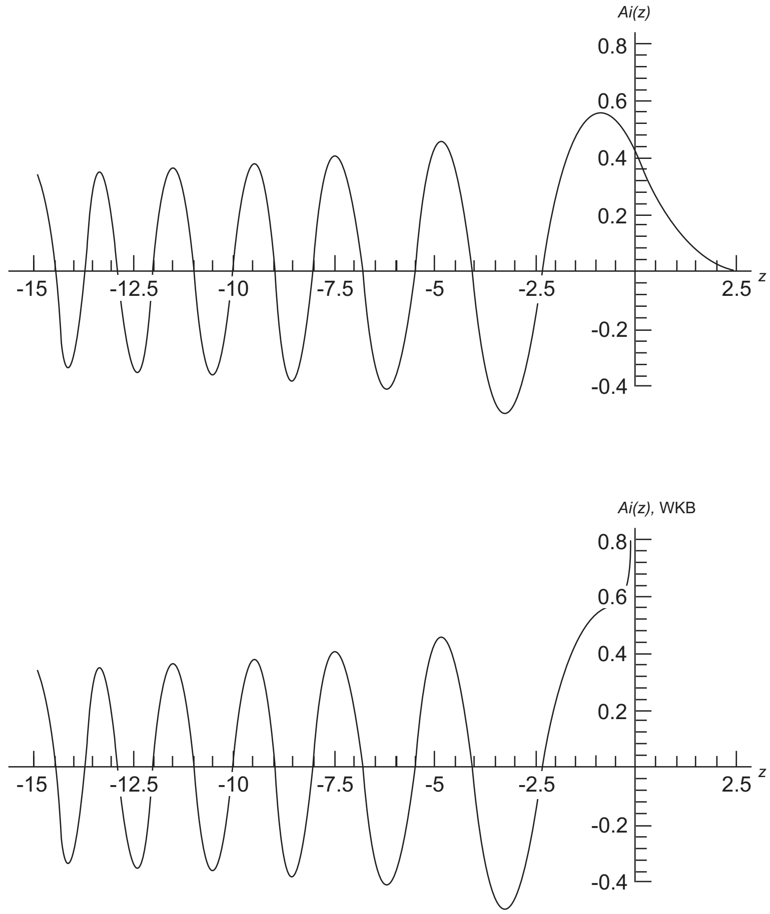
$$Bi(z) \sim e^{+\phi(x)} \tag{3.20b}$$

At Z large/negative (in the 'allowed region')

$$Ai(z) \sim \cos\left(\phi(x) - \frac{\pi}{4}\right) \tag{3.21a}$$

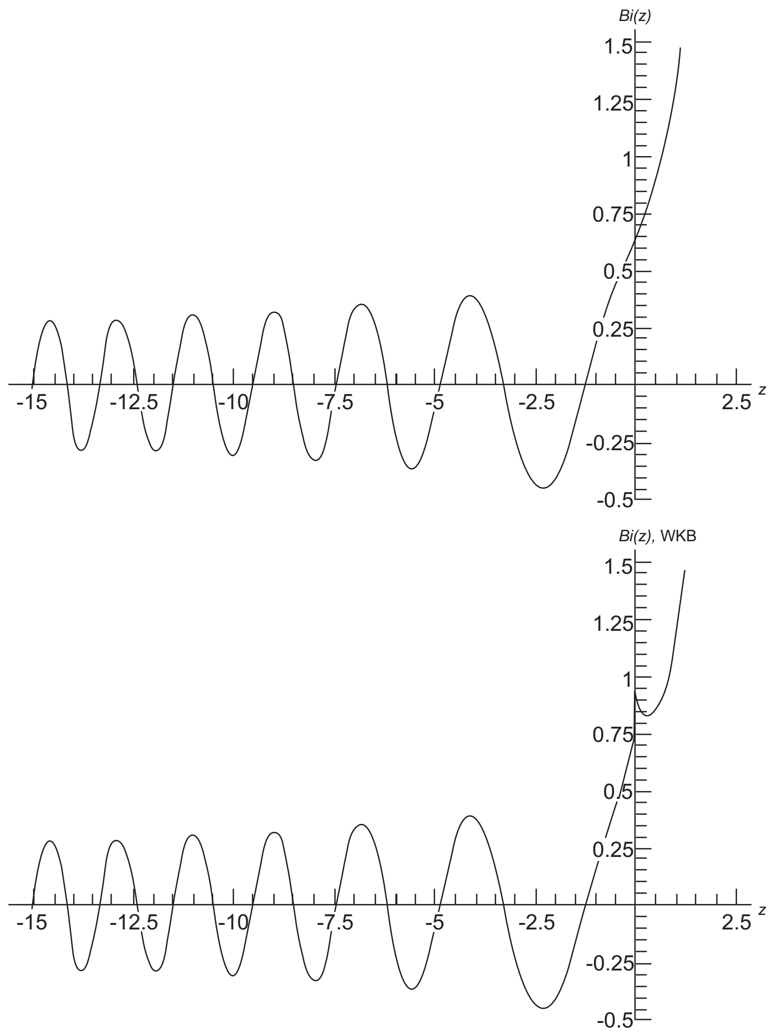
$$Bi(z) \sim \sin\left(\phi(x) - \frac{\pi}{4}\right) \tag{3.21b}$$

