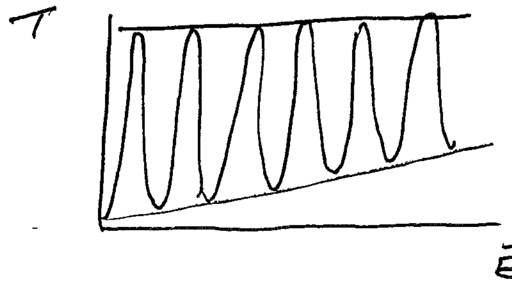


These large rapid wiggles ("resonances") are characteristic of low-energy scattering of a particle off of a highly attractive potential

From the optical viewpoint, constructive interference is enhancing the reflection off the attractive well.

The WKB Approximation

Wentzel Kramers Brillouin Jeffries Green

... is also called the semiclassical approximation and it is extremely useful. It is an expansion in the deBroglie wavelength, where the leading behavior is classical behavior, but we can also systematically study the quantum corrections (or semiclassical corrections) to classical behavior, when these are small.

What does it mean for the deBroglie wavelength to be small? Small compared to what? Our potential has a characteristic distance scale over which it changes appreciably... The WKB approximation is good when the fractional change in the wavelength is small over a distance of one wavelength (the wavelength is "slowly varying"):

$$\left|\frac{d\lambda}{dx}\lambda\right| \ll |\lambda| \quad \text{or} \quad \left|\frac{d\lambda}{dx}\right| \ll 1$$

Writing this as a condition on the potential, we have

$$1 \gg \left|\frac{d}{dx}\frac{1}{k}\right| \sim \left|\frac{1}{k^2}\frac{dk}{dx}\right| \sim \left|\frac{1}{k^3}\frac{dk^2}{dx}\right| = \left|\frac{1}{k^3}\frac{m}{\hbar^2}\frac{dV}{dx}\right|$$

— the force $\left|\frac{dV}{dx}\right|$ on the particle is small compared to $\frac{(\hbar k)^2}{m}k$ — the quantity with dimensions of force we can build out of $\hbar, k, m$

Formally, we can regard this as a small $\hbar$ approximation:

$$\hbar \left|\frac{m}{p^3}\frac{dV}{dx}\right| \ll 1$$

and quantum effects can be systematically studied in a power series expansion in $\hbar$ — the WKB or semiclassical expansion. (In the case of tunneling, the leading behavior for $\hbar$ small $\sim e^{-A/\hbar}$ — which vanishes as $\hbar \to 0$ faster than any power — but these effect can also be studied using the WKB method.) for $A \gg \hbar$

Note that for an abrupt step, the WKB approximation is maximally bad, and that is why we did not observe classical behavior for a wave packet reflecting from a step

We want to solve the time-independent Schrodinger equation

$$-\hbar^2\frac{\partial^2}{\partial x^2}\varphi = p^2(x)\varphi \qquad p^2(x) = 2m\,(E-V(x))$$

Write the solution as $\psi(x) = e^{iS(x)/\hbar}$

S(x) can be complex

Then $\dfrac{\partial \psi}{\partial x} = \frac{i}{\hbar} S'(x)\, e^{iS(x)/\hbar}$

$$\frac{\partial^2 \psi}{\partial x^2} = \left(-\frac{1}{\hbar^2} S'^2 + \frac{i}{\hbar} S''\right) e^{iS(x)/\hbar}$$

So $S(x)$ must satisfy

$$-\hbar^2\left(-\frac{1}{\hbar^2} S'^2 + \frac{i}{\hbar} S''\right) = p^2(x)$$

or $$\boxed{S'^2 - i\hbar S'' = p^2}$$

This is just a rewriting of the Schrodinger equation, but convenient because the second term on the LHS is small compared to the first if the WKB approximation is good. We will solve as a power series expansion in $\hbar$

$$S = S_0 + \hbar S_1 + \frac{\hbar^2}{2} S_2 + \cdots$$

In lowest order

$$S_0' = \pm p \quad \Rightarrow \quad S_0 = \pm \int^x p(x)\,dx + \text{const}$$

The leading order WKB soln is

$$\psi(x) = A\, e^{\frac{i}{\hbar}\int^x p(x)\,dx} + B\, e^{-\frac{i}{\hbar}\int^x p(x)\,dx}$$

— Like the free particle soln, but with a slowly varying p...

