Chapter 9 The WKB Approximation (semiclassical)

We know that if we have a flat potential the

$\psi(x) = A e^{ikx} + B e^{-ikx}$ where $\frac{\hbar^2 k^2}{2m} = KE$

$k = \sqrt{2m(E-V)}/\hbar$

For the case of a flat potential but $KE < 0$ (see Secs. 2.5 + 2.6

$\psi(x) = \alpha e^{-\kappa x} + \beta e^{\kappa x}$ where $\frac{\hbar^2 \kappa^2}{2m} = -KE$

$\kappa = \sqrt{2m(V-E)}/\hbar$

What does the wave function look like when your situation is nearly classical?

Look at highly excited wave functions

How to get approximate wave functions that reproduce the features: faster oscillation in space when $KE(x)$ is larger and smaller amplitude where $KE(x)$ is larger?

This can be derived using a phase amplitude method (Milne method [my first paper where I'm 1st author!])

The Schrodinger equation is

$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)$

$\frac{d^2\psi(x)}{dx^2} + k^2(x)\psi(x) = 0$

$\hbar^2 k^2(x)/2m = E - V(x) = KE(x)$

Define $\psi(x)$ using an amplitude and a phase

$\psi(x) \equiv A(x) e^{i\phi(x)}$

To get the equation for $A(x)$ and $\phi(x)$, substitute into the Schrodinger eq.

$$\psi' = (A' + i\phi' A) e^{i\phi}$$
$$\psi'' = (A'' + i\phi'' A + 2i\phi' A' - (\phi')^2 A) e^{i\phi}$$

Substitute back into the Sch. eq

$$A'' - (\phi')^2 A + i[\phi'' A + 2\phi' A'] = -k^2(x) A$$

This is one equation with two unknown functions. Need to impose another condition to define the A and ϕ.

The condition that I've always seen chosen is both A and ϕ are real.

$$A''(x) + k^2(x) A(x) - (\phi'(x))^2 A(x) = 0$$

$$\phi''(x) A(x) + 2\phi'(x) A'(x) = ([\phi'(x) A^2(x)]')/A(x) = 0$$

These equations do <u>not</u> define the A and ϕ. For example, choose $\phi(x) = 0$. The 2^{nd} equation is automatically satisfied and the 1^{st} equation becomes $A''(x) + k^2(x) A(x) = 0$ is the Schrodinger eq.

The Milne equation for A results by setting

$\phi'(x) = C^2 / A^2(x)$ this implies $A''(x) + k^2(x) A(x) = C^4 / A^3(x)$

The WKB approximation comes from setting $A''(x) \simeq 0$

This gives $A(x) \simeq \frac{C}{\sqrt{k(x)}}$ $\Rightarrow$ $\phi'(x) = k(x) = \sqrt{2m(E - V(x))}/\hbar$

This is a very good approximation when the position is <u>not</u> near a classical turning point.

The derivation did not depend on right/left moving particles.

$$\psi(x) \simeq \frac{1}{\sqrt{k(x)}} [C_+ e^{i\phi(x)} + C_- e^{-i\phi(x)}]$$

$$\simeq \frac{1}{\sqrt{k(x)}} [C_s \sin(\phi(x)) + C_c \cos(\phi(x))]$$

Example: An infinite square well has a small linear force added.

$$V(x) = F\cdot x \qquad 0 \le x \le a$$
$$= \infty \qquad x<0 \text{ or } x>a$$

Must have $\psi(0)=0 \Rightarrow \quad \psi(x) = \frac{C}{\sqrt{k(x)}} \sin\left[\int_0^x k(x')dx'\right]$

Get expression for $k(x) = \sqrt{2m(E_n - Fx)}/\hbar = \sqrt{k_n^2 - \beta x}$

$$k_n^2 = \frac{2mE_n}{\hbar^2} \qquad \beta = \frac{2mF}{\hbar^2}$$

Integrate $k(x)$ $\quad \int_0^x \sqrt{k_n^2 - \beta x'}\, dx' = \frac{-2}{3\beta}\left(k_n^2 - \beta x'\right)^{3/2}\Big|_0^x$

How to find the eigenstates? $\quad \psi(a)=0 \Rightarrow \phi(a) = n\pi$

$$\phi(a) = -\frac{2}{3\beta}\left[\left(k_n^2 - \beta a\right)^{3/2} - k_n^3\right] = \frac{2}{3\beta}\left[k_n^3 - k_n^3\left(1-\frac{\beta a}{k_n^2}\right)^{3/2}\right] = n\pi$$

