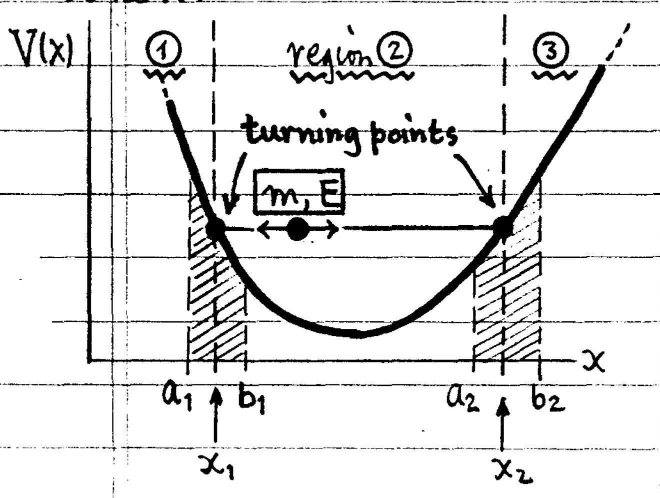
WKB (cont'd) Back to the turning point problem.

11) We have remarked before (e.g. on p. WKB 5) that the WKB (approximate) solution to $\psi'' + k^2\psi = 0$ does not work when $k^2 \to 0$... the solns $\propto 1/\sqrt{k}$ diverge, the "slowly-varying" condition $|k'/k^2| \ll 1$ can't be met, etc... everything seems to be a mess. Here we will see how something can be rescued from this mess.

It is easiest to begin sorting out the mess by talking about a physical example. We turn to QM... where a particle of mass m & energy E is trapped in a "potential well", i.e. a potential energy fcn $V(x)$ [1D motion] which looks like...



x_1 & x_2 are "turning points" of the motion (classical m turns around there), where...

$$V(x_1) = E = V(x_2),$$

$$\Rightarrow \hbar k(x) = \sqrt{2m[E - V(x)]} = 0, \text{ @ } x_1 \text{ \& } x_2,$$

and // WKB fails $\left(\text{for } \psi'' + k^2(x)\psi = 0\right)$,

in // regions: $a_1 < x < b_1$, $a_2 < x < b_2$. **(29)**

12) A classical m would never be found in regions ①&③, where $V(x) > E$; it would have to have (−)ve kinetic energy & imaginary velocity. This is reflected in QM by claiming the wavefcn $\psi(x)$ [with $|\psi|^2 \propto$ "presence" of m] must be "small" in ①&③ [m may be there, but not very often]. So we choose WKB forms

$$\left[\begin{array}{ll} \underline{\text{in region ①}}: \ \psi_1(x) = \dfrac{A}{\sqrt{\kappa(x)}}\, e^{-\int_x^{x_1} \kappa(\xi)\,d\xi}, & \underline{x < a_1} \\[2ex] \underline{\text{in region ③}}: \ \psi_3(x) = \dfrac{C}{\sqrt{\kappa(x)}}\, e^{-\int_{x_2}^{x} \kappa(\xi)\,d\xi}, & \underline{x > b_2} \end{array}\right\} \ \hbar\kappa(x) = \sqrt{2m[V(x) - E]}. \quad (30)$$

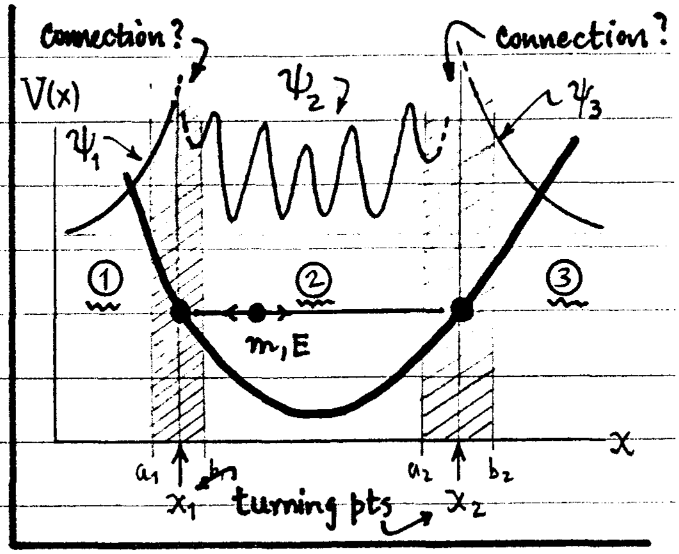
Both of these get suitably small as $|x| \to$ large. Anyway, we are adopting the point of view that WKB is $\sim$ OK as long as we exclude the shaded regions: $a_1 < x < b_1$ & $a_2 < x < b_2$ (size to be fixed later). In the

WKB (cont'd) Need for Connection Formulas across turning points.

