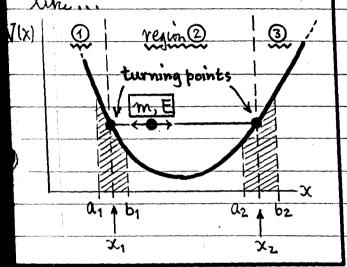
11) We have remarked before (e.g. on p. WKB 5) that the WKB (approximate) solution to \psi' + k^2 \psi = 0 does not work when k^2 \rightarrow 0... the solus \alpha 1/tk diverge, the slowly-verying condition |k'/k²| << 1 can't be met, etc... everything seems to be a mess. Here we will see how something can be rescued from tais 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 for V(x) [1D motion] which looks



(classical on turns around there), where ...

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

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

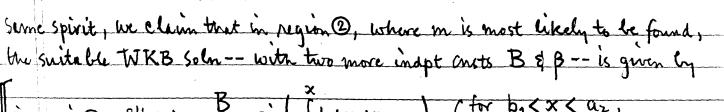
andy WKB fails (for Ψ"+ k2(x) ψ= 0),

in/1 regions: a1< x < b1, a2< x < b2, (29)

A classical on world never be found in regions () (3), where V(x) > E; it would have to have (-) ve kinetic energy of imaginary velocity. This is reflected in any claiming the wavefen \(\psi(x) \) [with \(\psi\) \(\pi \) presence of \(\mathred{m} \) must be "Small" in () (3) [m may be there, but not very often]. So we choose WKB forms

$$\frac{\sum_{x} \frac{x}{x} e_{x} e_{x}}{\sum_{x} \frac{x}{x}} = \frac{\sum_{x} \frac{x}{x} e_{x}}{\sum_{x} \frac{x}{x}} e_{x} + \sum_{x} \frac{x}{x} e_$$

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



 $\frac{\text{in region}(2): \Psi_2(x) = \frac{B}{Jk(x)} \sin\left(\frac{J}{x}k(\xi)d\xi + \beta\right) \int_{y}^{y} \frac{b_1 \langle x \langle a_2, y \rangle}{tk(x) = \sqrt{2m[E-V(x)]}}, \quad (31)$

Pictorially, we have the problem at right.

We have valid WKB 4's everywhere but
in shaded regions, near where K & k > 0.

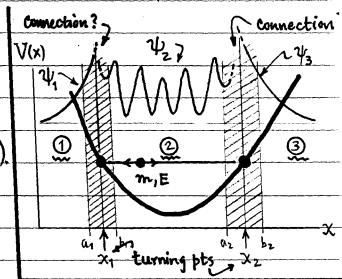
But in those regions, we know the "real"

4 must be continuous (and 4' continuous).

So what we want is a way of connecting

41 to 42, and 42 to 43 across the

turning point barriers.



STRATEGY: 4, 42, 43 of Eqs. (30) 4(31) contain 4 arbitrary costs A, B&B, C. Only 2 we necessary in soln to Ψ"+ k²(x) Ψ = 0. We will use the freedom of the two extra costs to connect 4, to Ψz at X1, and Ψz to Ψz at x2. This will result in what are called the WKB Connection Formulas, and it will solve the turning point problem.

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

... in IH shaded region, an < x < b1 ...

-Exact egtin is: $\psi'' + \frac{2m}{\hbar^2} [E-V(x)] \psi = 0$ (t) re or (-1 is

Near x_1 : $V(x) = V(x_1) + V'(x_1)(x-x_1) + \frac{1}{2}V''(x_1)(x-x_1)^2 + \cdots$