This is a transcendental equation that must be solved numerically.
If the semiclassical approximation is good, then $\beta a/k_n^2 \ll 1$
Taylor series expansion

$$(1-x)^{3/2} = 1 - \frac{3}{2}x + \frac{3}{8}x^2 + \frac{x^3}{16} \cdots$$

$$\phi(a) \simeq \frac{2}{3\beta}k_n^3\left[1 - \left(1 - \frac{3}{2}\frac{\beta a}{k_n^2} + \frac{3}{8}\frac{\beta^2 a^2}{k_n^4}\cdots\right)\right] = k_n a - \frac{1}{4}\frac{\beta a^3}{k_n a} = n\pi$$

$$k_n \simeq \frac{n\pi}{a} + \frac{1}{4}\frac{\beta a^2}{n\pi} \Rightarrow E_n \simeq \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2\pi^2}{2ma^2} + \frac{\hbar^2}{2m}\left(\frac{1}{2}\beta a\right) = \frac{\hbar^2 n^2\pi^2}{2m} + \frac{\hbar^2}{2m}\frac{1}{2}\frac{2mF}{\hbar^2}a$$
$$= E_n^{(0)} + \frac{1}{2}Fa$$

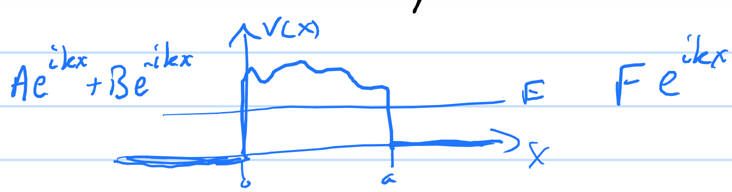
This is what you get from 1st order perturbation theory

If the x-region has $p^2(x) < 0$ (negative KE), then the wave function is a superposition of exponentially increasing and decreasing functions

$$\psi(x) \simeq \frac{C}{(-p^2(x))^{1/4}} e^{+\int\sqrt{-p^2(x)}\,dx/\hbar} + \frac{D}{(-p^2(x))^{1/4}} e^{-\int\sqrt{-p^2(x)}\,dx/\hbar}$$

Suppose the potential has some shape where $E < V(x)$

Scattering example



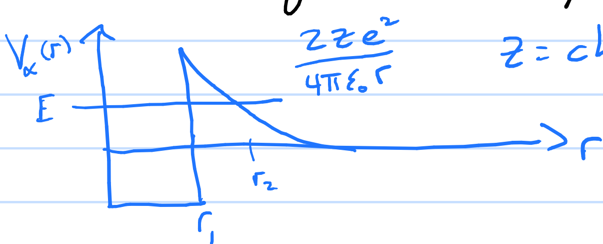
If the region between 0 and a is broad or $\sqrt{-p^2(x)}$ is large, then the coefficient in front of the exponentially increasing function is small

Refl Prob $= \left|\frac{B}{A}\right|^2$ Transm Prob $= \left|\frac{F}{A}\right|^2 \equiv T$

At this level of approximation $\left|\frac{F}{A}\right| \simeq e^{-\int_0^a \sqrt{-p^2(x)}\,dx/\hbar}$

$T = e^{-2\gamma}$ $\gamma \simeq \int_0^a \sqrt{-p^2(x)}\,dx/\hbar$

The most famous example is Gamow's theory of α-decay.



Z = charge left

$$\gamma = \frac{1}{\hbar}\int_{r_1}^{r_2} \sqrt{2m\left(\frac{e^2\,2Z}{4\pi\varepsilon_0 r} - E\right)}\,dr = \frac{\sqrt{2mE}}{\hbar}\int_{r_1}^{r_2}\sqrt{\frac{r_2}{r}-1}\,dr \qquad E = \frac{2Ze^2}{4\pi\varepsilon_0 r_2}$$

$$r = r_2 \sin^2 u \qquad \sqrt{\frac{r_2}{r}-1} = \left(\frac{1-\sin^2 u}{\sin^2 u}\right)^{1/2} = \frac{\cos u}{\sin u} \qquad dr = r_2\, 2\sin u \cos u\, du$$

$$\gamma = \frac{\sqrt{2mE}}{\hbar}\,2r_2\int_{\operatorname{asin}(\sqrt{r_1/r_2})}^{\pi/2} \cos^2 u\,du = \frac{\sqrt{2mE}}{\hbar}\,r_2 \int_{\operatorname{asin}(\sqrt{r_1/r_2})}^{\pi/2} 1+\cos 2u\,du$$

$$= \frac{\sqrt{2mE}}{\hbar}\,r_2\left[\frac{\pi}{2} - \operatorname{asin}\left(\sqrt{\frac{r_1}{r_2}}\right) - \frac{1}{2}\sin\left(2\operatorname{asin}\left(\sqrt{\frac{r_1}{r_2}}\right)\right)\right]$$

$$\sin\left(\operatorname{asin}\sqrt{\frac{r_1}{r_2}}\right)\sqrt{1-\sin^2\left(\operatorname{asin}\sqrt{\frac{r_1}{r_2}}\right)}$$