Same spirit, we claim that in region ②, where m is most likely to be found, the suitable WKB soln -- with two more indpt cnsts B & β -- is given by

$$\left[\text{in region ②}: \ \psi_2(x) = \frac{B}{\sqrt{k(x)}} \sin\left(\int_{x_1}^{x} k(\xi)\,d\xi + \beta \right) \right. \quad \text{for } b_1 < x < a_2, \quad \text{w/ } \hbar k(x) = \sqrt{2m[E - V(x)]}. \tag{31}$$

Pictorially, we have the problem at right. We have valid WKB ψ's everywhere but in shaded regions, near where K & $k \to 0$. But in those regions, we know the "real" ψ must be continuous (and ψ' continuous). So what we want is a way of connecting ψ_1 to ψ_2, and ψ_2 to ψ_3 across the turning point barriers.



STRATEGY: ψ_1, ψ_2, ψ_3 of Eqs. (30) & (31) contain 4 arbitrary cnsts A, B & β, C. Only 2 are necessary in soln to $\psi'' + k^2(x)\psi = 0$. We will use the freedom of the two extra cnsts to connect ψ_1 to ψ_2 at x_1, and ψ_2 to ψ_3 at x_2. This will result in what are called the WKB Connection Formulas, and it will solve the turning point problem.

---

13) Look at the Schrödinger problem in neighborhood of a turning point. Have...

... in LH shaded region, $a_1 < x < b_1$ ...

Exact eqtn is: $\psi'' + \frac{2m}{\hbar^2}[E - V(x)]\psi = 0$ — the [ ] is (+)ve or (−)ve.

Near x_1: $V(x) = \cancel{V(x_1)}^{\,E} + \underbrace{V'(x_1)}_{\text{this is (−) ve}}(x - x_1) + \cancel{\tfrac{1}{2}V''(x_1)(x-x_1)^2 + \cdots}^{\,0,\ \text{ignore (small)}}$

so $\boxed{\psi'' + \frac{2mF_1}{\hbar^2}(x - x_1)\psi \simeq 0}$, near $x = x_1$, w/ $F_1 = |V'(x_1)|$. (32)

WKB (cont'd) Airy Eqtn near turning point.

It is convenient to write this eqtn in dimensionless form, as...

Airy's → diff. eq.
$$\boxed{\frac{d^2\psi}{d\xi^2} - \xi\psi = 0, \quad \text{w/} \quad \xi = \left(\frac{2m}{\hbar^2}F_1\right)^{\frac{1}{3}}(x_1 - x) \quad [\text{as } x \to x_1]}. \tag{33}$$

TACTICS: Solve this for $\psi = \psi(\xi)$; Connect $\begin{cases} \psi \text{ to } \psi_1 \text{ @ } x = a_1 \\ \psi \text{ to } \psi_2 \text{ @ } x = b_1 \end{cases}$.

Solutions to Eq. (33) thus provide the needed bridge $\psi_1 \curvearrowright \underset{(x_1)}{\overset{\psi}{\uparrow}} \curvearrowright \psi_2$. It is clear that a_1 & b_1 should be chosen so that...

$\left[\begin{array}{l} \psi_1(\text{WKB}) \text{ "good" up to } x = a_1, \\ \psi_2(\text{WKB}) \text{ "good" down to } x = b_1; \end{array}\right\} \psi(\text{Eq.(33)}) \text{ "good" in } a_1 \leq x \leq b_1.$ (34)

→ requires: $\left|\frac{1}{k^2}(dk/dx)\right| \ll 1$ @ $x = a_1$ & $x = b_1$,

... with: $\hbar k(x) = \sqrt{2m[E - V(x)]} = \sqrt{2mF_1(x - x_1)}$ here...

