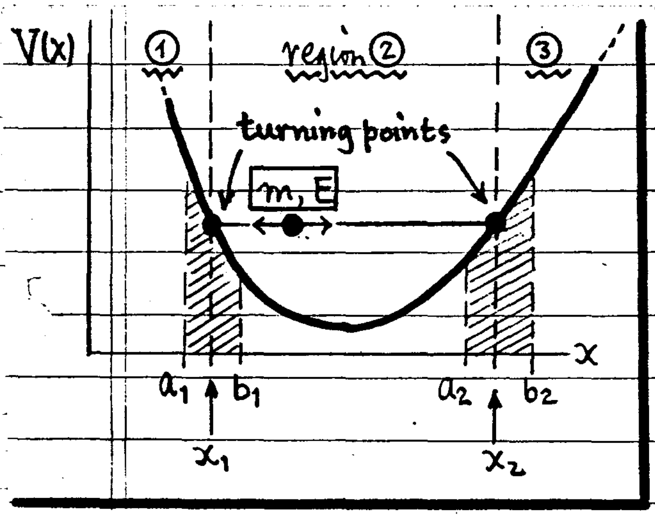
The QM Turning-Point Problem for Bound States.

3) Turning-point Problem. WKB Connection Formulas.

● We have discussed the "turning-point" problem on p. W5, i.e. the fact that the WKB sol$^{\underline{n}}$s fail at points where $k^2 \to 0$. In QM, this happens when the particle total energy becomes wholly potential: $E \to V(x)$. To see how this affects a WKB approx$^{\underline{n}}$ to the Schrödinger Eq., we consider a specific example: a particle of mass m & energy E trapped in a 1D potential well $V(x)$...



x_1 & x_2 are "turning-points" of m's motion (a classical m turns around there), with...

$$\left[\begin{array}{l} V(x_1) = E = V(x_2), \\ \text{so}/\ \hbar k(x) = \sqrt{2m[E-V(x)]} = 0 \ @\ x_1 \ \&\ x_2, \\ \text{and}/\ \text{WKB sol}^{\underline{n}} \text{ to } \psi'' + k^2\psi = 0 \ \underline{\text{fails}} \\ \text{in regions: } a_1 < x < b_1,\ a_2 < x < b_2. \end{array}\right. \tag{18}$$

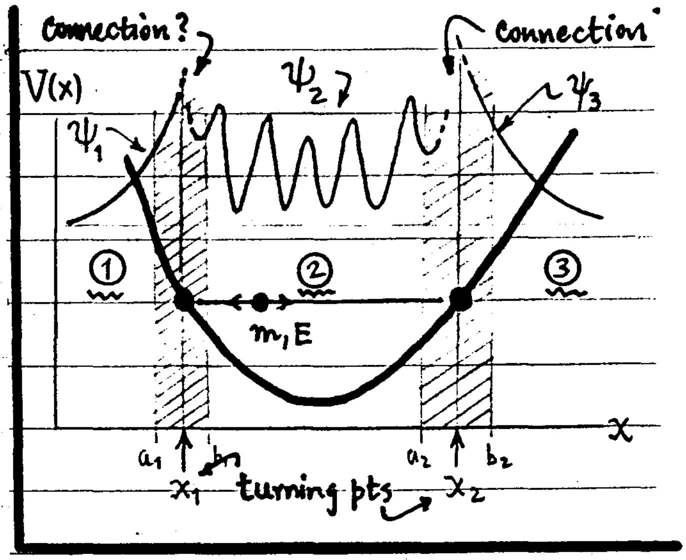
● The wavefcn $\psi(x)$ must be "small" in regions ① & ③, where even a QM particle rarely penetrates. Excluding x_1 & x_2, we can use WKB solutions...