 $\frac{500}{4} + \frac{2mF_1}{h^2} (x-x_1) + \frac{2}{4} = |V'(x_1)|. \quad (32)$

```
It is convenient to write this extre in dimensionless form, as.
y's \Rightarrow \frac{d^2\psi}{d\xi^2} - \xi\psi = 0, \chi = (\frac{2m}{k^2}F_1)^{\frac{1}{3}}(\chi_1 - \chi) [as \chi \to \chi_1]
                                                                                                                                                                                                                                                     (33)
   TACTICS; Solve trus for \psi = \psi(\xi); Connect { \psi to \psi_1 @ x = a_1
        Solutions to Eq. (33) thus provide the needed bridge 4, 4 4. It is clear
         that and by Should be chosen so that ...
                 4, (WKB) " good" up to x=a1,
                                                                                                                        → (Eq.(33)) "good" in a, < x < b,.
                 1 /2 (WKB) "good" down to x = b1;
                    → requires: | 1/2 | dk/dx) << 1 @ x=a1 & x=b1,
                                          with ! to k(x) = \( 2m[E-V(x)] = \sqrt{2m F_1 (x-x_1)} \) here...
                      WKB"goodness" requires: \(\left(\frac{2mF_1}{\pi^2}\right)^{1/2} \left(\chi^2\right)^{3/2} \right| \frac{1}{7} \right| \frac{5}{7} \right| \frac{1}{7} \right| \frac{5}{7} \right| \frac{1}{7} \right| \frac{1
               This is a big relief ... it means we need only asymptotic solutions to Eq. (33): \psi'' - \xi \psi = 0, for |\xi| \rightarrow large, at the endpoints a_1 \not\in b_1.
        14) The extra 4"- & 4 = 0 is solved most efficiently by Fornier transforms. We look for a solution in terms of a Fourier integral...
                         \Psi(\xi) = \int \varphi(k) e^{ik\xi} dk \leftarrow \varphi(k) to be found, to satisfy: \Psi'' - \xi \Psi = 0.
                       Show spectrum for is: 9(k) = 1 5 4(x) e-ik & dx (Fourier inverse).
                     If we can find an extra for 4lks, and solve it, we can at least write
                     4(E) as an integral.
```

WKB (cont'd) Airy Egtr Solved by Fourier Integral.

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

1 $i\left(\frac{d\varphi}{dk}\right) = \frac{1}{2\pi} \int [\xi] \psi(\xi) e^{-ik\xi} d\xi$

The further sunder the $\int_{\xi}^{\xi} i \left(\frac{d\varphi}{dk}\right) d\xi$

2) $\frac{1}{2\pi} \int \psi'(\xi) e^{-ik\xi} d\xi = ik \varphi(k) \leftarrow \text{partial integration (assume } \psi \rightarrow 0 \text{ as } |\xi| \rightarrow a)$.

3 1/2π [ψ"(ξ)] e-ikξ dξ = -k² φ(k) ← repent②(ξψ'→0 ω(ξ)-νω).

Then can convert the 2nd order 4 epts to a 1st order 9 extr...

 $\frac{1}{2\pi}\int_{-\infty}^{\infty}(\psi''-\xi\psi)e^{-ik\xi}d\xi \Rightarrow \frac{d\psi}{db} = +ik^{2}\phi$ use 3 use 1

(37)

(38)

The O extr is trivial, and has solution: (1/k) = cust. e3iks. Then the

the solution to Eq. (33): 4"- 824 = 0 takes the Former form [Eq. (36)]:

ψ(ξ) = \$ 9(k)eik\$ dξ = cnst. Sei(ξk+ 1/2 k3) αk

 $\Psi(\xi) = \text{cost. Ai}(\xi), \quad \text{Ai}(\xi) = \frac{1}{\pi} \int \cos(\xi k + \frac{1}{3}k^3) dk$

15) Ai(E) is called an "Airy Function"; it is closely related to Bessel for of

order V= ± 1/3. Asymptotic forms for [E] > large are... $\frac{(1/2\sqrt{\pi}) \xi^{-1/4} e^{-\xi}, \text{ for } \xi >>+1; [exponential]}{(1/\sqrt{\pi}) |\xi|^{-1/4} \sin(|\xi| + \frac{\pi}{4}), \xi <<-1; [0scilla=]}$

W/ 5=(2/3) 53/2.