WKB "goodness" requires: $\left|\left(\frac{2mF_1}{\hbar^2}\right)^{1/2}(x - x_1)^{3/2}\right| = \boxed{|\xi|^{3/2} \gg \frac{1}{2}}$. (35)

(at $x = a_1, b_1$)

This is a big relief... it means we need only asymptotic solutions to Eq. (33): $\psi'' - \xi\psi = 0$, for $|\xi| \to$ large, at the endpoints a_1 & b_1.

---

14) The eqtn $\psi'' - \xi\psi = 0$ is solved most efficiently by Fourier transforms. We look for a solution in terms of a Fourier integral...

$$\left[\psi(\xi) = \int_{-\infty}^{\infty} \varphi(k)\, e^{ik\xi}\, dk \leftarrow \varphi(k) \text{ to be found, to satisfy: } \psi'' - \xi\psi = 0.\right. \tag{36}$$

Show spectrum fcn is: $\varphi(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \psi(\xi)\, e^{-ik\xi}\, d\xi$ (Fourier inverse).

If we can find an eqtn for $\varphi(k)$, and solve it, we can at least write $\psi(\xi)$ as an integral.

WKB (cont'd) Airy Eqtn solved by Fourier Integral.

To convert the Airy Eqtn [Eq. (33)] to a Fourier problem, note identities...

① $i\left(\frac{d\varphi}{dk}\right) = \frac{1}{2\pi}\int_{-\infty}^{\infty}[\xi]\psi(\xi)\,e^{-ik\xi}\,d\xi$ ← just differentiate under the $\int_{-\infty}^{\infty}$;

② $\frac{1}{2\pi}\int_{-\infty}^{\infty}\psi'(\xi)\,e^{-ik\xi}\,d\xi = ik\,\varphi(k)$ ← partial integration★ (assume $\psi \to 0$ as $|\xi| \to \infty$);

③ $\frac{1}{2\pi}\int_{-\infty}^{\infty}[\psi''(\xi)]\,e^{-ik\xi}\,d\xi = -k^2\varphi(k)$ ← repeat ② ($\xi\psi' \to 0$ as $|\xi| \to \infty$).

Then can convert the 2nd order ψ eqtn to a 1st order φ eqtn...

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}(\underbrace{\psi''}_{\text{use ③}} - \underbrace{\xi\psi}_{\text{use ①}})\,e^{-ik\xi}\,d\xi \Rightarrow \boxed{\frac{d\varphi}{dk} = +ik^2\varphi} \tag{37}$$

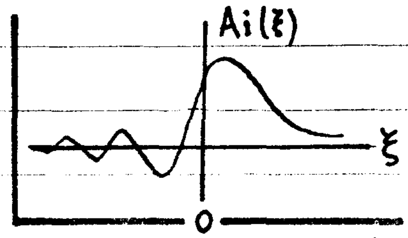
The φ eqtn is trivial, and has solution: $\varphi(k) = \text{cnst}\cdot e^{\frac{1}{3}ik^3}$. Then the the solution to Eq. (33): $\psi'' - \xi^2\psi = 0$ takes the Fourier form [Eq. (36)]:

$$\psi(\xi) = \int_{-\infty}^{\infty}\varphi(k)\,e^{ik\xi}\,d\xi = \text{cnst}\cdot\int_{-\infty}^{\infty}e^{i(\xi k + \frac{1}{3}k^3)}\,dk$$ ← exp. is odd in k

w/ $$\boxed{\psi(\xi) = \text{cnst}\cdot Ai(\xi), \quad Ai(\xi) = \frac{1}{\pi}\int_0^{\infty}\cos(\xi k + \tfrac{1}{3}k^3)\,dk}. \tag{38}$$

---

15) $Ai(\xi)$ is called an "Airy Function"; it is closely related to Bessel fcns of order $\nu = \pm 1/3$.¶ Asymptotic forms for $|\xi| \to$ large are...



$$\rightarrow Ai(\xi) \sim \begin{cases} (1/2\sqrt{\pi})\,\xi^{-1/4}\,e^{-\zeta}, & \text{for } \xi \gg +1; \text{ [exponential]} \\ (1/\sqrt{\pi})\,|\xi|^{-1/4}\sin(|\zeta| + \frac{\pi}{4}), & \xi \ll -1; \text{ [oscillatory]} \end{cases}$$

w/ $\zeta = (2/3)\,\xi^{3/2}$. (39)

¶ NBS Math Handbook, Ch. 10, Sec. 4. E.g. $Ai(z) = (1/\pi\sqrt{3})\,z^{1/2}K_{\frac{1}{3}}(\frac{2}{3}z^{3/2})$.