$$= \frac{\sqrt{2mE}}{\hbar}\,r_2\left[\frac{\pi}{2} - \operatorname{asin}\left(\sqrt{\frac{r_1}{r_2}}\right) - \sqrt{\frac{r_1}{r_2}}\sqrt{1-\frac{r_1}{r_2}}\right]$$

$$\simeq \frac{\sqrt{2mE}}{\hbar}\left[\frac{\pi}{2}r_2 - 2\sqrt{r_1 r_2}\right] \qquad \text{used } r_1 \ll r_2$$

$$= K_1 Z/\sqrt{E} - K_2\sqrt{Z r_1} \qquad K_1 = \frac{e^2}{4\pi\varepsilon_0}\frac{\pi\sqrt{2m}}{\hbar} = 1.980\ \text{MeV}^{1/2}$$
$$K_2 = \left(\frac{e^2}{4\pi\varepsilon_0}\right)^{1/2}\frac{4\sqrt{m}}{\hbar} = 1.485\ \text{fm}^{-1/2}$$

To get the lifetime, think semiclassically: the α particle will hit the barrier with a period $2r_1/v$ and, each time it hits, it has a probability $e^{-2\gamma}$ to go through.

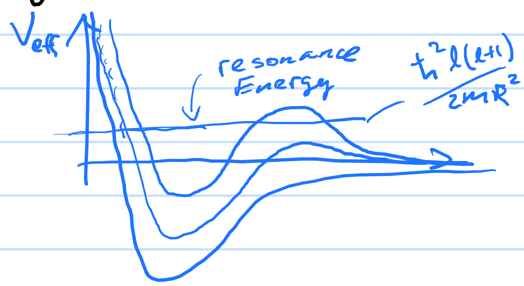
Lifetime $\tau \simeq \frac{2r_1}{v}e^{2\gamma}$

See plots

A similar effect happens in electron-molecule or atom-atom etc scattering. The short range potential (few Å) is very attractive. As the system goes to higher ℓ, the effective potential

$V_{eff}(r) = V(r) + \hbar^2 \ell(\ell+1)/2MR^2$

can get an inner well. "Shape resonance"



Another important example is the tunnel ionization of electrons pulled from atom/molecule in strong electric field. Very important in strong, low frequency laser.

One of the important questions is how to connect the classically allowed region to the classically not-allowed region. The derivation below takes a slightly different method from the book but has less restrictions.

The problem with the WKB approximation is it uses sin/cos or exponentials to carry the info about how Ψ should oscillate or diverge/converge.

$\Psi(x) = A(x)\, Y(\phi(x))$ in WKB $Y(\phi) = e^{\pm i\phi}$

The $Y(\phi)$ is defined by $\frac{d^2Y}{d\phi^2} + K^2(\phi)Y(\phi) = 0$

Choose the Y so that $K^2(\phi)$ has the same behavior as $k^2(x)$ but is simpler so that the Y are known

Use $A_x \equiv \frac{\partial A}{\partial x}$ and $Y_\phi \equiv \frac{\partial Y}{\partial \phi}$ etc.

$$\Psi_x = A_x Y + A Y_\phi \phi_x$$
$$\Psi_{xx} = A_{xx} Y + 2A_x Y_\phi \phi_x + A Y_{\phi\phi} \phi_x^2 + A Y_\phi \phi_{xx}$$

Schrodinger's Eq: $A_{xx} Y + 2A_x Y_\phi \phi_x - AYK^2 \phi_x^2 + AY_\phi \phi_{xx} + k^2 AY = 0$

As with the substitution, there are 2 unknown functions and one equation. Make the choice that the coefficient of Y and of Y_ϕ are separately 0.

Generalized Milne equations

$$A_{xx} + A\left(k^2 - K^2\phi_x^2\right) = 0 \qquad 2A_x\phi_x + A\phi_{xx} = \frac{1}{A}\frac{d}{dx}\left(A^2\phi_x\right) = 0$$

$$K^2(\phi)\left(\frac{d\phi}{dx}\right)^2 = k^2(x) \quad \underline{\underline{\text{Approx}}} \qquad A = \frac{C}{\sqrt{d\phi/dx}} \quad \text{Same form as WKB}$$

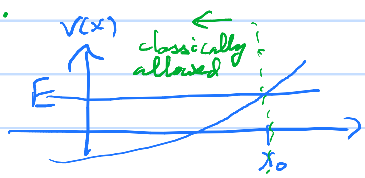
WKB: $K^2(\phi) = 1$ if $k^2(x) > 0$ $\quad Y = e^{\pm i\phi}$

$\qquad\qquad = -1$ if $k^2(x) < 0$ $\quad Y = e^{\pm\phi}$

The equation for ϕ: $\underbrace{\int_{\phi_0}^{\phi}\sqrt{\pm K^2(\phi')}\,d\phi' = \int_{x_0}^{x}\sqrt{\pm k^2(x')}\,dx'}_{\text{transformation of variables}}$ $\left[\begin{array}{l} + \text{ with } + \\ - \text{ with } - \end{array}\right.$

Show WKB result.