$$\left.\begin{array}{l} \underline{\text{in region ①}}: \ \psi_1(x) = \dfrac{A}{\sqrt{K(x)}} \exp\left[-\int_x^{x_1} K(\xi)\,d\xi\right], \ \underline{x < a_1} \\ \underline{\text{in region ③}}: \ \psi_3(x) = \dfrac{C}{\sqrt{K(x)}} \exp\left[-\int_{x_2}^{x} K(\xi)\,d\xi\right], \ \underline{x > b_2} \end{array}\right\} \begin{array}{l} A \ \&\ C = \text{free cnsts}, \\ K = \sqrt{\dfrac{2m}{\hbar^2}(V-E)}. \end{array} \tag{19A}$$

Both ψ's vanish as $|x| \to \infty$. Our point of view is that WKB sol$^{\underline{n}}$s are OK so long as we exclude the shaded regions in the above sketch, w/ size to be fixed later. In the same spirit, we write a WKB sol$^{\underline{n}}$ in the central region:

$$\underline{\text{in region ②}}: \ \psi_2(x) = \frac{B}{\sqrt{k(x)}} \sin\left(\int_{x_1}^{x} k(\xi)\,d\xi + \beta\right), \ \underline{b_1 < x < a_2} \ \int \begin{array}{l} B \ \&\ \beta = \text{free cnsts}, \\ k = \sqrt{\dfrac{2m}{\hbar^2}(E-V)}. \end{array} \tag{19B}$$

Airy's ODE for ψ near a turning-point.



● We now have the problem at right. The WKB solⁿs ψ_1, ψ_2 & ψ_3 are valid everywhere but in the shaded regions, where K and $k \to 0$. Since we know that the physical ψ must be continuous (also ψ') across those regions, we need a way of connecting ψ_1 to ψ_2, and ψ_2 to ψ_3 across the turning-point "barriers". This is made possible by the fact that ψ_1, ψ_2 & ψ_3 in Eqs. (19) contain 4 free cnsts (A, B & β, C), while only 2 cnsts are needed for a solⁿ to $\psi'' + k^2\psi = 0$ everywhere. The two extra cnsts can be adjusted to match $\psi_1 \to \psi_2$ near x_1, and $\psi_3 \to \psi_2$ near x_2. The results are called the WKB Connection Formulas.

● Details of the matching procedure are fairly intricate. Briefly...

1. One expands $V(x)$ near the turning points, e.g. $V(x) = E + V'(x_1)(x - x_1) + \cdots$ near $x = x_1$. The Schrödinger Eq. is then: $\psi'' - \frac{2mF_1}{\hbar^2}(x_1 - x)\psi = 0$, near x_1, w/ $F_1 = |V'(x_1)|$. This eqtn can be written in dimensionless form as...

$$\rightarrow d^2\psi/d\xi^2 - \xi\psi = 0, \quad \text{w/ } \xi = (2mF_1/\hbar^2)^{\frac{1}{3}}(x_1 - x), \text{ as } x \to x_1. \tag{20}$$

The solⁿ ψ to this eqtn can be used to match $\psi_1 \leftarrow \psi$ @ $x = a_1$, and $\psi \to \psi_2$ @ $x = b_1$. So this ψ serves as a "bridge" over the turning-point at x_1.

2. The length scale for $(x_1 - a_1)$ & $(b_1 - x_1)$ can be fixed by invoking the "slowly-varying" condition... if ψ_1(WKB) is good up to $x = a_1$, and ψ_2(WKB) is good down to $x = b_1$, then we must have $\left|\frac{1}{k^2}(dk/dx)\right| \ll 1$ @ $x = a_1$ & b_1. This yields...

$$\rightarrow \psi_{1,2}(\text{WKB}) \text{ "good" to } x = a_1, b_1 \text{ iff : } \left|\left(\frac{2mF_1}{\hbar^2}\right)^{1/2}(x - x_1)^{3/2}\right| = |\xi|^{3/2} \gg \frac{1}{2}. \tag{21}$$

and it means we need only asymptotic solⁿs to Eq. (20), as $|\xi| \to \infty$, for matchups.

Asymptotic Forms for Airy Functions : Matching Procedure.

