16.2 The Wentzel-Kramers-Brillouin (WKB) semiclassical method

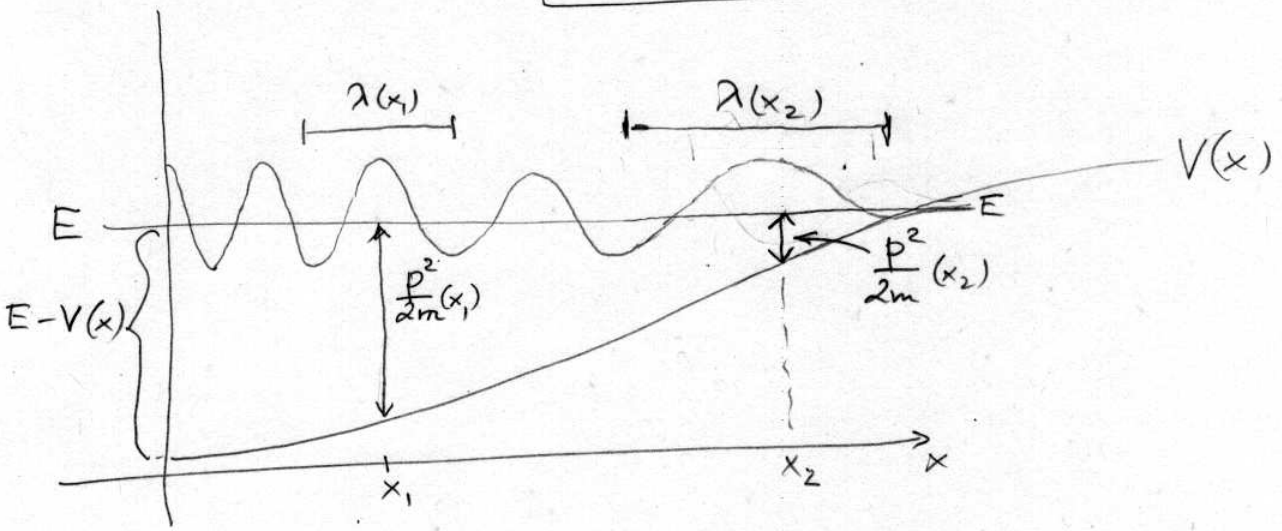
In a constant potential a particle of energy E moving in 1 dimension in a constant potential V has eigenfunction

$$\psi(x) = \psi(0)\, e^{\pm i p x/\hbar}, \qquad p = \sqrt{2m(E-V)}$$

The real and imaginary parts of ψ oscillate in space with wavelength

$$\lambda = \frac{2\pi}{k} = \frac{2\pi\hbar}{p}$$

Now, if the potential varies very slowly, such that its variation over a wavelength λ is small compared to $|E-V|$, then we expect the wavefunction to look like a slightly distorted plane wave, with slowly varying wavelength $\boxed{\lambda(x) = \frac{2\pi\hbar}{p(x)} = \frac{2\pi\hbar}{\sqrt{2m(E-V(x))}}}$:



Since λ varies with x, the accumulated phase between $x=0$ and x instead of $p \cdot x$ given by $\int_0^x p(x')\,dx'$, hence

$$\psi(x) = \psi(0)\, e^{\pm \frac{i}{\hbar}\int_0^x p(x')\,dx'}$$

or, more generally,

$$\boxed{\psi(x) = \psi(x_0)\, e^{\pm \frac{i}{\hbar}\int_{x_0}^{x} p(x')\,dx'}} \qquad (*)$$

(The general solution for a state of energy E is a linear combination of left- and right-moving such waves.)