Turning point



Choose $K^2(\phi) = -\phi$ $\qquad Y_{\phi\phi} - \phi Y = 0$

$Y(\phi) = A_i(\phi)$ or $B_i(\phi)$ (or linear combination)

$\phi >> 1 \qquad A_i(\phi) \simeq \frac{1}{2\sqrt{\pi}\,\phi^{1/4}}\,e^{-\frac{2}{3}\phi^{3/2}} \qquad B_i \simeq \frac{1}{\sqrt{\pi}\,\phi^{1/4}}\,e^{\frac{2}{3}\phi^{3/2}}$

$\phi << -1 \qquad A_i(\phi) \simeq \frac{1}{\sqrt{\pi}(-\phi)^{1/4}}\sin\left[\frac{2}{3}(-\phi)^{3/2} + \frac{\pi}{4}\right] \qquad B_i \simeq \frac{1}{\sqrt{\pi}(-\phi)^{1/4}}\cos\left[\frac{2}{3}(-\phi)^{3/2} + \frac{\pi}{4}\right]$

power series $\quad f(\phi) = 1 + \frac{1}{3!}\phi^3 + \frac{1\cdot 4}{6!}\phi^6 + \frac{1\cdot 4\cdot 7}{9!}\phi^9 + \ldots$

$\qquad g(\phi) = \phi + \frac{2}{4!}\phi^4 + \frac{2\cdot 5}{7!}\phi^7 + \frac{2\cdot 5\cdot 8}{10!}\phi^{10} + \ldots$

$A_i = C_1 f - C_2 g \qquad C_1 = 3^{-2/3}/\Gamma(2/3) = 0.35502\ 80538\ \ldots$

$B_i = \sqrt{3}\,(C_1 f + C_2 g) \qquad C_2 = 3^{-1/3}/\Gamma(1/3) = 0.25881\ 94037\ \ldots$

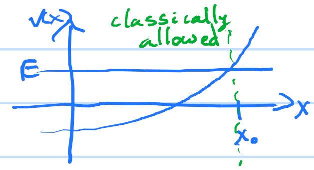
Look at plot of Airy functions

Apply the equations

$x > x_0$ and $\phi > 0 \qquad \int_0^{\phi}\sqrt{-K^2(\phi')}\,d\phi' = \int_0^{\phi}(\phi')^{1/2}d\phi' = \frac{2}{3}\phi^{3/2} = \int_{x_0}^{x}\left(-k^2(x')\right)^{1/2}dx'$

$x < x_0$ and $\phi < 0 \qquad \int_{\phi}^{0}\sqrt{K^2(\phi')}\,d\phi' = \int_{\phi}^{0}(-\phi')^{1/2}d\phi' = \frac{2}{3}(-\phi)^{3/2} = \int_{x}^{x_0}\left(k^2(x')\right)^{1/2}dx'$

Put it all together for the full solution



$$\psi(x) = \left(\frac{K^2(\phi)}{k^2(x)}\right)^{1/4}\left[C\, Ai(\phi(x)) + D\, Bi(\phi(x))\right]$$

Far from the turning pt., $|\phi| \gg 1$ so use the asymptotic form of the Airy functions to figure out what's going on

$x \gg x_0$ $$\psi(x) = \frac{\cancel{\phi^{1/4}}}{(-k^2(x))^{1/4}}\frac{1}{\sqrt{\pi}\,\cancel{\phi^{1/4}}}\left[\tfrac{1}{2} C\, e^{-\int_{x_0}^{x}(-k^2(x'))^{1/2}dx'} + D\, e^{\int_{x_0}^{x}(-k^2(x'))^{1/2}dx'}\right]$$

$x \ll x_0$ $$\psi(x) = \frac{\cancel{(-\phi)^{1/4}}}{(k^2(x))^{1/4}}\frac{1}{\sqrt{\pi}\,\cancel{(-\phi)^{1/4}}}\left\{C \sin\left[\int_x^{x_0} k(x')dx' + \tfrac{\pi}{4}\right] + D\cos\left[\int_x^{x_0} k(x') + \tfrac{\pi}{4}\right]\right\}$$

These are particular combinations of the WKB approximation but by using the Ai and Bi get more accurate results. Also get the connection between the classically allowed and not allowed regions. If the classically unallowed region goes to ∞, then $D=0$. Why? Compare to Eqs [8.46] of the book.