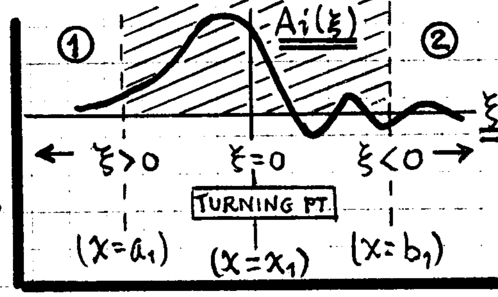
3. Eq.(20) is called Airy's Eqtn... it is "well-known" and its solutions (closely related to Bessel fcns of order $\nu = \pm 1/3$ *) are tabulated. An integral solⁿ is:

$$\rightarrow \psi(\xi) = \text{cnst} \cdot Ai(\xi), \quad \text{w/} \quad Ai(\xi) = \frac{1}{\pi}\int_0^\infty \cos(\xi k + \tfrac{1}{3}k^3)\,dk. \tag{22}$$

In accord with Eq.(21), tabulated asymptotic forms for $|\xi| \to \infty$ are...

$$Ai(\xi) \sim \begin{cases} (1/2\sqrt{\pi})\,\xi^{-1/4}\,e^{-\zeta}, & \text{for } \xi >> +1; \\ (1/\sqrt{\pi})\,|\xi|^{-1/4}\sin(|\zeta| + \frac{\pi}{4}), & \xi << (-)1; \end{cases}$$

$$\text{where: } \zeta = \tfrac{2}{3}\xi^{3/2} = (8mF_1/9\hbar^2)^{\frac{1}{2}}(x_1 - x)^{\frac{3}{2}}. \tag{23}$$



$Ai(\xi)$ vs. ξ is sketched at right. Notice that the exponential fall-off to the left (@ $\xi > 0$), followed by the distorted oscillation to the right (@ $\xi < 0$), closely resembles the behaviors of ψ_1 & ψ_2 in the diagram at the top of p. W8.

4. The asymptotic forms in Eq. (23) can be rewritten. Note that near region ①, i.e. $a_1 < x < x_1$, the wave# $K = \sqrt{\frac{2m}{\hbar^2}(V-E)} \to \sqrt{(2mF_1/\hbar^2)(x_1 - x)}$, and a simple integration shows that: $\int_x^{x_1} K(x')\,dx' = \frac{2}{3}\xi^{3/2} = \zeta$. Then, since $\xi^{-1/4} \propto 1/\sqrt{K(x)}$, we have...

$$\rightarrow \text{Airy sol}^{\underline{n}} \text{ is: } \psi(x) = \frac{D}{2\sqrt{K(x)}}\exp\left[-\int_x^{x_1} K(x')\,dx'\right], \text{ as } x \to a_1. \tag{24A}$$

D is a free cnst, to be used to match $\psi_1(\xi)$ of Eq.(19A) at $x = a_1$. In a similar way, in $x_1 < x < b$ near region ②: $\int_{x_1}^x k(x')\,dx' = |\zeta|$, and $|\xi|^{-1/4} \propto 1/\sqrt{k(x)}$, so...

$$\rightarrow \text{Airy sol}^{\underline{n}} \text{ is: } \psi(x) = \frac{D}{\sqrt{k(x)}}\sin\left[\int_{x_1}^x k(x')\,dx' + \frac{\pi}{4}\right], \text{ as } x \to b_1. \tag{24B}$$

The same cnst D appears in (24A) & (24B) because the ψ's refer to the same solⁿ.

5. At this point, joining the ψ's across the turning pt., i.e. $x \to a_1 \to (x_1) \leftarrow b_1 \leftarrow x$, is fairly easy. At the lefthand edge of the "barrier", $x = a_1$, we have $\psi_1(x)$ of Eq.(19A) as $x \to a_1$, and $\psi(x)$ of Eq.(24A) as $a_1 \leftarrow x$. The two versions of ψ

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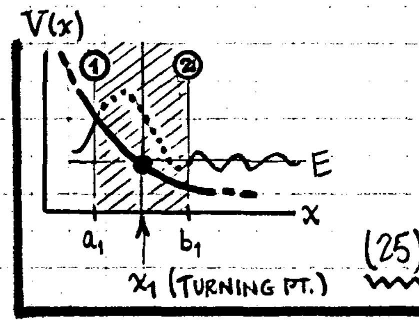
* NBS Math Handbook, Ch.10, Sec.4 : $Ai(z) = (1/\pi\sqrt{3})\,z^{\frac{1}{2}}\,K_{\frac{1}{3}}(\tfrac{2}{3}z^{3/2})$.

