Week 5

PHY 304 Quantum Mechanics-II
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7.6 The WKB or semi-classical approximation

The **W**entzel, **K**ramers, **B**rillouin approximation (also called "semi-classical approximation") provides help in finding solutions of the TISE in scenarios where most of the behaviour is very "classical". We had pointed out the hidden classical physics behind quantum mechanics in many places throughout this lecture. For example we had seen in example 13 that you can think of the eigenstates in the infinite square well as the particle bouncing back and forth with fixed momentum and thus wavelength, or in example 1 that a particle wavepacket in a potential valley mostly accelerates and decelerates in accordance with Newton's equations.

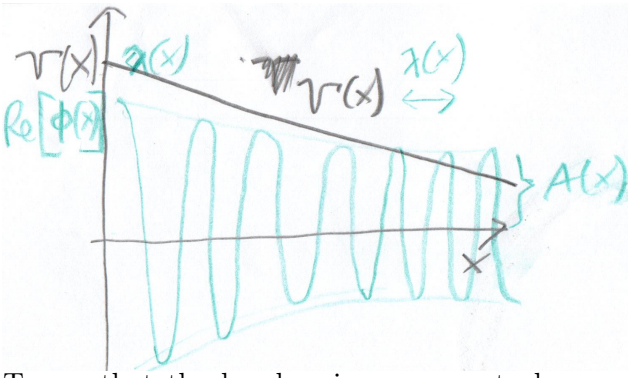
Let us revisit the free particle states from section 2.1: The solutions of the TISE

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V\right]\phi(x)=E\phi(x), \tag{7.117}$$

for a constant external potential $V(x)=V$ are:

$$\phi(x)=Ae^{\pm ikx} \tag{7.118}$$

with $k=\sqrt{2m(E-V)}/\hbar$ (and we have used a new name A for the amplitude/normalisation constant). This actually also works for $E<V$, only then we shall write $\phi(x)=Ae^{\pm\kappa x}$ with $\kappa=\sqrt{2m(V-E)}/\hbar$, to make the different behavior of $\phi(x)$ more apparent.



left: Now imagine instead of a constant V that $V(x)$ varies only little over the range of one de-Broglie wavelength $\lambda_{\rm dB}=2\pi/k$ with $k=\sqrt{2m(E-V)}/\hbar$. as shown on the left. We can then try to simply assign a local position dependent wavelength $\lambda(x)=h/\sqrt{2m(E-V(x))}$ and position dependent amplitude $A(x)$.

To see that the handwaving argument above can be mathematically justified, we can do steps similar to those in section 1.6.4 for the TISE (1.62) instead of the TDSE. First let us reshuffle (7.117) for a spatially varying potential $V\to V(x)$ into

$$\frac{\partial^2}{\partial x^2}\phi(x)=-\frac{p(x)^2}{\hbar^2}\phi(x), \tag{7.119}$$

with $p(x) = \sqrt{2m[E - V(x)]}$. Similar to (1.47), we now write the wavefunction in its polar representation as an amplitude and a phase, both real ($A \in \mathbb{R}$, $\varphi \in \mathbb{R}$):

$$\phi(x) = A(x)e^{i\varphi(x)}. \tag{7.120}$$

Through double application of the product rule, we then have

$$\frac{\partial^2}{\partial x^2}\phi(x) = \left[A'' + 2iA'\varphi' + iA\varphi'' - A\varphi'^2\right] e^{i\varphi(x)}, \tag{7.121}$$

which we can insert into (7.119) and then divide by $e^{i\varphi(x)}$ to reach

$$A'' + 2iA'\varphi' + iA\varphi'' - A\varphi'^2 = -\frac{p^2}{\hbar^2}A, \tag{7.122}$$

All variables in (7.122) are real, hence it is easy to separately equate the real part and the imaginary part of the equation.