This form of the wave function can be formally derived as follows (and this will elucidate the limitations of this approximation):

We want to solve

$$\left(\frac{d^2}{dx^2} + \underbrace{\frac{2m}{\hbar^2}[E - V(x)]}_{k^2(x) = \frac{p^2(x)}{\hbar^2}}\right)\psi(x) \equiv \left[\frac{d^2}{dx^2} + k^2(x)\right]\psi(x) = 0$$

Let us write $\psi(x) = e^{i\phi(x)/\hbar}$.

where $\phi(x)$ is complex,

and expand $\phi(x)$ in powers of $\hbar$:

$$\phi(x) = \phi_0(x) + \hbar\,\phi_1(x) + \hbar^2\phi_2(x) + \cdots \qquad (**)$$

$$\Rightarrow \left[\frac{d^2}{dx^2} + \frac{p^2(x)}{\hbar^2}\right] e^{i\phi(x)/\hbar} = \left[-\left(\frac{\phi'}{\hbar}\right)^2 + \frac{i\phi''}{\hbar} + \frac{p^2(x)}{\hbar^2}\right] e^{i\phi(x)/\hbar} = 0$$

As $\hbar \to 0$, the wavelength $\lambda = \frac{2\pi\hbar}{p}$ tends to zero; in this limit <u>any</u> potential can be considered "slowly varying" and the ansatz (*) should become increasingly accurate. Any correction to (*) thus must be due to $\hbar$ being not exactly zero. In situations where $\hbar$ can be considered a small number ($\to$ classical physics) we should be able to compute these corrections as a Taylor series in $\hbar$.

The "semiclassical" WKB approximation keeps only the first 2 terms in the expansion:

$$\phi(x) \cong \phi_0(x) + \hbar\,\phi_1(x):$$

If we plug (**) into our differential eq. for ϕ:

$$-\frac{(\phi_0' + \hbar\phi_1' + O(\hbar^2))^2}{\hbar^2} + \frac{i}{\hbar}\left(\phi_0'' + \hbar\phi_1'' + O(\hbar^2)\right) + \frac{p^2(x)}{\hbar^2} = 0 \quad | \cdot \hbar^2$$

$$-(\phi_0')^2 + p^2(x) + \hbar\left(i\phi_0'' - 2\phi_0'\phi_1'\right) + O(\hbar^2) = 0$$

This holds for any value of $\hbar$ if

$$\phi_0' = \pm p(x) \quad \Longrightarrow \quad \phi_0(x) = \phi_0(x_0) \pm \int_{x_0}^{x} p(x')\,dx'$$

and $i\phi_0'' = 2\phi_0'\phi_1' \quad \Rightarrow \quad \frac{\phi_0''}{\phi_0'} = -2i\phi_1'$

$$\Rightarrow \ln|\phi_0'| = -2i\phi_1 + c$$

$$\Rightarrow \phi_1 = \frac{i}{2}\ln|\phi_0'| + \frac{c}{2i} = i\ln\sqrt{|p(x)|} + \tilde{c}$$

Keeping terms only up to order $\hbar$, we get for the wave function

$$\psi(x) = e^{i\phi(x)/\hbar} = e^{i\phi_0(x)/\hbar} e^{\pm \frac{i}{\hbar}\int_{x_0}^{x} p(x')dx'} e^{-\ln\sqrt{|p(x)|} + \frac{C}{2}}$$

$$= \psi(x_0)\sqrt{\left|\frac{p(x_0)}{p(x)}\right|}\, e^{\pm i/\hbar \int_{x_0}^{x} p(x')dx'} \quad \text{(WKB)}$$

The propability density goes like $|\psi(x)|^2 \sim \frac{1}{|p(x)|} \sim \frac{1}{v(x)}$ as expected classically. If we had taken this requirement into account, we would have obtained the WKB wave function correctly normalised already on page (12) (instead of (*)).