Matching Procedure → WKB Connection Formulas.

(and their derivatives ψ') match if: $A = \frac{D}{2}$. At the righthand edge of the "barrier", $x = b_1$, we can match $\psi_2(x)$ of Eq. (19B) to $\psi(x)$ of Eq. (24B) if we choose $B = D$ and $\beta = \pi/4$. Then the connection between WKB sol$^{\underline{n}}$s to the left and right of the turning-point at $x = x_1$ is...

$$\boxed{\begin{aligned} &\psi_1(x \leq a_1) = (A/\sqrt{\kappa(x)})\exp\left[-\int_x^{x_1}\kappa(x')\,dx'\right], \text{ in region ①;} \\ &\text{thru } x_1 \\ &\psi_2(x \geq b_1) = (2A/\sqrt{k(x)})\sin\left[\int_{x_1}^{x} k(x')\,dx' + \frac{\pi}{4}\right], \text{ in ②.} \end{aligned}}$$

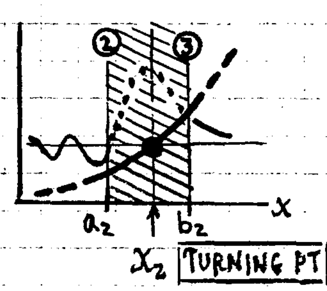


(25)

w/ $\hbar\kappa(x) = \sqrt{2m[V(x)-E]}$ & $\hbar k(x) = \sqrt{2m[E-V(x)]}$ for our QM problem. So, as ψ evolves from exponential to oscillatory behavior, the amplitude $A \to 2A$, and the oscillation is born with a phase $\frac{\pi}{4}$ (equal admixture of sin & cos$[\int k\,dx']$).

6. We can repeat the above procedure at the other turning-point, i.e. $x = x_2$ in the sketch on p. W8 (this just requires changing notation in (25)). Result is...

$$\boxed{\begin{aligned} &\psi_2(x \leq a_2) = (2C/\sqrt{k(x)})\sin\left[\int_x^{x_2} k(x')\,dx' + \frac{\pi}{4}\right], \text{ in ②;} \\ &\text{thru } x_2 \\ &\psi_3(x \geq b_2) = (C/\sqrt{\kappa(x)})\exp\left[-\int_{x_2}^{x}\kappa(x')\,dx'\right], \text{ region ③.} \end{aligned}}$$



(26)

Eqs. (25) & (26) are known as "WKB Connection Formulas". The two cnsts A & C are free (and sufficient) to fit initial conditions for the sol$^{\underline{n}}$ to $y'' + k^2 y = 0$.

7. Eqs. (25) & (26) connect an exponentially decreasing WKB solution to an oscillatory one across a turning-point. For completeness (and later use), we also need connection formulas for exponentially increasing WKB → oscillatory WKB. Calculations similar to the above produce the following results, in a form suitable for QM problems [formulas ⓐ & ⓑ are ≡ (25) & (26) above; formulas $\tilde{ⓐ}$ & $\tilde{ⓑ}$ are new].

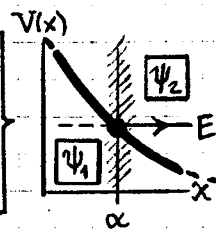
Let: $\hbar k(x) = \sqrt{2m[E-V(x)]}$, $\hbar\kappa(x) = \sqrt{2m[V(x)-E]} = i\,k(x)$.

Then WKB solutions to $\left\{\begin{array}{l} \psi'' + k^2\psi = 0 \text{ (in bound state regions)} \\ \psi'' - \kappa^2\psi = 0 \text{ (in "forbidden" regions)} \end{array}\right\}$ are...

Complete WKB Connection Formulas. Bohr Sommerfeld Quantization.