$$A'' - A\varphi'^2 = -\frac{p^2}{\hbar^2}A, \tag{7.123}$$

$$2A'\varphi' + A\varphi'' = 0. \tag{7.124}$$

We divide the first equation by A and then assume that A''/A can be neglected compared to φ'^2 and $p^2/\hbar^2$. This is a slowly varying envelope approximation. With it, the first equation turns into $\varphi'^2 = p^2/\hbar^2$ or $\varphi' = \pm p/\hbar$, which we can formally integrate to reach

$$\varphi(x) = e^{\pm\frac{1}{\hbar}\int^x dx'\, p(x')dx'}. \tag{7.125}$$

We also have to solve the earlier equation (7.124), which can first be reshaped into $(A^2\varphi')' = 0$ from which $A^2\varphi' = const$, from which we know $A = const/\sqrt{|\varphi'|}$. Putting it all together, we found the

Wavefunction in the WKB approximation

$$\phi(x) = \frac{const}{\sqrt{p(x)}} e^{\pm\frac{i}{\hbar}\int_{x_0}^x dx'\, p(x')}, \tag{7.126}$$

with $p(x) = \sqrt{2m[E - V(x)]}$ the classical momentum.

- Note that the lower integration limit x_0 in the exponent as not been specified yet, it can be chosen as convenient for a given problem, since changes in it can be absorbed into *const*.
- The expression (7.126) encapsulates the scenario we tried to draw above, where the particle is slower once it climbed higher in the potential, and hence the wavelength there is larger.
- It also makes sense that $|\phi(x)|^2 \sim 1/p(x)$, since the particle is less likely to be found in a region where it is faster and hence spends less time. We had used a similar argumentation in example 15 to understand the structure of high harmonic oscillator states, based on the classical probability distribution of the oscillator.

- The WKB wavefunction (7.126) can also be found through (the right) expansion of the TISE to leading order in $\hbar$, see Griffith.

- Since we (approximately) solved a second order differential equation in x, we get two linearly independent solutions as usual, represented by the two signs $\pm$ in (7.126). To find the complete solution, we combine these to satisfy boundary conditions as usual, and then adjust normalisation to one to specify *const*.

- To reach (7.126), we used $|A''/A| \ll p^2/\hbar^2$ in (7.123) (note that $\varphi'^2 = p^2/\hbar^2$ as well). Now that we know that $A = \frac{const}{\sqrt{p(x)}}$, this amounts to

$$\frac{3p'(x)^2}{4p(x)^2} - \frac{C}{2p(x)}p''(x) \ll \frac{p(x)^2}{\hbar^2}. \tag{7.127}$$

  Focussing only on the first term, ditching the factor 3/4 and inserting the de-Broglie wavelength $\lambda(x) = h/p(x)$ we reach the condition (exercise)

$$\lambda(x)'\lambda(x) \ll \lambda(x), \tag{7.128}$$

  where we again dropped a factor of (2π). All up, this means that the change of the wavelength over one wavelength must be much less than the wavelength itself.

- A complemetary way to think about the conditions used, again starting from $|\hbar p'/p| \ll p$, is found by inserting $p(x) = \sqrt{2m[E - V(x)]}$ and hence $p'(x) = -2mV'(x)/[2p(x)]$. Then

$$\left|\hbar m\frac{V'(x)}{p(x)^2}\right| = \left|\frac{1}{2\pi}\lambda(x)m\frac{V'(x)}{p(x)}\right| \ll p(x) \Leftrightarrow$$

$$\left|\lambda(x)V'(x)\right| \ll \frac{p(x)^2}{2m}, \tag{7.129}$$

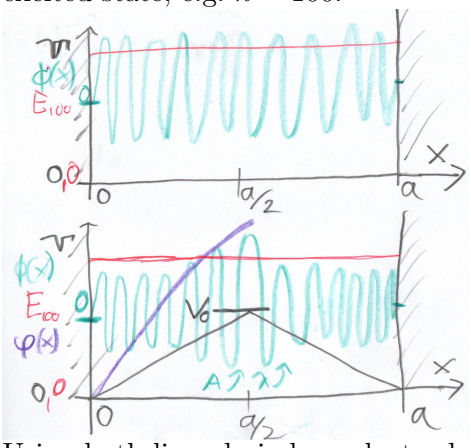
  which tells us that the change of the potential energy over one de-Broglie wavelength must be much less than the kinetic energy.

- Note that the approach here conceptually requires us to work in one-dimension (1D). The WKB can be generalized to higher dimensions, but becomes more clumsy then, so it is most useful for 1D problems.