The WKB approximation is valid as long as it is justified to ignore the terms $O(\hbar^2)$ in (**) in p. (12). Since we haven't worked out those terms, we will use instead the criterium that the term $\sim\hbar$ is much smaller than the term $\sim\hbar^0$. If that's the case, one is justified to assume that the terms $O(\hbar^2) \ll O(\hbar)$. So we look at

$$\frac{-(\phi_0')^2 + p^2(x)}{\hbar^2} + \frac{i\phi_0'' - 2\phi_0'\phi_1'}{\hbar} + O(\hbar^0) = 0$$

and require that the terms in the first term are much larger than the terms in the second term, etc.

$$\Rightarrow \left|\frac{\phi_0'}{\hbar}\right|^2 \gg \left|\frac{\phi_0''}{\hbar}\right| \qquad \left(p^2(x) = \phi_0',\ 2\phi_0'\phi_1' = i\phi_0''\right)$$

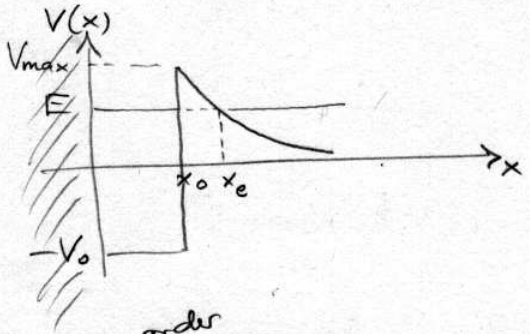
This can be written as

$$\hbar \left|\frac{d}{dx}\left(\frac{1}{\phi_0'}\right)\right| \leq 1 \quad \text{or} \quad \left|\frac{d}{dx}\left(\frac{\hbar}{p(x)}\right)\right| = \frac{1}{2\pi}\left|\frac{d\lambda}{dx}\right| \ll 1$$

just as we had heuristically argued at the beginning of this subsection.

Tunneling amplitudes

Consider a particle trapped in a potential:



In first order WKB approximation (i.e. ignoring the factor $\sqrt{\left|\frac{p(x_0)}{p(x_e)}\right|}$ which is not well-defined and requires a more careful study) we get

$$\psi(x_e) = \psi(x_0)\, e^{\frac{i}{\hbar}\int_{x_0}^{x_e} dx\ i\sqrt{2m(V(x)-E)}} \equiv \psi(x_0)\, e^{-\gamma/2}$$

for an outward-moving particle (since $E - V(x) < 0$ under the barrier, we pick up a factor i). The tunneling factor $e^{-\gamma}$ defined in this way is real.

The mean lifetime of the bound state against decay by tunneling through the barrier can be estimated as follows: Inside the well the particle has kinetic energy $T = E - V = E + V_0$, with classical velocity $v = \frac{\sqrt{2m(E+V_0)}}{m}$. Therefore it bangs its head against the outer wall with frequency $f = \frac{v}{2x_0}$. Each time this happens, it escapes with probability $e^{-\gamma}$. So the rate of successful escape attempts per second is

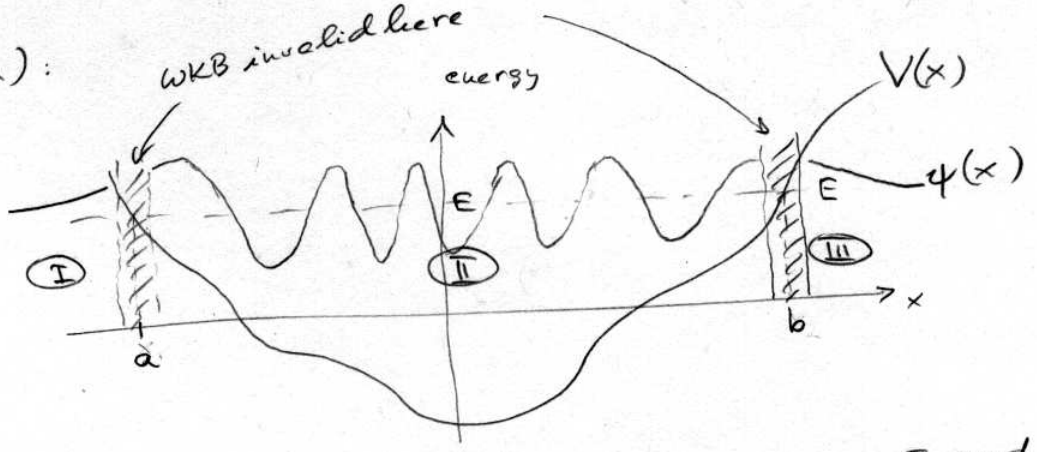
$$\frac{1}{N}\frac{dN}{dt} = R = \frac{\sqrt{2m(E+V_0)}}{m\,2x_0}\,e^{-\gamma}$$

The mean lifetime is $\tau = \frac{1}{R}$.

