QUANTUM PHYSICS III

Solutions to Problem Set 3 23 September 2025

1. On validity of the leading-order (LO) WKB approximation

1. Substituting the wave function

$$\psi = e^{\frac{i}{\hbar}S} \;, \quad S = S_0 + \frac{\hbar}{i}S_1 + \left(\frac{\hbar}{i}\right)^2 S_2 + ... \tag{1}$$

into the Schroedinger equation, we get

$$-i\hbar S'' + S'^2 = p^2 \; . \tag{2}$$

Expanding this up to $O(\hbar^2)$ and equating the $\hbar^2$-terms, we obtain

$$S_1'' + 2S_0'S_2' + S_1^2 = 0 \quad \Rightarrow \quad S_2' = -\frac{1}{2S_0'}(S_1'' + S_1'^2) \; . \tag{3}$$

Recall that

$$S_0' = \pm p \;, \quad S_1 = -\frac{1}{4}\log p^2 \; . \tag{4}$$

Hence,

$$S_2' = \frac{1}{8p^3}(2pp'' - 3p'^2) \;, \tag{5}$$

or, using the relation $p = \sqrt{2m(E-V)}$,

$$S_2' = -\frac{1}{32\sqrt{2m}}\left(\frac{5V'^2}{(E-V)^{5/2}} + \frac{4V''}{(E-V)^{3/2}}\right) \; . \tag{6}$$

2. The LO WKB approximation is applicable if

$$\psi = e^{\frac{i}{\hbar}(S_0 + \frac{\hbar}{i}S_1)}(1 + o(1)) \; . \tag{7}$$

This means that all exponents containing the higher-order terms must be close to one,

$$|e^{i\hbar^{n-1}S_n}| = 1 + o(1) \quad \Rightarrow \quad |\hbar^{n-1}S_n| \ll 1 \;, \;\; n \geqslant 2 \; . \tag{8}$$

3. We notice that S_2' can be rewritten as

$$S_2' = \frac{1}{4}\frac{d}{dx}\left(\frac{p'}{p^2}\right) + \frac{1}{8}\frac{p'^2}{p^3} \;, \tag{9}$$

and, hence,

$$\begin{aligned} |\hbar S_2| &= \left|\frac{1}{4}\hbar\frac{p'}{p^2} + \frac{1}{8}\int^x \hbar\frac{p'^2}{p^3}dx\right| \\ &\leqslant \frac{1}{4}\left|\frac{\hbar p'}{p^2}\right| + \frac{1}{8}\int^x \left|\frac{\hbar p'^2}{p^3}\right| dx = \frac{1}{4}|\lambda\!\!\!^{-}{}'| + \frac{1}{8}\int^x \left|\frac{\lambda\!\!\!^{-}{}'^2}{\lambda\!\!\!^{-}}\right| dx \; . \end{aligned} \tag{10}$$

Thus, from $|\lambda\!\!\!^{-}{}'| \ll 1$ and $\int^x |\lambda\!\!\!^{-}{}'^2 \lambda\!\!\!^{-}{}^{-1}|\, dx \ll 1$ it follows that $|\hbar S_2| \ll 1$.

4. Differentiating the expression for the momentum, we find

$$p' = \frac{-2mV'}{2p} = \frac{m}{p}F \ , \quad F = -V' \ . \tag{11}$$

Next, we notice that

$$\frac{\hbar}{p}F = \lambda F \sim \delta A \ , \tag{12}$$

where δA is a work done by the force F on the distance λ. Finally,

$$T_{kin} = \frac{p^2}{2m} \ , \tag{13}$$

and we have

$$|\lambda'| = \left|\hbar\frac{p'}{p^2}\right| = \left|\frac{\hbar}{p}\frac{pp'}{m}\frac{m}{p^2}\right| \sim \left|\lambda F\frac{2m}{p^2}\right| \sim \left|\frac{\delta A}{T_{kin}}\right| \ll 1 \ . \tag{14}$$

2. On accuracy of the LO WKB approximation

1. In the classically forbidden region, the exponentially decaying LO WKB wave function is given by (up to a constant multiplier)

$$\psi = \frac{1}{\sqrt{|p|}}e^{-\frac{1}{\hbar}\int_{x_0}^{x}|p|dx} \ . \tag{15}$$

For the potential

$$V(x) = V_0\sqrt{\frac{x}{x_0}} \ , \quad x > 0 \tag{16}$$

we have at $x > x_0$

$$|p| = \sqrt{2V_0\left(\sqrt{\frac{x}{x_0}} - 1\right)} \ . \tag{17}$$

Integrating $|p|$, we arrive at

$$\psi = \left(2V_0\left(\sqrt{\frac{x}{x_0}} - 1\right)\right)^{-1/4} \exp\left[-\frac{4\sqrt{2V_0}}{15\hbar}x_0\left(\sqrt{\frac{x}{x_0}} - 1\right)^{3/2}\left(3\sqrt{\frac{x}{x_0}} + 2\right)\right] \ . \tag{18}$$

In the limit $x \gg x_0$, this simplifies to

$$\psi \sim V_0^{-1/4}(x/x_0)^{-1/8}e^{-\frac{4\sqrt{2V_0}}{15\hbar}x_0^{-1/4}x^{5/4}} \ . \tag{19}$$