7.7 In the classical region

The WKB approximation (7.126) can be used for $E > V(x)$ (in the classically allowed region) as well as for $E < V(x)$ in the classically forbidden region. Let us look at an example for the former first. In yet another variation of example 45, let us look at the

Example 60, Infinite square well potential with a broad bump: and go to a highly excited state, e.g. $n = 100$.



left: The drawing on the left first sketches[a] the state $n = 100$ for the usual infinite square potential, see Eq. (2.18). Below we show the wavefunction for the modified potential $V(x) = 2V_0 x$ for $0 < x < a/2$, infinity outside $[0, a]$ and symmetric wrt. $x = a/2$. Let us set $\hbar = m = a = 1$, then $E_{100} \approx 50000$ and choose $V_0 = 35000$.

[a] I was too lazy to draw the correct number of nodes

Using both linearly independent solutions in the WKB approximation we start with

$$\phi(x) \approx \frac{const}{\sqrt{p(x)}} \left(C_+ e^{+i\varphi(x)} + C_- e^{-i\varphi(x)} \right), \tag{7.130}$$

with $\varphi(x) = \int_0^x dx' p(x')/\hbar$, choosing $x_0 = 0$ here. We can instead directly write this as

$$\phi(x) \approx \frac{const}{\sqrt{p(x)}} \left(C_1 \sin\left[i\varphi(x)\right] + C_2 \cos\left[i\varphi(x)\right] \right), \tag{7.131}$$

so that we see $C_2 = 0$ due to the boundary condition $\phi(0) = 0$. Now we (mathematica) can actually do the integration (assuming $0 < x < a/2$)

$$\begin{aligned} \varphi(x) &= \int_0^x dx' \underbrace{\sqrt{2m[E - 2V_0 x]}}_{=p(x)} /\hbar \\ &= \frac{2V_0 x\sqrt{2m(E - 2V_0 x/a)} + aE(\sqrt{2mE} - \sqrt{2m(E - 2V_0 x/a)})}{3V_0}. \end{aligned} \tag{7.132}$$

This turns out to be almost but not quite linear, see violet line in drawing. Alltogether we reach the wavefunction shown in green above, where we can see the wavelength and the amplitude getting slightly larger[b] on the bump. Quantisation of energy arises, just as in the ordinary particle in the box, by requiring that $\varphi(a) = 0$ (we are not doing that now). We do not need to do the calculation for $x > a/2$, since we can use the symmetry or anti-symmetry of the wavefunction. Finally, you can verify all the above using the full solution in the app http://www.falstad.com/qm1d/ , choose particle in the box, "draw" the above potential landscape, and then select a high energy eigenstate.
While we do not show this now, the WKB approximation works here only for large n. If you'd try to use it for lower ones (e.g. $n = 1$), you run into trouble since (7.128) breaks down.

[b] Incidentally the amplitude getting larger was already visible in example 45.

7.8 In the classically forbidden region

To obtain the result (7.126), we did not have to demand that $p(x)$ be real, so it works just fine if $V(x) > E$ and $p(x)$ hence imaginary. Just to make the changing character of the exponential function more obvious, we can then write

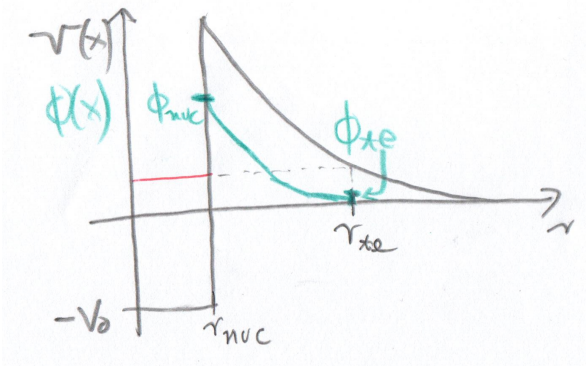
Wavefunction in the WKB approximation in the classically forbidden region $V(x) > E$

$$\phi(x) = \frac{const}{\sqrt{|p(x)|}} e^{\pm\frac{1}{\hbar}\int_{x_0}^{x} dx' \, |p(x')|}, \tag{7.133}$$

with $|p(x)| = \sqrt{2m[V(x) - E]}$ the magnitude of the (imaginary) classical momentum.