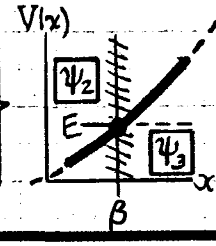
$$\textcircled{\alpha}\quad \psi_1(x<\alpha) = \frac{A}{\sqrt{k}}\, e^{-\int_x^{\alpha} k(\xi)\,d\xi} \rightarrow \psi_2(x>\alpha) = \frac{2A}{\sqrt{k}} \sin\left(\int_{\alpha}^{x} k(\xi)\,d\xi + \frac{\pi}{4}\right),$$

$$\widetilde{\textcircled{\alpha}}\quad \psi_1(x<\alpha) = \frac{\tilde{A}}{\sqrt{k}}\, e^{+\int_x^{\alpha} k(\xi)\,d\xi} \rightarrow \psi_2(x>\alpha) = \frac{\tilde{A}}{\sqrt{k}} \cos\left(\int_{\alpha}^{x} k(\xi)\,d\xi + \frac{\pi}{4}\right); \tag{27A}$$



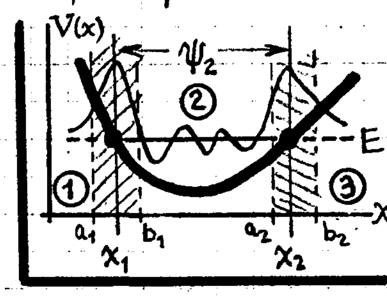
$$\textcircled{\beta}\quad \psi_2(x<\beta) = \frac{2C}{\sqrt{k}} \sin\left(\int_x^{\beta} k(\xi)\,d\xi + \frac{\pi}{4}\right) \leftarrow \psi_3(x>\beta) = \frac{C}{\sqrt{k}}\, e^{-\int_{\beta}^{x} k(\xi)\,d\xi},$$

$$\widetilde{\textcircled{\beta}}\quad \psi_2(x<\beta) = \frac{\tilde{C}}{\sqrt{k}} \cos\left(\int_x^{\beta} k(\xi)\,d\xi + \frac{\pi}{4}\right) \leftarrow \psi_3(x>\beta) = \frac{\tilde{C}}{\sqrt{k}}\, e^{+\int_{\beta}^{x} k(\xi)\,d\xi}. \tag{27B}$$



These are the complete WKB Connection Formulas. A & $\tilde{A}$, and C & $\tilde{C}$, are free cnsts.

● **ASIDE** Bohr-Sommerfeld Quantization Rule



For the bound state problem, we have two equivalent expressions for ψ_2 in the interior region, $b_1 < x < a_2$. By continuity of ψ...

$$\underbrace{\frac{2A}{\sqrt{k}} \sin\left(\int_{x_1}^{x} k(\xi)\,d\xi + \frac{\pi}{4}\right)}_{\text{from left: ①→②, Eq. (25)}} = \psi_2(x) = \underbrace{\frac{2C}{\sqrt{k}} \sin\left(\int_{x}^{x_2} k(\xi)\,d\xi + \frac{\pi}{4}\right)}_{\text{from right: ②←③, Eq. (26)}}$$

... cancel $2/\sqrt{k}$, and use: $\int_x^{x_2} = \int_{x_1}^{x_2} - \int_{x_1}^{x}$ ... define: $\phi = \int_{x_1}^{x} k(\xi)\,d\xi + \frac{\pi}{4}$ ...

$$\text{so}/\!/\quad A\sin\phi = C\sin(\phi_0 - \phi),\quad {}^{w}/\!/\ \ \phi_0 = \int_{x_1}^{x_2} k(\xi)\,d\xi + \frac{\pi}{2}. \tag{28}$$

This identity ensures ψ_2 is continuous in the interior. It is always true only if

→ $\underbrace{\phi_0 = (n+1)\pi}$, and: $C = (-)^n A$, for: $n = 0, 1, 2, 3, \ldots$

$$\text{i.e.}/\!/\quad \int_{x_1}^{x_2} k(\xi)\,d\xi = \left(n+\tfrac{1}{2}\right)\pi,\quad \text{for}: n = 0,1,2,3,\ldots \tag{29}$$