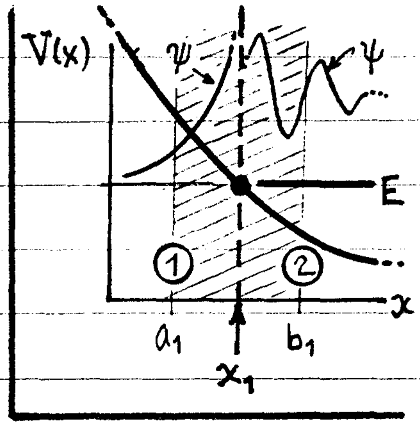
★ $$\int_{-\infty}^{\infty}\psi'(\xi)e^{-ik\xi}d\xi = \int e^{-ik\xi}d\psi = \cancelto{0}{\psi e^{-ik\xi}\Big|_{\xi=-\infty}^{\xi=+\infty}} - \int_{-\infty}^{\infty}\psi(\xi)\frac{d}{d\xi}e^{-ik\xi}\,d\xi \Rightarrow ②.$$

WKB (Cont'd) Asymptotic forms for $\psi(\xi)$ near turning point.

The asymptotic forms for $Ai(\xi)$ in Eq. (39) can be verified by direct substitution.*

SUMMARY: we have now solved the Schrödinger problem near the LH turning pt:

$\rightarrow d^2\psi/d\xi^2 - \xi\psi = 0$, w/ $\xi = (2mF_1/\hbar^2)^{\frac{1}{3}}(x_1 - x)$, and $F_1 = \left|\frac{dV}{dx}\right|_{x=x_1}$.



$\Rightarrow$ Region ①: $x < x_1$, and $\xi \gg +1$ for $x \to a_1$:

$$\rightarrow \psi(\xi) \propto \frac{1}{2}\xi^{-1/4} e^{-\frac{2}{3}\xi^{3/2}} \quad \text{exponential decline.} \tag{40}$$

Region ②: $x > x_1$, and $\xi \ll (-)1$ for $x \to b_1$:

$$\rightarrow \psi(\xi) \propto |\xi|^{-1/4} \sin\left(\frac{2}{3}|\xi|^{3/2} + \frac{\pi}{4}\right) \quad \text{oscillatory character.} \tag{41}$$

phase is important!

Now we need to join up all the pieces of ψ [ψ(Airy) from left & right, and ψ(WKB) from left & right], smoothly, in the neighborhood $x \sim x_1$.

---

16) Since the ψ(WKB)'s are quoted in terms of $K = \sqrt{\frac{2m}{\hbar^2}(V-E)}$ & $k = \sqrt{\frac{2m}{\hbar^2}(E-V)}$, it is convenient to express the ψ(Airy)'s in the same terms.

In ①: $a_1 < x < x_1$, and: $K(x) = [(2mF_1/\hbar^2)(x_1 - x)]^{1/2}$.

So// $\frac{2}{3}\xi^{3/2} = \frac{2}{3}\sqrt{\frac{2mF_1}{\hbar^2}}(x_1 - x)^{3/2} = \int_x^{x_1} K(x')\,dx'$, ← nice trick!

and// $\xi^{-1/4} \propto 1/\sqrt{K(x)}$.

$$\psi(\xi) = \frac{D}{2\sqrt{K(x)}} e^{-\int_{x \to a_1}^{x_1} K(x')\,dx'}. \tag{42}$$

---

* For $\xi \to +\infty$, put $\psi(\xi) = \xi^{-1/4} \cdot e^{-\frac{2}{3}\xi^{3/2}}$ into Airy's Eqtn [Eq. (33)]...

$\psi'' = \xi\left(1 + \frac{5}{16}\xi^{-3}\right)\psi$, so: $\psi'' - \xi\psi \simeq 0$, neglecting $\mathcal{O}(\xi^{-3})$. OK

Do same with asymptotic form for $\xi \to (-)\infty$. Note that...