The paradigmatic case where the classically forbidden region is quantum tunnelling, which we had seen in section 2.2.4 for a simple square barrier. The cases where the WKB is most useful, are when the barrier is more complicated than square, for example in

Example 61, Nuclear alpha decay: In PHY106, week 9, we had already seen how nuclear alpha decay is related to quantum tunnelling. The WKB approximation works well for a simpler method (Gamow theory) to calculate the decay rate than we have seen earlier.



left: While the α particle is within the nucleus, it feels the strong force giving rise to a constant potential well $V(r) = -V_0$, once it exits the nucleus, it only feels the Coulomb repulsion with all other protons, $V_{\text{coul}}(r) = \frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{r}$ as shown on the left. We assume the α particle has an energy $E > 0$ within the well shown.

Since the tunneling probability is just the ratio of the probability density at the entrance and at the exit of the tunnelling region (compare section 2.2.4), we only require a WKB approximation to the wavefunction within the classically forbidden region, to in the end take the tunnelling probability as $T = |\phi_{te}|^2/|\phi_{\text{nuc}}|^2$ (see sketch).
We set up the linear combination in the tunnelling region based on (7.133), yielding

$$\phi(r) \approx \frac{1}{\sqrt{|p(r)|}} \left(C_+ e^{+\varphi(r)} + C_- e^{-\varphi(r)} \right), \tag{7.134}$$

with $\varphi(r) = \int_{r_{\text{nuc}}}^{r_{te}} dr' \sqrt{2m(V_{\text{coul}}(r') - E)}$, where the "tunnel exit" is defined by $V_{\text{coul}}(r_{te}) = E$. Since $\varphi(r)$ keeps increasing for a quite broad tunnelling barrier, we need $C_+ = 0$ for a reasonable solution where $|\phi_{te}|^2 < |\phi_{\text{nuc}}|^2$ (in a more complete treatment this is made certain of by the boundary conditions).

Example continued: We can then read off the drawing that

$$T = \frac{|\phi(r_{te})|^2}{|\phi(r_{\rm nuc})|^2} = \frac{\left|C_- e^{-\frac{1}{\hbar}\int_{r_{\rm nuc}}^{r_{te}} dr' |p(r')|} / \sqrt{|p(r_{te})|}\right|^2}{\left|C_- e^0 / \sqrt{|p(r_{nuc})|}\right|^2} \tag{7.135}$$

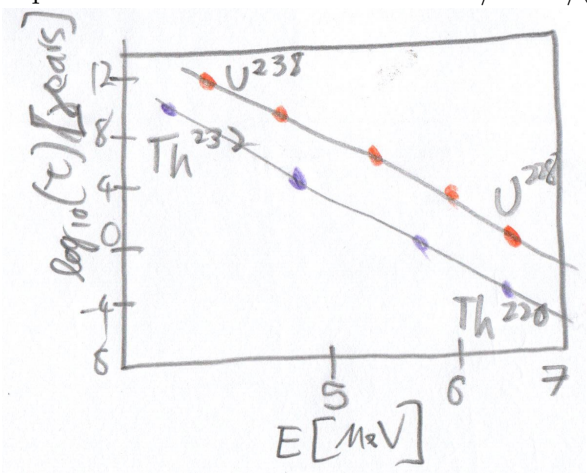
We can pick $V_{\rm coul}(r_{te}) = V_{\rm coul}(r_{nuc})$ and hence $p(r_{nuc}) = p(r_{te})$, which gives us a tunelling probability

$$T = e^{-2\gamma}, \tag{7.136}$$

with $\gamma = \int dr' |p(r')|/\hbar$. So far the discussion was not dependent on the shape of the potential $V(r)$ through which we are tunneling. For the coulomb potential the integral is doable (see Griffith), and assuming $r_{\rm nuc} \ll r_{\rm te}$ we reach in the end

$$\gamma = K_1 \frac{Z}{\sqrt{E}} - K_2 \sqrt{Z r_{\rm nuc}}, \tag{7.137}$$

where $K_1 = 1.98$ MeV$^{1/2}$ and $K_2 = 1.485$ fm$^{-1/2}$ arise from a collection of fundamental constants (see Griffith).
To find an α decay rate Γ (and from that a lifetime) we have to multiply T with an "escape attempt frequency ν" (see Griffith), which however does not change the extreme exponential dependence of the final lifetime $\tau = 1/\Gamma = 1/(\nu T)$ on the energy E.