(LOOK AT FIGS: The $Bi(z)$ connect with each other, the $Ai(z)$ too.)

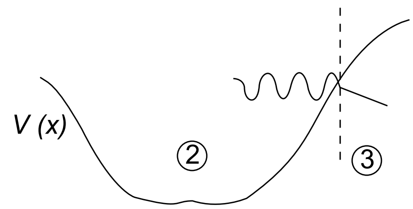

Ai(z)
0.8
0.6
0.4
0.2
-0.2
-0.4
-15
-12.5
-10
-7.5
-5
-2.5
2.5
z
Ai(z), WKB
0.8
0.6
0.4
0.2
-0.2
-0.4
-15
-12.5
-10
-7.5
-5
-2.5
2.5
z

(*a*)

Figure 1: (a)The Airy function $Ai(z)$, and (b) the Airy function $Bi(z)$, and their asymptotic (WKB) approximations, for real-valued z. The approximation diverge at $z = 0$.



We use this to obtain CONNECTION FORMULAE:



a is the turning point on the right hand side of the well.

C.1:

$$\frac{2A}{\sqrt{k(x)}}\cos\left[\int_x^a k(x')dx' - \frac{\pi}{4}\right] \leftarrow \frac{A}{\sqrt{q(x)}}e^{-\int_a^x q(x')dx'}$$

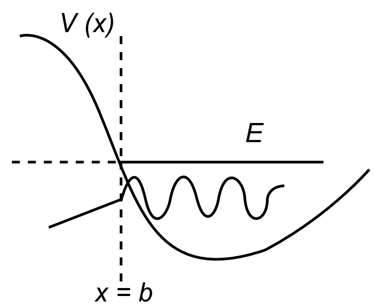
C.2:

$$\frac{B}{\sqrt{k(x)}}\sin\left[\int_x^a k(x')dx' - \frac{\pi}{4}\right] \rightarrow \frac{-B}{\sqrt{q(x)}}e^{-\int_a^x q(x')dx'}$$

Integrand limits come from detailed analysis. But just remember to integrate with increasing x (from LEFT TO RIGHT). In the -classically allowed- potential well region, the integration limits go from an arbitrary point $x_{(L)}$ (left of the turning point) up to a.

In the -classically forbidden- barrier region, they go FROM a to an arbitrary point $x_{(R)}$ to the right of the turning point, incrementing the phase ("action") of a 1D classical path from $X_{(L)}$ TO $X_{(R)}$.