$\xi < 0 \Rightarrow |\xi| = -\xi$, and: $\xi^{3/2} = -i|\xi|^{3/2}$, $\xi^{-1/4} = e^{-i\frac{\pi}{4}}|\xi|^{-1/4}$;

so// $\xi^{-1/4} e^{-\frac{2}{3}\xi^{3/2}} = |\xi|^{-\frac{1}{4}} e^{i\left(\frac{2}{3}|\xi|^{3/2} - \frac{\pi}{4}\right)} \xrightarrow[\text{part}]{\text{Re}} |\xi|^{-\frac{1}{4}} \sin\left(|\xi| + \frac{\pi}{4}\right)$. OK

WKB (cont'd) Behavior of Airy solution $\psi(\xi)$ near WKB boundaries.

This result is ~ pleasing, because it resembles the ψ_1(WKB) form we wrote down in Eq. (30)... ψ_1 exponentially declining @ $x < a_1$. As for $x > x_1$...

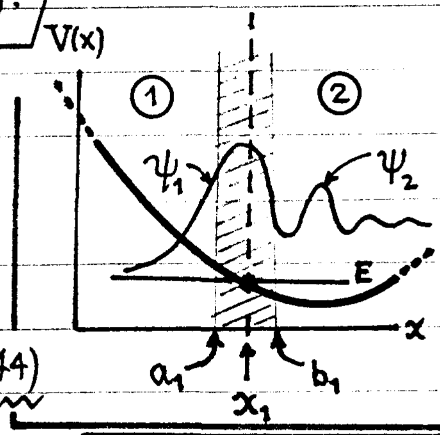
In ②: $x_1 < x < b_1$, and: $k(x) = [(2mF_1/\hbar^2)(x - x_1)]^{1/2}$.

So// $\frac{2}{3}|\xi|^{3/2} = \frac{2}{3}\sqrt{\frac{2mF_1}{\hbar^2}}(x - x_1)^{3/2} = \int_{x_1}^{x} k(x')\,dx'$, ← same trick works

and// $|\xi|^{-1/4} \propto 1/\sqrt{k(x)}$.

$$\psi(\xi) = \frac{D}{\sqrt{k(x)}} \sin\left(\int_{x_1}^{x \to b_1} k(x')\,dx' + \frac{\pi}{4}\right). \tag{43}$$

Again ~ pleasing... because ψ(Airy) resembles the oscillatory ψ_2(WKB) form in Eq. (31). NOTE: the same amplitude cnst D is used in both $\psi(\xi)$'s here [Eqs. (42) & (43)], because both ψ's refer to the same solution. Also... we still don't have a valid ψ at $x = x_1$ (this would entail the $|\xi| \to 0$ version of $Ai(\xi)$ in Eq. (38), rather than the $|\xi| \to \infty$ version we have used). But we don't need ψ(Airy) at $x = x_1$; it is sufficient for matching purposes to know how ψ(Airy) behaves at the WKB boundaries $x \to a_1$ & $x \to b_1$. Just such information is provided by Eqs. (42) & (43).



17) Now, finally, we can connect solutions. We have...

→ REGION ①: declining exponential.

$$\text{[Eq.(30)] WKB } (x \le a_1):\ \psi_1(x) = \frac{A}{\sqrt{k(x)}} e^{-\int_x^{x_1} k(x')\,dx'},$$

$$\text{[Eq.(42)] Airy } (x \ge a_1):\ \psi(x) = \frac{1}{2}\frac{D}{\sqrt{k(x)}} e^{-\int_x^{x_1} k(x')\,dx'}. \tag{44}$$

ψ is continuous across boundaries at a_1 & b_1 (and even in $a_1 \le x \le b_1$)

→ REGION ②: distorted oscillation.

$$\text{[Eq.(43)] Airy } (x \le b_1):\ \psi(x) = \frac{D}{\sqrt{k(x)}} \sin\left(\int_{x_1}^{x} k(x')\,dx' + \frac{\pi}{4}\right),$$

$$\text{[Eq.(31)] WKB } (x \ge b_1):\ \psi(x) = \frac{B}{\sqrt{k(x)}} \sin\left(\int_{x_1}^{x} k(x')\,dx' + \beta\right). \tag{45}$$

So// ψ continuous at $x = a_1$ & $x = b_1$ $\Rightarrow$ $\boxed{2A = D = B, \text{ and } \beta = \frac{\pi}{4}}$. (46)