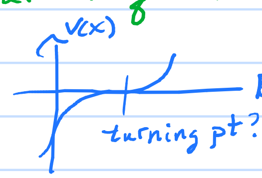
Does anything nasty happen near $x = x_0$

$$k^2(x) = \alpha_1(x-x_0) + \tfrac{1}{2}\alpha_2(x-x_0)^2 + \tfrac{1}{6}\alpha_3(x-x_0)^3 \ldots \qquad \alpha_1 < 0$$

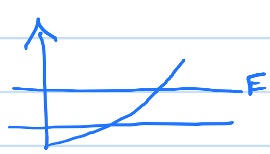
$x > x_0$ $$\tfrac{2}{3}\phi^{3/2} = \int_{x_0}^{x}\left(-k^2(x')\right)^{1/2}dx' = (-\alpha_1)^{1/2}\int_{x_0}^{x}(x'-x_0)^{1/2}\left[1 - \frac{\alpha_2}{2\alpha_1}(x'-x_0) - \frac{\alpha_3}{6\alpha_1}(x'-x_0)^2 \ldots\right]^{1/2}dx'$$
$$= (-\alpha_1)^{1/2}\int_{x_0}^{x}(x'-x_0)^{1/2} - \frac{\alpha_2}{4\alpha_1}(x'-x_0)^{3/2} \ldots dx'$$
$$= (-\alpha_1)^{1/2}\left[\tfrac{2}{3}(x-x_0)^{3/2} - \tfrac{2}{5}\frac{\alpha_2}{4\alpha_1}(x-x_0)^{5/2} \ldots\right]$$
$$\phi = (-\alpha_1)^{1/3}(x-x_0)\left[1 - \frac{3\alpha_2}{20\alpha_1}(x-x_0) \ldots\right]^{2/3}$$
$$= (-\alpha_1)^{1/3}(x-x_0)\left[1 - \frac{\alpha_2}{10\alpha_1}(x-x_0) \ldots\right] = \text{linear} + \text{quadratic} + \ldots$$

Same eq. from $x < x_0$

Nothing bad happens unless $\alpha_1 \approx 0$



Suppose you have a potential like



well with ∞ wall at $x=0$

We know that $D=0$ and $\psi(0)=0$

The eigenstates are found for

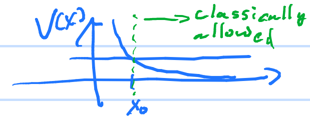
$$Ai(\phi(0)) = 0$$

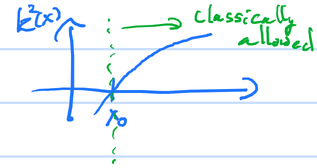
If we use the asymptotic form of the Ai function

$$\sin\left(\int_0^{x_0} k(x')dx' + \tfrac{\pi}{4}\right) = 0 \Rightarrow \int_0^{x_0} k(x)dx = (n - \tfrac{1}{4})\pi$$

determines the eigenenergies

What about the case





Choose $K^2(\phi) = \phi$ $\qquad Y_{\phi\phi} - \phi Y = 0$

$Y(\phi) = Ai(-\phi)$ or $Bi(-\phi)$ (or linear combination)

Apply the equations

$x < x_0$ and $\phi < 0$ $\qquad \int_\phi^0 \sqrt{-K^2(\phi')}\, d\phi' = \int_\phi^0 (-\phi')^{1/2} d\phi' = \frac{2}{3}(-\phi)^{3/2} = \int_x^{x_0} \sqrt{-k^2(x')}\, dx'$

$x > x_0$ and $\phi > 0$ $\qquad \int_0^\phi \sqrt{K^2(\phi')}\, d\phi' = \int_0^\phi (\phi')^{1/2} d\phi' = \frac{2}{3}\phi^{3/2} = \int_{x_0}^x \sqrt{k^2(x')}\, dx'$

Put it all together for the full solution

$$\psi(x) = \left(\frac{K^2(\phi)}{k^2(x)}\right)^{1/4} \left[A\ Ai(-\phi(x)) + B\ Bi(-\phi(x))\right]$$

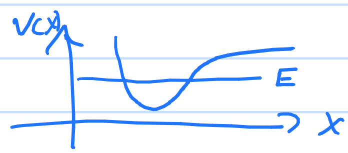
As before, far from the turning pt. $|\phi| \gg 1$, so we can use the asymptotic form of the Airy functions to figure out what's going on

$x \ll x_0 \qquad \psi(x) = \frac{1}{(-k^2(x))^{1/4}} \frac{1}{\sqrt{\pi}} \left[\frac{1}{2} A\, e^{-\int_x^{x_0}\sqrt{-k^2(x')}\, dx'} + B e^{\int_x^{x_0}\sqrt{-k^2(x')}\, dx'}\right]$

$x \gg x_0 \qquad \psi(x) = \frac{1}{(k^2(x))^{1/4}} \frac{1}{\sqrt{\pi}} \left\{A \sin\left[\int_{x_0}^x k(x')\, dx' + \frac{\pi}{4}\right] + B \cos\left[\int_{x_0}^x k(x')\, dx' + \frac{\pi}{4}\right]\right\}$

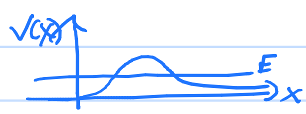
This completes the treatment of the case with 1 turning pt.