Next order, we match terms that are linear order in $\hbar$

$$2\hbar S_0' S_1' - i\hbar S_0'' = 0$$

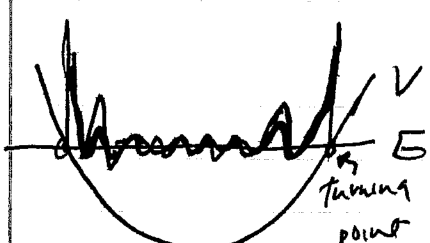
This determines S_1 as $S_1' = \frac{i}{2}\frac{S_0''}{S_0'} = \frac{i}{2}\frac{d}{dx}\ln|S_0'|$

$\Rightarrow \quad S_1 = \frac{i}{2}\ln|S_0'| + \text{constant} = \frac{i}{2}\ln|p| + \text{const}$

And $\quad e^{iS_1} \doteq C e^{-\frac{1}{2}\ln|p|} = \frac{C}{\sqrt{|p(x)|}}$

So including the next to leading semiclassical correction, we have a solution

$$\varphi(x) = \frac{1}{\sqrt{K(x)}}\left[A e^{i\int^x K dx} + B e^{-i\int^x K dx}\right]$$



This is like the free particle solution, but with amplitude $\propto K^{-\frac{1}{2}}$ -- small amplitude where wavelength is small

Interpretation $\quad |\varphi|^2 \sim \frac{1}{K} \propto \frac{m}{\hbar K} \sim \frac{1}{v}$

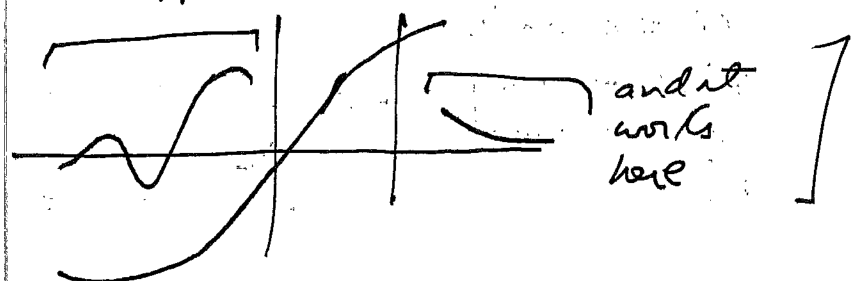
So $\quad P dx \propto \frac{dx}{v} = dt$

Probability of finding particle near x is proportional to time it spends there

(Since this is a stationary state, probability flux is constant - i.e. x-independent, and $J \equiv v|\varphi|^2$ means $|\varphi|^2 \sim \frac{1}{v}$)

Our WKB solution actually <u>blows up</u> at the classical turning point, where $v \to 0$.
But we should not take this seriously.
The approximation works for small $\lambda(x) = 2\pi/k(x)$
— but $\lambda(x) \to \infty$ at the turning point —
the approximation breaks down.

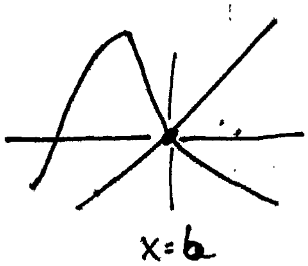
WKB works here



But can we <u>match</u> the two solutions across the turning point?

In fact, we <u>can</u>. But before we do, let's see why this is important by considering how WKB solutions are applied...

What we will show is that if the turning point is at $x = b$,



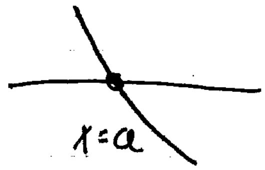
then the exponentially decaying solution

$$\frac{1}{\sqrt{\kappa(x)}} \exp\left(-\int_b^x \kappa(x)\,dx\right)$$

continued across the turning point matches

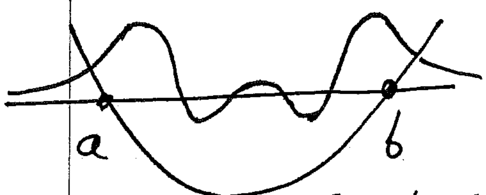
$$\frac{2}{\sqrt{k(x)}} \sin\left(\int_x^b k(x)\,dx + \pi/4\right)$$

on the other side



or $\frac{1}{\sqrt{K(x)}} \exp\left(\int_a^x K(x)\,dx \right)$

matches $\frac{2}{\sqrt{k(x)}} \sin\left(\int_a^x k(x)\,dx + \frac{\pi}{4} \right)$



The two decaying solutions have same sign if # of nodes is even; opposite sign if # of nodes is odd

These "connection formulas" tell us the conditions for a bound state in the WKB approximation - i.e. a solution that is exponentially decaying in both classically forbidden regions.