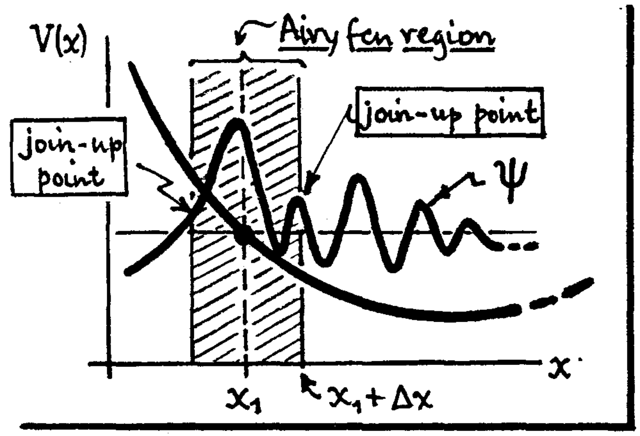
So the WKB phase integral ϕ_0 is quantized as a result of continuity in ψ. This is a classical result... using only $\psi \sim \psi(\text{WKB})$ & continuity of ψ. But in QM, we write $p = \hbar k$ for the particle momentum, and (29) becomes...

$$\boxed{\int_{x_1}^{x_2} p(x)\,dx = \int_{x_1}^{x_2} \sqrt{2m[E - V(x)]}\,dx = \left(n+\tfrac{1}{2}\right)\pi\hbar,\ {}^{w}/\ n = 0,1,2,3\ldots} \tag{30}$$

Eq. (30) can be satisfied only for quantized values of the total energy: $E = E_n$. So we get energy quantization from classical restraints! Eq. (30) is the Bohr-Sommerfeld Rule.

WKB: A Physical Accuracy Criterion

- We can state a "physical" criterion for accuracy of the WKB approx^n in terms of the de Broglie wavelength $\lambda = 2\pi/k$ of the particle (mass m) described by ψ. Recall that in Eq.(21) we found that ψ could be continued thru a turning point by means of the Airy-fcn analysis if we joined up the WKB solutions to an appropriate Airy fcn in the asymptotic region $|\xi|^{\frac{3}{2}} \gg 1/2$ (to left & right of turning pt x_1 shown).



In fact, in that notation, $|\xi|^{\frac{3}{2}} \gg 1/2$, was equivalent to the WKB "goodness" criterion $|k'/k^2| \ll 1$. This asymptotic condition can be converted to a statement about the size of the well in units of λ.

Consider a "join-up point" (Airy→WKB) @ $x_1 + \Delta x$ as shown. Compare the size of Δx with $\lambda = 2\pi/k$, where $k = \sqrt{(2mF_1/\hbar^2)\Delta x}$ at that point. Then...

$$\left[\!\left[\ \frac{\Delta x}{\lambda} = \frac{1}{2\pi}\left(\sqrt{(2mF_1/\hbar^2)\Delta x}\right)\Delta x = \frac{1}{2\pi}\left[\left(\frac{2mF_1}{\hbar^2}\right)^{\frac{1}{3}}\Delta x\right]^{\frac{3}{2}} = \frac{1}{2\pi}|\xi|^{3/2} \gg 1. \qquad (55)\right.\right.$$

We have recognized ξ by its definition in Eq.(20), p.W8 [note $\hbar^2$ there]. This condition says that a successful Airy↔WKB join-up can only occur when well is big enough so that there are allowed regions $\underline{\Delta x \gg \lambda}$ on either side of a turning point. To the extent this condition is weakened, the WKB approx^n to ψ will become less accurate.

In these terms, we can see immediately that for the bound state problem we have done, **WKB will be accurate only if** the energy E is high enough so that the distance between the turning points $(x_2 - x_1) \gg \lambda$. This condition is successively weakened as the particle sinks down to the bottom of the well, since $(x_2 - x_1)$ decreases while λ increases. So WKB results here are expected to be ~ poor for the lowest lying states, but they improve as E increases.