If we have the forbidden region on the left the analysis can be repeated to obtain two more connection formulae:



C.3:

$$\frac{A}{\sqrt{q(x)}}e^{-\int_x^b q(x')dx'} \rightarrow \frac{2A}{\sqrt{k(x)}}\cos\left[\int_b^x k(x')dx' - \frac{\pi}{4}\right]$$

C.4:

$$\frac{-B}{\sqrt{q(x)}}e^{\int_x^b q(x')dx'} \leftarrow \frac{B}{\sqrt{k(x)}}\sin\left[\int_b^x k(x')dx' - \frac{\pi}{4}\right]$$

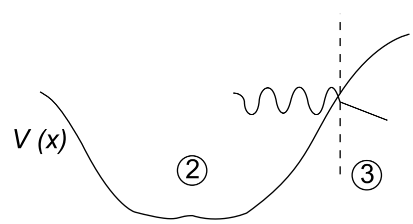
Once again, we integrate from left to right (see integration limits)

$$x \rightarrow b \text{ in barrier } b \rightarrow x \text{ in the well}$$

Why the arrows in the connection formulae?

While $\cos\phi$ and $\sin\phi$ solutions are always of the same order of magnitude at any range of x, (since $-1 \leq \cos\phi, \sin\phi \leq +1$), the $\exp \pm \phi$ terms, which might be of reasonable magnitude at the turning points, will either blow-up or vanish as $|x| \rightarrow \infty$. We can magnify small inaccuracies in the calculation, thus producing qualitatively incorrect solutions.

FOR EXAMPLE:



use C.1 with arrow reversed: we know $\psi_2 \simeq \cos\phi(x)$ but have a tiny uncertainty in the phase, producing a small uncertainty in $\sin\phi(x)$ component ie:

$$\begin{aligned}\psi_2(x) \simeq \cos(\phi(x)+\varepsilon) &= \cos\phi\cos\varepsilon + \sin\varepsilon\sin\phi \\ &\simeq \cos\phi + \varepsilon\sin\phi \text{ connects with } \varepsilon e^{+\phi}\end{aligned}$$

Regardless of how small ε is, at sufficiently large x, the $\varepsilon e^{+\phi}$ term, which is of uncertain amplitude will dominate $\psi_3(x)$.

While the small uncertainty ε does not perturb $\psi_2(x)$ much, it will means we know nothing of ψ_3 as $x \rightarrow \infty$. It could be exponentially decaying or growing; we are not sure.

An exercise: explain the arrow in C.2

HINT: If we *know* $\psi_3(x) \simeq A\exp + \phi$ at x *large*, can we be sure that, near the turning point, we still have: $\psi_3(x_T) \simeq Ae^{+\phi}$?

WKB CRIBSHEET

1) $\psi(x) = e^{iu(x)} = e^{is(x)/\hbar}$

2) **GEN. SOLUTIONS:**

$$\psi(x) = \frac{1}{\sqrt{k(x)}} \left[Ae^{i\int k(x')dx'} + Be^{-i\int k(x')dx'} \right]$$

'ALLOWED' REGION
E > V

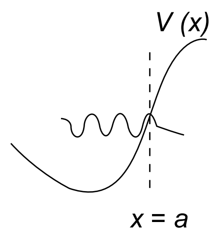
$$\psi(x) = \frac{1}{\sqrt{q(x)}} \left[Ae^{i\int q(x')dx'} + Be^{-i\int q(x')dx'} \right]$$

'FORBIDDEN' REGION
E < V

3) **CONNECTION FORMULAE**

$$\text{C1}: \quad \frac{A}{\sqrt{q(x)}} e^{-\int_a^x q(x')dx'} \rightarrow \frac{2A}{\sqrt{k(x)}} \cos\left[\int_x^a k(x')dx' - \frac{\pi}{4}\right]$$

$$\text{C2}: \quad \frac{B}{\sqrt{k(x)}} \sin\left[\int_x^a k(x')dx' - \frac{\pi}{4}\right] \rightarrow \frac{-B}{\sqrt{q(x)}} e^{-\int_a^x q(x')dx'}$$



$$\text{C3}: \quad \frac{A}{\sqrt{q(x)}} e^{-\int_x^b q(x')dx'} \rightarrow \frac{2A}{\sqrt{k(x)}} \cos\left[\int_b^x k(x')dx' - \frac{\pi}{4}\right]$$

$$\text{C4}: \quad \frac{-B}{\sqrt{q(x)}} e^{\int_x^b q(x')dx'} \leftarrow \frac{B}{\sqrt{k(x)}} \sin\left[\int_b^x k(x')dx' - \frac{\pi}{4}\right]$$