What to do with the case
$K^2(\phi) = 1 - \phi^2$



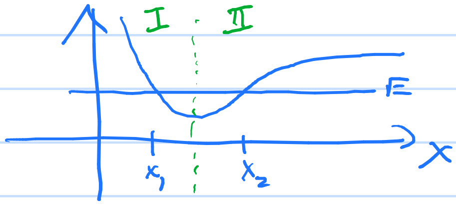
most bound state problems

What to do with the case
$K^2(\phi) = -1 + \phi^2$



reflection from a barrier

Instead of doing these special cases (parabolic cylinder functions), will just cobble together the Airy approximation in each region



Find WKB bound states for this case

$$\psi_I(x) = \left(\frac{\Phi_I(x)}{k^2(x)}\right)^{1/4} A\, Ai(-\Phi_I(x))$$

what happened to $Bi(-\Phi_I)$?

$$\psi_{II}(x) = \left(\frac{-\Phi_{II}(x)}{k^2(x)}\right)^{1/4} C\, Ai(\Phi_{II}(x))$$

what happened to $Bi(\Phi_{II})$?

$$\frac{2}{3}\left[\pm\Phi_I(x)\right]^{3/2} = \pm\int_{x_1}^{x}\sqrt{\pm k^2(x')}\,dx' \qquad + \Rightarrow x > x_1,\quad - \Rightarrow x < x_1$$

$$\frac{2}{3}\left[\pm\Phi_{II}(x)\right]^{3/2} = \pm\int_{x_2}^{x}\sqrt{\mp k^2(x)}\,dx' \qquad \text{upper } x > x_2,\quad \text{lower } x < x_2$$

How to get eigenvalues? The ψ_I and ψ_{II} should be the same in the classically allowed region. From asymptotic approximation

$$A\sin\left[\int_{x_1}^{x} k(x')dx' + \frac{\pi}{4}\right] = C\sin\left[\int_{x}^{x_2} k(x')dx' + \frac{\pi}{4}\right]$$

$A = \pm C$

Use $$\int_{x}^{x_2} k(x')dx' + \frac{\pi}{4} = \underbrace{\int_{x_1}^{x_2} k(x')dx' + \frac{\pi}{2}}_{\Delta} - \Big[\underbrace{\int_{x_1}^{x} k(x')dx' + \frac{\pi}{4}}_{\Theta(x)}\Big] \equiv \Delta - \Theta(x)$$

$$\sin[\Theta(x)] = \mp\sin[\Theta(x) - \Delta] = \mp\sin[\Theta(x)]\cos(\Delta) \pm \cos[\Theta(x)]\sin(\Delta)$$

This equation can only be satisfied if $\sin(\Delta) = 0$

$$\Delta = \int_{x_1}^{x_2} k(x')dx' + \frac{\pi}{2} = n\pi \qquad n = 1, 2, \ldots$$

WKB Quantization $$\int_{x_1}^{x_2} k(x')dx' = \left(n - \tfrac{1}{2}\right)\pi \qquad n = 1, 2, \ldots$$

Example: In the limit of large n, show $E_{n+1} - E_n \cong h f_{cl}(E_{n+1/2})$ where $f_{cl}(E)$ is the classical frequency at energy E.

$$\frac{E_{n+1} - E_n}{n+1-n} \simeq \left.\frac{dE}{dn}\right|_{n+1/2}$$

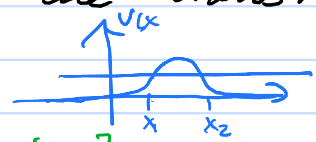
Take derivative of WKB $$\frac{d}{dn}\int_{x_1}^{x_2}\sqrt{\frac{2m}{\hbar^2}}\,(E - V(x))^{1/2}dx = \frac{d}{dn}\left[\left(n - \tfrac{1}{2}\right)\pi\right] = \pi$$

$$= \frac{dE}{dn}\,\frac{1}{2}\sqrt{\frac{2m}{\hbar^2}}\int_{x_1}^{x_2}\frac{1}{\sqrt{E - V(x)}}dx = \frac{1}{\hbar}\frac{dE}{dn}\int_{x_1}^{x_2}\frac{1}{\sqrt{\frac{2}{m}(E - V(x))}}dx$$

$$= \frac{1}{\hbar}\frac{dE}{dn}\int_{x_1}^{x_2}\frac{1}{v(x)}dx = \frac{1}{\hbar}\frac{dE}{dn}\,\frac{T}{2} \quad \leftarrow \text{period}$$

Move to right hand side $$\frac{dE}{dn} = 2\pi\hbar\frac{1}{T} = h f(E_{n+1/2})$$ ✓✓

Prob 9.11 Find the WKB approx to the transmission and reflection through a barrier.