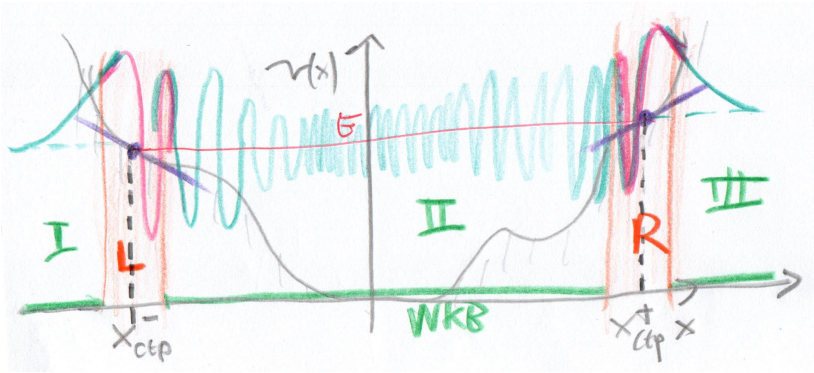


left: The latter very nicely captures what is experimentally observed, as shown on the left for two different types of nuclei that decay via alpha decay. Note that in reality this is a many-body problem of nuclear physics. The energy E that you associate with the α-particle inside the nucleus for our present single body picture, is actually the energy difference between the complete nucleus and the nucleus after decay plus one alpha particle.
This E must be positive for α decay to be possible, and varies depending on the configuration of the nucleus, i.e. number of neutrons, as visible in the graph on the left (see Griffith and references therein for the proper version of the sketch).

7.9 Connecting both regions

Clearly the requirement that we started with for the WKB aproximation, of the potential to be slowly varying over one de-Broglie wavelength, cannot be fulfilled near the classical turning point $x_{\rm ctp}$ where $V(x_{\rm ctp}) = E$, since there the classical momentum $p(x)$ approaches zero and $\lambda = h/p(x)$ hence diverges. The most important quantum problems (unlike the examples cunningly chosen

above) contain all three regions, classically allowed, forbidden and crossing regions.



left: This is shown in the sketch to the left. Regions I and III are classically forbidden and II classically allowed, and in all of these the WKB approximation can work fine, giving us a WKB wavefunction (green).

Near the two classical turning points $x^{\pm}_{ctp}$ it breaks down, but there we can hope to approximate the potential as linear $V(x) \approx V_0 + V'(x - x^{\pm}_{ctp})$ and then use the solution of the TISE in a linear potential, based on Airy functions (red, see QM-I assignment 4).

For a linear potential, we have seen in that assignment that the general solution of the TISE is

$$\phi(x) = A\mathrm{Ai}(\alpha x) + B\mathrm{Bi}(\beta x) \tag{7.138}$$

with Airy functions of the first kind $\mathrm{Ai}(x)$ and second kind $\mathrm{Bi}(x)$. We now patch[16] a WKB solution from the classically allowed region (7.126), onto the solution for a linear potential (7.138) and then also patch the solution (7.138) onto the solution in the classically forbidden region (7.133). The calculation is described in Griffith, but is only needed to once find the

WKB connection formula For a WKB solution that crosses a classical turning point x_{ctp} (where $E > V(x)$ for $x < x_{\mathrm{ctp}}$, we need to use

$$\phi(x) = \begin{cases} \frac{2D}{\sqrt{p(x)}} \sin\left[\frac{\pi}{4} + \frac{1}{\hbar}\int_x^{x_{\mathrm{ctp}}} dx' p(x')\right] & \text{for } x < x_{\mathrm{ctp}}, \\ \frac{D}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_{x_{\mathrm{ctp}}}^{x} dx' |p(x')|} & \text{for } x > x_{\mathrm{ctp}}. \end{cases} \tag{7.139}$$