NBS Math Handbook, Ch. 10, Sec. 4. E.g. Ai (z) = (1/11/3) 21/2 Kz (32312).

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

Region 2: x>x1, and \$<<(-)1 for x > b1:

-> \(\xi\) \(\chi\) \(\xi\) \

Now we need to join up all the pieces of 4 [4(Airy) from left & right, and 4 (TVKB) from left & right I, smoothly, in the neighborhood x ~ X.

Since the 4 (WKB)'s are quoted in time of $K = \sqrt{\frac{2m}{h^2}}(V-E) \notin k = \sqrt{\frac{2m}{h^2}}(E-V)$, it is convenient to express the Y(Airy)'s in the same terms

1. 1 : a, (x < x, and: K(x) = [(2m F,/h2)(x,-x)]1/2. $\frac{3}{50\%} \frac{2}{3} \xi^{3/2} = \frac{2}{3} \sqrt{\frac{2mF_1}{k^2}} (x_1 - x)^{3/2} = \int_{x}^{x_1} \kappa(x') dx'_1 \psi(\xi) = \frac{D}{2\sqrt{\kappa(x)}} e^{-\int_{x}^{x} \kappa(x') dx'}.$ and &=1/4 oc 1/VK(x). Unice trick!

k For &>+0, put 4(8) = }-1/4:0-3 \ into Airys Eqt. [Eq. (33)]...

Do same with asymptotic form for \$ > (-) 00. Note that.

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

 $|\xi^{-1/4}| e^{-\frac{2}{3}\xi^{3/2}} = |\xi|^{-\frac{1}{4}} e^{\frac{1}{3}(\frac{2}{3}|\xi|^{3/2} - \frac{\pi}{4})} \xrightarrow{\text{Re}} |\xi|^{-\frac{1}{4}} \sin(|\xi| + \frac{\pi}{4}).$

This result is ~ pleasing, because it resembles the 4(WKB) form we wrote down in Eq. (30)... 4 exponentially declining @ X < a. As for X > x... In @: x1<x<b1, and: k(x) = [(2mF1/t2)(x-x1)]/2 $50/1 \frac{2}{3} |\xi|^{3/2} = \frac{2}{3} \sqrt{\frac{2mF_1}{k^2}} (x - x_1)^{3/2} = \int |k(x')dx'|,$ $\psi(\xi) = \frac{D}{\sqrt{k(x)}} \sin\left(\int_{x}^{x+b_1} k(x') dx' + \frac{\pi}{4}\right)$ only 151-14 oc 1/JRIX). Come trick works Again ~ pleasing. because 4 (Airy) resembles the oscillatory 42 lWKB) form in Eq. (31). NOTE: the same amplitude cost D is used in both Y(E)'s here [Eqs. (42) of (43)], because both 4's refer to the same solution. Also. we still don't have a valid 4 at x=x, (this would entail the 15170 version of Ai(3) in Eq. (38), rather than the 181 > 00 version we have used). But he don't need 4 (Awy) at x= x, it is sufficient for matching purposes to know how 4 (Airy) behave at the WKB boundaries X > a, & x > b, . Just such information is provided by Eqs. (42) & (43). 3) Now, finally, we can connect solutions. We have > REGION 1 : declining exponential. (30)] WKB (x < a1): 4(x) = A e x (x') dx' (42)] Airy (x) a1): Y(x) = 1/2 D e-5 K(x') dx' V is continuous across -> REGION@ : distorted oscillation. boundaries at a1 & b1 (43)] Awy (x < b1): $\psi(x) = \frac{D}{\sqrt{h(x)}} \sin(\int k(x')dx' + \frac{\pi}{4})$, (and even in a 1 & x & b, (45) (31)] WKB (X2b1): $\psi(x) = \frac{B}{\sqrt{k(x)}} \sin(\int k(x')dx' + \beta)$ Soll Ψ continuous at $x=a_1 \notin x=b_1 \Rightarrow 2A=D=B$, and $\beta=\frac{\pi}{4}$

(46)