What kind of wave function in each region?

slightly change from Book

$$\psi(x) = \frac{1}{\sqrt{k(x)}}\left[A e^{-i\int_x^{x_1} k(x')\,dx'} + B e^{i\int_x^{x_1} k(x')\,dx'} \right] \qquad x < x_1$$

which is left/right going

$$\frac{1}{(-k^2(x))^{1/4}}\left[C e^{-\int_x^{x_2}\sqrt{-k^2(x')}\,dx'} + D e^{\int_x^{x_2}\sqrt{-k^2(x')}\,dx'} \right] \qquad x_1 < x < x_2$$

which is exp increasing as x increases

$$\frac{1}{\sqrt{k(x)}} F e^{i\int_{x_2}^{x} k(x')\,dx'}$$

Look at the wave fct from pg 8 of notes

$$B_{pg8} = e^{-i\pi/4} F\sqrt{\pi} \qquad A_{pg8} = i B_{pg8} = i e^{-i\pi/4} F\sqrt{\pi}$$

$$C = \frac{A_{pg8}}{2}\sqrt{\pi} = \frac{1}{2} i e^{-i\pi/4} F\sqrt{\pi} \qquad D = B_{pg8}\sqrt{\pi} = e^{-i\pi/4} F\sqrt{\pi}$$

Now look at pg 7 notes

$$\gamma = \int_{x_1}^{x_2}\sqrt{-k^2(x')}\,dx'$$

$$D_{pg7}\, e^{\gamma} = C\sqrt{\pi} = \frac{1}{2} i e^{-i\pi/4} F \qquad \frac{1}{2} C_{pg7} e^{-\gamma} = D\sqrt{\pi} = e^{-i\pi/4} F$$

$$D_{pg7} = \frac{1}{2} i e^{-i\pi/4} e^{-\gamma} F \qquad C_{pg7} = 2 e^{-i\pi/4} e^{\gamma} F$$

$$C_{pg7} \sin\left[\int_x^{x_1} k(x')\,dx' + \frac{\pi}{4}\right] + D_{pg7} \cos\left[\int_x^{x_1} k(x')\,dx' + \frac{\pi}{4}\right]$$

$$= \underbrace{\frac{1}{2}\left(D_{pg7} + i C_{pg7}\right) e^{-i\pi/4}}_{A} e^{-i\int_x^{x_1} k(x')\,dx'} + \underbrace{\frac{1}{2}\left(D_{pg7} - i C_{pg7}\right) e^{i\pi/4}}_{B} e^{i\int_x^{x_1} k(x')\,dx'}$$

$$A = \frac{1}{2} e^{-i\pi/2}\, i \left(\frac{e^{-\gamma}}{2} + 2e^{\gamma}\right) F \qquad B = \frac{1}{2} i \left(\frac{e^{-\gamma}}{2} - 2e^{\gamma}\right) F$$

$$T = \left|\frac{F}{A}\right|^2 = \frac{4}{\left(4e^{2\gamma} + 2 + \frac{1}{4}e^{-2\gamma}\right)} = \frac{e^{-2\gamma}}{\left(1 + \frac{e^{-2\gamma}}{2} + \frac{1}{16}e^{-4\gamma}\right)}$$

$$R = \left|\frac{B}{A}\right|^2 = \frac{1 - \frac{1}{2}e^{-2\gamma} + \frac{1}{16}e^{-4\gamma}}{1 + \frac{1}{2}e^{-2\gamma} + \frac{1}{16}e^{-4\gamma}} \qquad R + T = 1 \checkmark$$

does this match expectation?

See footnote 16 on pg 371.

There's a problem applying WKB to the radial equation.

Eq 4.36 $\quad u(r) = r R(r) \qquad -\frac{\hbar^2}{2m}\frac{d^2 u_{n\ell}(r)}{dr^2} + \left(V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right) u_{n\ell}(r) = E\, u_{n\ell}(r)$

Suppose $V(r) r^2 \to 0$ as $r \to 0$, then the equation as $r \to 0$ is

$$\frac{d^2 u}{dr^2} = \frac{\ell(\ell+1)}{r^2} u \qquad u(r) = C\, r^{\ell+1} + D\, r^{-\ell}$$ which to choose?