This type of calculation allows to compute the lifetime of α-emitting radioactive isotopes, as well as the fusion rates for hydrogen and deuterium to ^3He or ^4He in the center of the sun. For decays in which the α-particle emerges with nonzero orbital angular momentum, the centrifugal barrier must be added to the Coulomb potential for $V(x)$ under the barrier. Obviously, the decay rate drops exponentially with the barrier height $V_{max} - E$.

Bound states

We can use the WKB approximation for the wave function to obtain approximate energy eigenvalues for bound states. Consider a particle bound by a potential



We have the classically forbidden regions I and III, and the classically allowed region II. Near the classical turning points, the WKB wave function becomes invalid, since $\frac{1}{\sqrt{|p(x)|}}$ blows up. Formally, we can see the breakdown from the condition

$$\left|\frac{\psi_0''}{\hbar}\right| \ll \left|\frac{\psi_0'}{\hbar}\right|^2 \quad \Rightarrow \quad \hbar\left|\frac{d}{dx}p(x)\right| \ll |p(x)|^2 \qquad p(x)=\sqrt{2m(E-V(x))}$$

$$\Rightarrow \hbar\frac{2m\left|\frac{dV}{dx}\right|}{\left|\sqrt{2m(E-V(x))}\right|} \ll p^2(x)$$

$$\Rightarrow \boxed{\frac{\lambda(x)}{2\pi}\left|\frac{dV}{dx}\right| \ll \left|\frac{p^2(x)}{2m}\right| = |T(x)|}$$

which is violated near the classical turning points where $T(x)=0$ while $\left|\frac{dV}{dx}\right| \neq 0$ and $\lambda(x) \to \infty$.

On the other hand we can use WKB both in region II and regions I, III if we stay far

enough away from the turning points (even though $p(x)$ is imaginary in regions I and III). In these regions we have

$$\psi_I(x) \sim \frac{1}{\sqrt{2m(V(x)-E)}}\, e^{-\frac{1}{\hbar}\int_x^a \underbrace{\sqrt{2m(V(x')-E)}}_{\kappa(x')}\, dx'}$$

$$\psi_{III}(x) \sim \frac{1}{\sqrt{2m(V(x)-E)}}\, e^{-\frac{1}{\hbar}\int_b^x dx' \underbrace{\sqrt{2m(V(x')-E)}}_{\kappa(x')}} \qquad (*)$$

$$\psi_{II}(x) = \frac{A}{\sqrt{2m(E-V(x))}} \cos\left(\frac{1}{\hbar}\int_a^x \underbrace{\sqrt{2m(E-V(x)}}_{k(x')}\, dx' + B\right)$$

$$= \frac{A}{\sqrt{2m(E-V(x))}} \cos\left(\frac{1}{\hbar}\int_x^b \sqrt{2m(E-V(x'))}\, dx' + B'\right)$$

(The last eq. is a superposition of left- and right-moving WKB waves, with A and B ensuring smooth matching to the solutions in regions I and III, see below.)

Q: Given the fact that the equations (*) all break down near $x=a$ and $x=b$, how do we match the solutions to each other?

A: Near $x=a$ and $x=b$, the potential can in almost all cases be approximated by a linear function (unless $V(x)$ is discontinuous at $x=a$ or $x=b$):

$$V(x) = V(a) + (x-a)V'(a) + O((x-a)^2) = E + (x-a)V'(a) + \ldots$$

$$V(x) = V(b) + (x-b)V'(b) + O((x-b)^2) = E + (x-b)V'(b) + \ldots$$

The S. Eq. for a linear potential can be solved exactly. We use that exact solution to both sides of $x=a$ and

$x = b$ until the WKB solutions become valid, and match it to them.