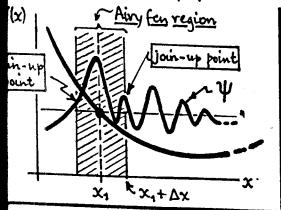
WKB (cont'd) First WKB Connection Formula. A Quantization Condition. WKB (7)

Now we know how a V(WKBexp2) connects to a V(WKB(OSC2) through a turning point, namely... $\mathcal{Y}_{1}(x < \alpha_{1}) = \left(A/\sqrt{k(x)}\right) e^{-\frac{x_{1}}{x}} \frac{x_{1}}{k(x') dx'}, \text{ in region } 0;$ $\Psi_2(x>b_1) = (2A/\sqrt{k(x)}) \sin\left(\int_{x_1}^x k(x') dx' + \frac{\pi}{4}\right), \text{ in region } 2.$ where: to KIX)= 12m[VIX)-E] & to KIX)= 12m[E-VIX)], for QM problem (as above). So it evolves from an exponential -> oscillation, the amplitude A > 2A, and the oscillation pichs up a phase fector of T/4. We can repeat the procedure at the other turning point, i.e. at X= Xz in diagram on p. WKB 12. This just amounts to changing notation in Eq. (47). Have. $\gamma \Psi_2(x \leq a_2) = (2C/\sqrt{k(x)}) \sin(\int k(x') dx' + \frac{\pi}{4})$, in region ②, $\psi_3(x)b_2 = (C/\sqrt{\kappa(x)})e^{-\int_{x_2}^{x}\kappa(x')dx'}, \text{ in region 3.}$ 19) This "bookkeeping" actually has some physical content. We have two equivalent expressions for \$\for \psi in the interior region: b_1 < x < az. By continuity of \$\psi\$, claim: $(2A/\sqrt{k}) \sin (\int k(x')dx' + \frac{\pi}{4}) = \psi_2(x) = (2C/\sqrt{k}) \sin (\int k(x')dx' + \frac{\pi}{4})$ from right: 2+3, Eq. (48) from Left: 10+0, Eq. (47) => A sin $\left(\int_{x}^{x} + \frac{\pi}{4}\right) = C sin \left(\int_{x}^{x} + \frac{\pi}{4}\right) \sim use : \int_{x}^{x} = \int_{x}^{x} - \int_{x}^{x} define : \phi = \int_{x}^{x} + \frac{\pi}{4}$ $A \sin \phi = C \sin (\phi_0 - \phi)$, where $: \phi_0 = \int k(x') dx' + \frac{\pi}{2}$. This identity ensures 42 is continuous in the interior. It can only be true (for all interior of & \$) if he have!

 $\rightarrow \phi_0 = (n+1)\pi$, and $C = (-)^n A$, n = 0,1,2,...