Apply WKB at small r $\qquad k^2(r) = \frac{2m}{\hbar^2}\left[E - V(r) - \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right]$

$$u(r) = \frac{1}{(-k^2(r))^{1/4}}\left[C\, e^{\int^r \sqrt{-k^2(r')}\,dr'} + D\, e^{-\int^r \sqrt{-k^2(r')}\,dr'}\right]$$

$$k^2(r) \simeq -\frac{\ell(\ell+1)}{r^2} \quad \Rightarrow \quad \int^r \frac{\sqrt{\ell(\ell+1)}}{r'}\,dr' = \sqrt{\ell(\ell+1)}\,\ln r$$

Combine (and remember $e^{a\ln x} = e^{\ln(x^a)} = x^a$)

$$u(r) \propto r^{1/2}\left[C\, r^{\sqrt{\ell(\ell+1)}} + D\, r^{-\sqrt{\ell(\ell+1)}}\right] = C\, r^{\sqrt{\ell(\ell+1)}+1/2} + D\, e^{-\sqrt{\ell(\ell+1)}+1/2}$$

The WKB for radial coordinate gives incorrect behavior at small r. The problem is that the condition for accurate WKB is violated at small r. We need to stretch the coordinate.

$r = e^s \qquad r \to 0$ as $s \to -\infty$ and $r \to \infty$ as $s \to \infty$

$$dr = e^s\, ds \quad \Rightarrow \quad \frac{d^2}{dr^2} = \frac{1}{e^s}\frac{d}{ds}\frac{1}{e^s}\frac{d}{ds}$$

The Sch. eq in terms of s $\qquad \frac{1}{e^s}\frac{d}{ds}\left(\frac{1}{e^s}\frac{du}{ds}\right) + k^2(e^s)\, u = 0$

This equation has both 1st and 2nd derivatives. The trick to get rid of the 1st derivative is to use

$u(s) = e^{s/2}\, w(s)$

$$\frac{du}{ds} = \frac{1}{2} e^{s/2} w(s) + e^{s/2}\frac{dw}{ds}$$

$$\frac{1}{e^s}\frac{d}{ds}\left[e^{-s}\frac{du}{ds}\right] = \frac{1}{e^s}\frac{d}{ds}\left(\frac{1}{2}e^{-s/2} w + e^{-s/2}\frac{dw}{ds}\right) = e^{-\frac{3}{2}s}\left[-\frac{1}{4} w(s) + \frac{d^2 w}{ds^2}\right]$$

The new equation is

$$\frac{d^2 w}{ds^2} + \left[e^{2s}\, k^2(e^s) - \frac{1}{4}\right] w = 0$$

This doesn't look like much of a change but it completely fixes the small r problem

$$e^{2s}\, k^2(e^s) - \frac{1}{4} = e^{2s}\left[k^2(e^s) - \frac{1}{4e^{2s}}\right] = e^{2s}\, \tilde{k}^2(e^s)$$

Now do the WKB approx for w

$$u = e^{s/2}\, w(s) = e^{s/2} \frac{1}{(-e^{2s}\tilde{k}^2(e^s))^{1/4}} \left[C e^{\int^{e^s} (-e^{2s'}\tilde{k}^2(e^{s'}))^{1/2} ds'} + D e^{-\int^{e^s} (-e^{2s'}\tilde{k}^2(e^{s'}))^{1/2} ds'} \right]$$

Carefully look at each term

Prefactor $\displaystyle \frac{e^{s/2}}{(-e^{2s}\tilde{k}^2(e^s))^{1/4}} = \frac{1}{(-\tilde{k}^2(e^s))^{1/4}}$

Integrals $\displaystyle \int^{e^s} (-e^{2s'}\tilde{k}^2(e^{s'}))^{1/2} ds' = \int^{e^s} (-\tilde{k}^2(e^{s'}))^{1/2} e^{s'} ds'$

$$= \int^{r} (-\tilde{k}^2(r'))^{1/2} dr'$$

The net effect of these manipulations is only to replace $k^2(r)$ with $\tilde{k}^2(r)$

$$\tilde{k}^2(r) = k^2(r) - \frac{1}{4r^2} = \frac{2m}{\hbar^2}\left[E - V(r) - \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right] - \frac{1}{4r^2}$$

$$= \frac{2m}{\hbar^2}\left[E - V(r) - \frac{\hbar^2(\ell+1/2)^2}{2mr^2}\right] \qquad \ell(\ell+1) + \frac{1}{4} = (\ell + 1/2)^2$$

The net effect is to replace $\ell(\ell+1) \longrightarrow (\ell+1/2)^2$

Check with the small r behavior

$$u(r) = C\, r^{\sqrt{(\ell+1/2)^2} + 1/2} + D\, r^{-\sqrt{(\ell+1/2)^2} + 1/2} = C\, r^{\ell+1} + D\, r^{-\ell}$$

Gives exact behavior at small r

Homework will show gives exact hydrogen energies