Near $x = a$, the S.Eq. reads approximately

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + g(x-b) \right] \psi(x) = 0 \qquad g = V'(b) > 0$$

substitute $z = \left(\frac{2mg}{\hbar^2}\right)^{1/3}(x-b)$

$$\Rightarrow \quad \frac{d^2\psi}{dz^2} = z\psi \qquad (**)$$

We have $k^2 = \underbrace{-\frac{2mg}{\hbar^2}}_{<0}(x-b) = -\left(\frac{2mg}{\hbar^2}\right)^{2/3} z$ (real k for $x<b$, imag. k for $x>b$)

and we need $|z|^{3/2} \gg 1$ for the WKB approximation

$\left|\frac{dV}{dx}\right| \ll \frac{p^3(x)}{2m\hbar} = \frac{\hbar^2 k^3(x)}{2m}$ to become valid.

The solutions of this S.Eq. $^{(**)}$ are the Airy functions $Ai(z)$ and $Bi(z)$; for large $|z|$ they are approximately given by

$$Ai(z) \xrightarrow[z\gg 1]{} \frac{1}{2\sqrt{\pi}}\frac{1}{z^{1/4}} e^{-\frac{2}{3}z^{3/2}}$$

$$Bi(z) \xrightarrow[z\gg 1]{} \frac{1}{\sqrt{\pi}}\frac{1}{z^{1/4}} e^{\frac{2}{3}z^{3/2}}$$

$$Ai(z) \xrightarrow[z\ll -1]{} \frac{1}{\sqrt{\pi}}\frac{1}{|z|^{1/4}} \cos\left(\frac{2}{3}|z|^{3/2} - \frac{\pi}{4}\right)$$

$$Bi(z) \xrightarrow[z\ll -1]{} -\frac{1}{\sqrt{\pi}}\frac{1}{|z|^{1/4}} \sin\left(\frac{2}{3}|z|^{3/2} - \frac{\pi}{4}\right)$$

These asymptotic forms are nothing but the WKB approximations for a linear potential, since

$$\int_x^b k(x')\,dx' = \frac{2}{3}\left(\frac{2mg}{\hbar^2}\right)^{1/2}(b-x)^{3/2} = \frac{2}{3}|z|^{3/2}$$

$$\int_b^x \kappa(x')\,dx' = \frac{2}{3}\left(\frac{2mg}{\hbar^2}\right)^{1/2}(x-b)^{3/2} = \frac{2}{3}|z|^{3/2}$$

By identifying these WKB solutions for the linear potential around $x=b$ (i.e. the Airy functions for $|z|\gg 1$) with the WKB solutions (*) outside the shaded regions, we find the "matching formulae"

$$\frac{2A_{\text{II}}}{\sqrt{k(x)}}\cos\left(\int_x^b k(x')\,dx' - \frac{\pi}{4}\right) - \frac{B_{\text{II}}}{\sqrt{k(x)}}\sin\left(\int_x^b k(x')\,dx' - \frac{\pi}{4}\right) \longleftrightarrow$$

(II)

$$\longleftrightarrow \frac{A}{\sqrt{\kappa(x)}}\,e^{-\int_b^x \kappa(x')\,dx'} + \frac{B}{\sqrt{\kappa(x)}}\,e^{\int_b^x \kappa(x')\,dx'}$$

(III)

to match ψ_{II} to ψ_{III}, and similarly

$$\frac{\tilde{A}}{\sqrt{\kappa(x)}}\,e^{-\int_x^a \kappa(x')\,dx'} + \frac{\tilde{B}}{\sqrt{\kappa(x)}}\,e^{\int_x^a \kappa(x')\,dx'} \longleftrightarrow$$