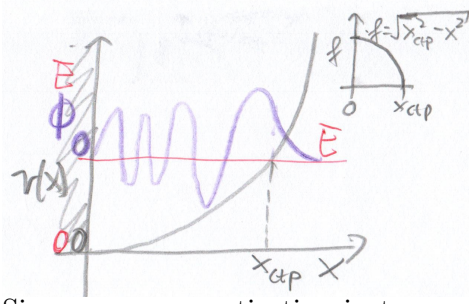
for the same constant D (which is later fixed by the overall normalisation).

- We still have to stay away from $x = x_{\mathrm{ctp}}$ when using (7.139) (or use (7.138) there), since $p(x_{\mathrm{ctp}}) = 0$, however the advantage of (7.139) is that the wavefunctions on either side are now connected with the correct phase relation (for the sine) and thus one can properly apply boundary conditions etc, see example below.

Let's see at least one example of an application for the connection formula, the

[16] that means make them match exactly in the region drawn in red in the diagram above

Example 62, Half of a harmonic oscillator: with a potential $V(x) = m\omega^2 x^2/2$ for $x > 0$ and $V(x) = \infty$ for $x < 0$.



left: For a fixed energy E, this potential one classical turning point $x_{\rm ctp}$ on the right. As in our solutions for the infinite square well potential, we have to satisfy the boundary condition $\phi(0) = 0$. The drawing also sketches the function $f(x) = \sqrt{x_{\rm ctp}^2 - x^2}$, to be integrated over later.

Since energy quantisation just comes from the boundary condition, we don't even have to worry about the region II outside $x_{\rm ctp}$, instead we just use (7.139) for $x < x_{\rm ctp}$

$$\phi(x) = \frac{2D}{\sqrt{p(x)}} \sin\left[\frac{\pi}{4} + \frac{1}{\hbar}\int_x^{x_{\rm ctp}} dx' p(x')\right], \tag{7.140}$$

and check when the condition $\phi(0) = 0$ is fulfilled.
We write

$$p(x) = \sqrt{2m(\underbrace{E}_{=\frac{1}{2}m\omega^2 x_{\rm ctp}^2} - \frac{1}{2}m\omega^2 x^2)} = m\omega\sqrt{x_{\rm ctp}^2 - x^2}, \tag{7.141}$$

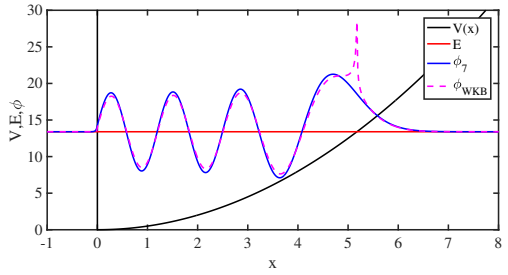
thus

$$\int_0^{x_{\rm ctp}} dx' p(x') = m\omega \underbrace{\int_0^{x_{\rm ctp}} \sqrt{x_{\rm ctp}^2 - x^2}}_{=\pi x_{\rm ctp}^2/4} = \frac{\pi E}{2\omega}, \tag{7.142}$$

since the integration essentially asks us to find the area of a fourth of a circle, see $f(x)$ in the drawing above. For $\phi(0) = 0$, we need

$$\frac{1}{\hbar}\int_0^{x_{\rm ctp}} dx' p(x') + \frac{\pi}{4} = n\pi \qquad \text{for } n = 1, 2, \cdots \Leftrightarrow E = \hbar\omega\left(2n - \frac{1}{2}\right). \tag{7.143}$$

These are exactly all the oscillator energies with odd n, which is incidentally the correct (approximation free) answer (Q: why does that answer make sense?).



left: Finally, we compare on the left the numerical half-oscillator state for $n = 6$ (blue), with the WKB solution (7.139) (magenta dashed). The potential $V(x)$ is black, and the energy E_n (red) provides the line $\phi = 0$ for the wavefunctions. We can see that the WKB solution blows up on the turning point. Elsewhere it would agree perfectly, but the spike causes normalisation issues.