KB (cont'd) Bohr-Sommenfeld Quantization. Connection Formula Collection. WKB (18
So the WKB phase integral ϕ_0 is quantized as a result of continuity in ψ : $\phi_0 = (n+1)\pi = \begin{cases} x_2 \\ x_3 \\ x_4 \end{cases} k(x) dx = (n+\frac{1}{2})\pi \left[n=0,1,2, \end{cases} $ (51)
This is a <u>classical</u> result involving use of \$\psi\psi\psi\wedge \psi\text{VWKB}) & \$\psi\$ continuous, only. In QM, we write momentum \$p = \text{the}, so that this condition is
In QM, we write momentum $\beta = hk$, so that this condition is $\int_{x_2}^{x_2} \frac{x_2}{\int p(x) dx} = \int_{x_1}^{x_2} \sqrt{2m(E-V(x))} dx = (n+\frac{1}{2})\pi k$, $n=0,1,2,3$ (52)
This condition can be satisfied only for quantized values of but total energy, i.e. E = En. So every am particle on in a well V(x) has quantized En. This important result is known as the Bohr-Sommerfeld Quantization.
The Connection Formulas in Eq. (47) & (48) connect an exponentially decreasing WKF solution to an oscillatory one across a turning point. For completeness, we also need the connection for exponentially increasing WKB -> oscillatory WKB. Calculations Similar to the above produce the following results (in a form suitable for QM problems) Tion Let: trkix) = \(\frac{2m[E-V(x)]}{2m[E-V(x)]} \), trkix) = \(\frac{2m[V(x)-E]}{2m[V(x)-E]} = \frac{1}{2}klx \).
Then WKB solutions to $\{\psi'' + k^2 \psi = 0 \leftarrow \text{bound-state regions} \text{ are}$ (1) (2) $\{\psi'' - \kappa^2 \psi = 0 \leftarrow \text{"forbidden" regions} \text{ are}$ $\{\psi'' - \kappa^2 \psi = 0 \leftarrow \text{"forbidden" regions} \text{ are}$ $\{\psi'' - \kappa^2 \psi = 0 \leftarrow \text{"forbidden" regions} \text{ are}$
$\frac{1}{a} \times \left(\frac{\psi_1(x < a) = \tilde{A}}{\sqrt{\kappa}} e^{+\int_{-\kappa}^{\kappa} \kappa(\xi) d\xi} \rightarrow \psi_2(x > a) = \frac{\tilde{A}}{\sqrt{\kappa}} \cos\left(\frac{x}{2} \log \frac{\pi}{4}\right); (53)}{(53)} \right)$
$ \frac{2}{\sqrt{3}} \left\{ \frac{\psi_{2}(x < b) = \frac{2C}{\sqrt{k}} \text{ sin} \left(\int_{x}^{x} k(\xi) d\xi + \frac{\pi}{4} \right) \leftarrow \psi_{3}(x > b) = \frac{C}{\sqrt{k}} e^{-\int_{x}^{x} k(\xi) d\xi}, \right. \\ \left[\frac{\psi_{2}(x < b) = \frac{C}{\sqrt{k}} \cos \left(\int_{x}^{x} k(\xi) d\xi + \frac{\pi}{4} \right) \leftarrow \psi_{3}(x > b) = \frac{C}{\sqrt{k}} e^{+\int_{x}^{x} k(\xi) d\xi} \left(\frac{54}{\sqrt{k}} \right) \right] $
A, A & C, C are all adjustable enste. 19 & 3rd connections are Eqs. (47) & (48); 2nd & 4th connections are "Similar Calculations". Free e.g. "J. Powell & B. Croseman "ann" (Addison-Wesley 1961), b. 148 et sea.

24) We can state a "physical" criterion for accuracy of the WKB approxim in terms of



the <u>de Broglie</u> wavelength $\lambda = 2\pi/k$ of the particle (mass m) described by Ψ . Recall that on β . 13 we found that Ψ could be continued thru a turning point by means of the Airy-fon analysis if we joined up the WKB solutions to an appropriate Airy for in the asymptotic region $|\xi|^2 >> \frac{1}{2}$ (to left 4 right of turning $\beta t \times_1 5 hown$).

In fact, in that notation, $|\xi|^2 >> 1/2$ was equivalent to the WKB goodness criterion $|k'/k^2| << 1$. 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 $k = \sqrt{(2mF_1/k^2)}\Delta x$ at that point. Then...

$$\left[\frac{\Delta x}{\lambda} = \frac{1}{2\pi} \sqrt{(2mF_1/k^2)\Delta x}\right] \Delta x = \frac{1}{2\pi} \left[\left(\frac{2mF_1}{k^2}\right)^{\frac{1}{3}} \Delta x\right]^{\frac{3}{2}} = \frac{1}{2\pi} |\xi|^{3/2} >> 1. \quad (55)$$

We have recognized & by its definition in Eq. (33), p. 13 [note the three]. This condition says that a successful Airy &> WKB join-up can only occur when well is big enough so that there are allowed regions $\Delta x >> \lambda$ on either side of a turning point. To the extent this condition is weakened, the WKB approximents & 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 (x2-x1) >> 2. 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 a poor for the lowest lying states, but they improve as E increases.