(I)

$$\longleftrightarrow \frac{2\tilde{A}}{\sqrt{k(x)}}\cos\left(\int_a^x k(x')\,dx' - \frac{\pi}{4}\right) - \frac{\tilde{B}}{\sqrt{k(x)}}\sin\left(\int_a^x k(x')\,dx' - \frac{\pi}{4}\right)$$

(II)

to match ψ_{I} to ψ_{II}. For bound states we have

$\tilde{B} = B = 0$. Since ψ_{II} is unique, the term $\frac{2A}{\sqrt{k(x)}} \cos\left(\int_x^b k(x')dx' - \frac{\pi}{4}\right)$ obtained from the matching of ψ_{II} with ψ_{III} must agree with the term $\frac{2\tilde{A}}{\sqrt{k(x)}} \cos\left(\int_a^x k(x')dx' - \frac{\pi}{4}\right)$ obtained from the matching to ψ_I. Writing

$$A\cos\left(\int_x^b k(x')dx' - \frac{\pi}{4}\right) = A\cos\left(\int_a^b k(x')dx' - \int_a^x k(x')dx' - \frac{\pi}{4}\right)$$

$$= A\cos\left(\int_a^b k(x')dx' - \frac{\pi}{2} - \left(\int_a^x k(x')dx' - \frac{\pi}{4}\right)\right)$$

$$= \underbrace{A\sin\left(\int_a^b k(x')dx'\right)}_{\tilde{A}} \cos\left(\int_a^x k(x')dx' - \frac{\pi}{4}\right) - \underbrace{A\cos\left(\int_a^b k(x')dx'\right)}_{\tilde{B}} \sin\left(\int_a^x k(x')dx' - \frac{\pi}{4}\right)$$

$$= \tilde{A}\cos\left(\int_a^x k(x')dx' - \frac{\pi}{4}\right) + \tilde{B}\sin\left(\int_a^x k(x')dx' - \frac{\pi}{4}\right),$$

the bound state matching condition $\tilde{B} = 0$ implies

$$\cos\left(\int_a^b k(x')dx'\right) = 0 \quad \Longrightarrow \quad \boxed{\int_a^b k(x')dx' = \left(n + \tfrac{1}{2}\right)\pi}$$

This quantization condition leads to discrete allowed values for the energy E

$\longrightarrow$ discrete energy eigenvalues.

Let us apply this to the λx^4 potential:

$$\int_{a_n}^{b_n} \sqrt{2m(E_n - \lambda x^4)}\, dx = (n+\tfrac{1}{2})\pi\hbar = \sqrt{2mE_n}\int_{a_n}^{b_n} \left(1 - \frac{\lambda}{E_n}x^4\right)^{1/2} dx$$

At the classical turning points $E_n = V(a_n) = V(b_n) = \lambda b_n^4$

$$\Rightarrow \quad b_n = -a_n = \left(\frac{E_n}{\lambda}\right)^{1/4}$$

Use $y = \frac{x}{b_n}$ as integration variable:

$$(n+\tfrac{1}{2})\pi\hbar = \sqrt{2mE_n}\left(\frac{E_n}{\lambda}\right)^{1/4}\underbrace{\int_{-1}^{1} \sqrt{1-y^4}\, dy}_{\sqrt{\pi}\,\Gamma(5/4)/\Gamma(7/4) = 1.74804 \equiv c} = (2m)^{1/2} E_n^{3/4} \lambda^{-1/4} \cdot c$$

$\left(= \frac{\sqrt{\pi}}{3_2}$ ($_2$ from HW, Pr. 1)$\right)$

$$\Rightarrow \quad E_n^{3/4} = \frac{(n+1/2)\pi\hbar}{(2m)^{1/2} c}\,\lambda^{1/4}$$

$$\boxed{E_n^{WKB} = \frac{(n+1/2)^{4/3}\,\pi^{4/3}\,(\hbar^4)^{1/3}\,\lambda^{1/3}}{c^{4/3}\,2^{2/3}\,m^{2/3}} = \left(\frac{n+\frac{1}{2}}{c}\,\frac{\pi}{\sqrt{2}}\right)^{4/3}\left(\frac{\hbar^4\lambda}{m^2}\right)^{1/3}}$$