These two functions have to coincide up to a constant multiple

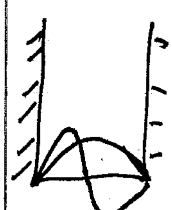
The two sine waves that match decaying solns agree up to a phase shift by π.

Since the sine function is odd, it works for

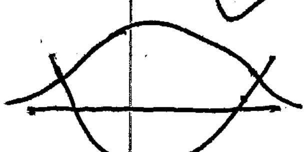
$$\frac{\pi}{4} + \int_a^x k\,dx = -\left(\frac{\pi}{4} + \int_x^b k\,dx \right) + \pi \cdot \text{integer}$$

$$\Rightarrow \int_a^b k\,dx = \pi\left(n + \tfrac{1}{2}\right)$$

(then two ways of calculating phase of wave at x agree)



For the ∞ly deep well, we needed to fit an integer no of half wavelengths into the well to have a bound state



But in the WKB approximation, we can remove an ~~extra~~ eighth of a wavelength from the vicinity of each turning point or a quarter of a wavelength all together

So the number of half wavelengths becomes integer + $\frac{1}{2}$
this becomes a good approximation for large n (short wavelength) as long as the potential is smooth.

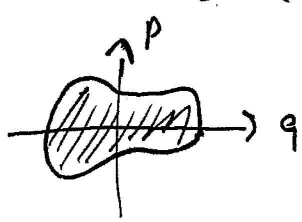
Lecture #17, 2002

The result is often stated as

$$\oint p\,dx = 2\pi\hbar\left(n+\tfrac{1}{2}\right)$$

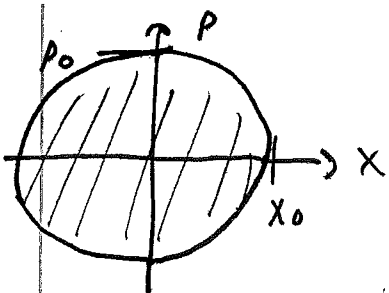
We can imagine that each quantum state occupies a cell in phase space, with area h

– Bohr-Sommerfeld quantization rule (integrating over a full orbit) – except B + S did not know about the $+\frac{1}{2}$



In terms of classical phase space – the quantity on the LHS is the area enclosed by the orbit (sometimes called the action) Action has the interesting property of being an adiabatic invariant – meaning that it remains unchanged if you vary the potential very slowly.. It therefore makes sense that the action is quantized... Slowly changing the potential should not excite the quantum system, or change its state.

In old quantum theory, h was called "quantum of action"



we can apply the Bohr-Sommerfeld rule to the harmonic oscillator

$$E = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2$$

$$\Rightarrow \quad p_0 = \sqrt{2mE} \qquad x_0 = \sqrt{\frac{2E}{m\omega^2}}$$

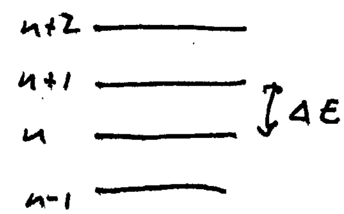
Recall area of an ellipse: $\quad A = \pi a b = \pi\left(2mE \cdot \frac{2E}{m\omega^2}\right)^{\frac{1}{2}}$

$$= \frac{2\pi E}{\omega} = 2\pi\hbar\,(n+\tfrac{1}{2})$$

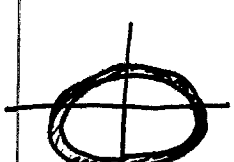
$$\Rightarrow \quad E = \hbar\omega\,(n+\tfrac{1}{2})$$

- the semiclassical energies coincide with the exact energy eigenvalues. This is just an accident, and will not be true for other potentials -- But this behavior will be seen for any smooth potential for sufficiently large n, if there are many bound states

What about the spacing in energy between the levels - how much does E increase when n increases by 1?