One finds that, except for $n = 0$ and 1, these values are in excellent agreement with the exact numerical values $E_n \equiv E_n$(numerical). Shankar quotes for $n = 0$ and 1

$$\frac{E_0^{WKB}}{E_0} = 0.716, \qquad \frac{E_1^{WKB}}{E_1} = 0.992.$$ *)

Note that $E_0^{WKB} < E_0$. This is because E_n^{WKB} is not obtained from an expectation value of $\hat{H}$ (which would always be $\geq E_0$), but from a periodicity condition on the phase of the WKB wavefunction.

*) For harmonic oscillator, WKB energy eigenvalues are <u>exact</u> $\forall n$!

The expectation value $\bar{E}_n = \langle \psi_n^{WKB} | \hat{H} | \psi_n^{WKB} \rangle$ differs from E_n^{WKB} and, for $n=0$, it is significantly larger.

Let us compare with our variational estimates for E_0:

$$\frac{E_0^{WKB}}{E_0^{gaussian}} = \frac{\left(\frac{\pi}{2\sqrt{2}c}\right)^{4/3}}{3/8\ 6^{1/3}} = \frac{0.5463}{0.6814} = 0.802$$

$$\frac{E_0^{WKB}}{E_0^{\exp(-\alpha x^4)}} = \frac{0.5463}{0.6814}\ \frac{1}{1.11} = 0.722$$

These values are in conflict with Shankar's ratio

$E_0^{WKB}/E_0^{exact} = 0.716$, since $E_0^{exact} \leq E_0^{gaussian}, E_0^{e^{-\alpha x^4}}$.

This must be a typo. H. Kleinert in his 1500 page tome on path integrals gives in Table 5.1 (p. 467) a comparison of exact and Gaussian variational ground state energies that shows a ratio

$$\frac{E_0^{gaussian}}{E_0} = 1.02$$ (i.e. a 2% error of the Gaussian variational ground state energy)

Compared to this, the error of the WKB approximation is astronomical; but for higher states the WKB approximation quickly gets exceedingly accurate. We thus realize that the variational and semi-classical WKB methods are complementary.

After this discussion of the WKB energy eigenvalues, let us close with a few words about the WKB wavefunctions. As we go up in energy, the region near the classical turning points where the approximation breaks down becomes, relatively speaking, less and less important. (This is why the energy eigenvalues get more and more accurate.) With the matching to Airy function, the artificial blow-up of the WKB functions at the turning points gets regulated and everything is continuous. The WKB function has exactly the correct number of nodes for the nth level (see the phase integral $\int_a^b k(x')dx' = (n+\frac{1}{2})\pi$): as x goes from a to b, the phase φ goes from $-\frac{\pi}{4}$ to $n\pi + \frac{\pi}{4}$, and $\cos\varphi$ vanishes n times. This phase integral is closely related to the "Bohr-Sommerfeld quantization rule"

$$\int_a^b p(x)\,dx = (n+1)\hbar\pi$$

The difference of $\frac{\hbar}{2}\pi$ comes from Bohr's assumption that the wavefunction vanishes exactly outside the region $a < x < b$; the WKB function has an exponential tail.

The WKB method can also be applied to the radial wavefunction in 3-d systems:

$$u_{nl}(r) = \frac{R_{nl}(r)}{r} \sim \frac{1}{\sqrt{|p_{nl}(r)|}} \sin\left(\frac{1}{\hbar}\int_0^r p_{nl}(r')\,dr'\right)$$

where $$p_{nl}(r) = \sqrt{2m\left(E_n - V(r) - \frac{l(l+1)\hbar^2}{2mr^2}\right)}$$

and $$\boxed{\int_0^{r_{max}} p_{nl}(r)\,dr = (n+\tfrac{3}{4})\pi\hbar}$$ (halfway between $n+\frac{1}{2}$ for two "hard" walls and $n+1$ for two "soft" walls ($r=0$ is a "hard wall").)