$$2\pi\hbar = \Delta\left(\oint p\,dx\right) = \Delta E \oint \frac{\partial p}{\partial E}\,dx + \text{higher order in } \Delta E$$



$$\text{and } \frac{\partial E}{\partial p} = \frac{p}{m} = v \Rightarrow 2\pi\hbar = \Delta E \oint \frac{dx}{v}$$

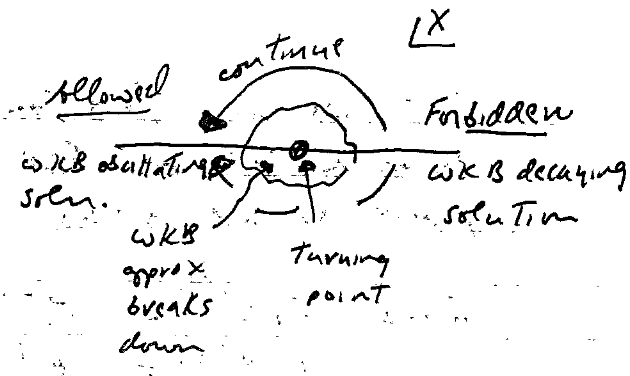
$$= \Delta E \oint dt = (\Delta E)\,T$$

$$\text{or } \Delta E = \frac{2\pi}{T}\hbar = \hbar\omega$$

- Not just for an oscillator but for any 1D potential.

cf. correspondence principle $\quad \underline{\updownarrow}\ \Delta E = \hbar\omega_\gamma$ ← circ. freq. of emitted photon

WKB Connection Formula



WKB approx breaks down near turning pt.

But we can continue around turning point in complex x-plane to find oscillating solution in allowed region that matches decaying solution in allowed region

In forbidden region $\frac{1}{\sqrt{K(x)}} \exp\left(-\int_b^x K(x)\,dx\right)$

where $K(x) = \frac{\sqrt{2m}}{\hbar}\left[V(x) - E\right]^{\frac{1}{2}}$ positive square root

This matches

$$\frac{C_1 e^{i\varphi_1}}{\sqrt{k(x)}} \exp\left(i\int_b^x k(x)\,dx\right) + \frac{C_2 e^{i\varphi_2}}{\sqrt{k(x)}} \exp\left(-i\int_b^x k(x)\,dx\right)$$

where $k(x) = \frac{\sqrt{2m}}{\hbar}\left[E - V(x)\right]^{\frac{1}{2}}$

positive square root.

When we continue in the upper half plane,

$-K(x)$ becomes $-ik(x)$

$\frac{1}{\sqrt{K(x)}}$ becomes $e^{-i\pi/4}\frac{1}{\sqrt{k(x)}}$

When we continue in the lower half plane

$-K(x)$ becomes $ik(x)$

$\frac{1}{\sqrt{K(x)}}$ becomes $e^{i\pi/4}\frac{1}{\sqrt{k(x)}}$

Why don't the two ways of continuing agree? It is because, in each half plane one of the exponentials becomes exponentially small compared to the other, and is lost in the leading WKB approx.

But we can legitimately find the coef of one exponential or the other by continuing in one half plane or the other

Thus $c_2 e^{i\varphi_2} = e^{-i\pi/4}$
$c_1 e^{i\varphi_1} = e^{i\pi/4}$

$$\frac{1}{\sqrt{K(x)}} \exp\left(-\int_b^x K(x)\,dx\right) \quad \text{continues to}$$

$$\frac{1}{\sqrt{K(x)}}\left(\exp\left(-i\int_b^x K(x)\,dx - i\pi/4\right) + \exp\left(i\int_b^x K(x)\,dx + i\pi/4\right)\right)$$

$$= \frac{2}{\sqrt{K(x)}} \cos\left(\int_b^x K(x)\,dx + \pi/4\right)$$

$$= \frac{2}{\sqrt{K(x)}} \cos\left(-\int_x^b K(x)\,dx - \pi/4\right) \quad \text{(reversing limits of integration)}$$

$$= \frac{2}{\sqrt{K(x)}} \sin\left(\int_x^b K(x)\,dx + \pi/4\right)$$

i.e. $\cos\left(\frac{\pi}{4} + A\right) = \sin\left(\frac{\pi}{2} - \frac{\pi}{4} - A\right)$
$= \sin(\pi/4 - A)$