2. One requires the LO result (18) to be accurate to 1 percent in the region $x > 2x_0$. This means, in particular, that the modulus of the NLO correction $\hbar S_2$ must not exceed 10^{-2} in that region, that is

$$|\hbar S_2|_{x>2x_0} \leqslant 10^{-2} \ . \tag{20}$$

To find S_2, we substitute the expression for the momentum (17) into eq. (5) and integrate over x. The result is

$$S_2 = \frac{3\dfrac{x}{x_0} - 4\sqrt{\dfrac{x}{x_0}} + 6 - 3\sqrt{\sqrt{\frac{x}{x_0}} - 1}\left(\sqrt{\dfrac{x}{x_0}} - \dfrac{x}{x_0}\right)\tan^{-1}\left(\sqrt{\sqrt{\frac{x}{x_0}} - 1}\right)}{96 x_0 \sqrt{2V_0}\sqrt{\dfrac{x}{x_0}}\left(\sqrt{\dfrac{x}{x_0}} - 1\right)^{3/2}} . \quad (21)$$

This is a monotonically decreasing function of x/x_0, hence the condition (20) implies

$$|\hbar S_2|_{x=2x_0} \leqslant 10^{-2} . \quad (22)$$

We have

$$|\hbar S_2|_{x=2x_0} \approx 0.14 \frac{\hbar}{\sqrt{V_0} x_0} , \quad (23)$$

so,

$$V_0 \gtrsim \frac{196\hbar^2}{x_0^2} . \quad (24)$$

3. On asymptotics of the potential in the WKB approximation

1. At first glance it may seem that the power-like decreasing potential cannot endanger the validity of the WKB approach, since in the classically forbidden region the WKB wave function decays much faster (exponentially fast). Let us see, however, that this is not so. We have to verify that

$$|\lambda\!\!\!^{-}{}'| \ll 1 , \quad |S_1| \gg |\hbar S_2| , \quad |\hbar S_2| \ll 1 , \quad x \to \infty . \quad (25)$$

Let the potential behave as

$$V(x) \sim x^{-n} , \quad n > 0 , \quad x \to \infty . \quad (26)$$

In the following reasoning it is important that the energy of the particle coincides with the asymptotics of the potential at infinity (in our case, zero). Then, for the momentum we have

$$p \sim x^{-n/2} . \quad (27)$$

We can now check if the conditions (25) hold in the limit $x \to \infty$. For example,

$$|\hbar S_2| \sim \hbar x^{n/2-1} \ll 1 \quad \Rightarrow \quad \frac{n}{2} - 1 < 0 \quad \Rightarrow \quad n < 2 . \quad (28)$$

Next,

$$|S_1| \sim \frac{n}{4} \log x \gg 1 \quad \text{for any } n > 0 . \quad (29)$$

Finally,

$$|\lambda\!\!\!^{-}{}'| \sim \hbar x^{n/2-1} \ll 1 \quad \Rightarrow \quad n < 2 . \quad (30)$$

Note that the case $n = 2$ is special and cannot be resolved without additional information about the potential. Hence, our best estimate is $n < 2$.

2. From the above we see that if the potential decreases faster than x^{-2}, the WKB approach fails to describe the decaying wave function at arbitrary large x. We also observe that any asymptotics of the form

$$V(x) \sim x^{-k} , \quad k < 2 \tag{31}$$

passes our tests of validity. But what if the potential falls off faster than any of (31), but still slower than x^{-2}? Long story short, anything can happen. As an example, consider the following behavior,

$$V(x) \sim \left(\frac{\log x}{x}\right)^2 . \tag{32}$$

Here we have

$$p \sim \frac{\log x}{x} , \quad p' \sim \frac{1}{x^2} - \frac{\log x}{x^2} \sim \frac{\log x}{x^2} , \quad p'' \sim \frac{\log x}{x^3} . \tag{33}$$

So, for example,

$$S_2' \sim \frac{1}{x \log x} \quad \Rightarrow \quad |\hbar S_2| \sim \hbar \log\log x . \tag{34}$$

This increases with x! Thus, the LO approximation is wrong in this case. Note in parentheses that the other two conditions in (25) are satisfied.

4*. WKB expansion beyond the LO

1. Substituting the expansion (1) into eq. (2) and extracting the $\hbar^n$-term, $n \geqslant 2$, we get

$$S''_{n-1} + \sum_{j=0}^{n} S'_j S'_{n-j} = 0 , \tag{35}$$

from which one concludes that

$$S'_n = -\frac{1}{2S'_0}\left(S''_{n-1} + \sum_{j=1}^{n-1} S'_j S'_{n-j}\right) , \quad n \geqslant 2 . \tag{36}$$

2. (a) From eqs. (4) and (36) it is clear that all S'_n are polynomial expressions of the momentum p and its derivatives. Since $p \sim (E-V)^{1/2}$, any S'_n contains multipliers of the form

$$(E-V)^{-n} , \quad (E-V)^{-n+\frac{1}{2}} \tag{37}$$

with n an integer number. Evidently, the term S'_n can be a non-real-valued function if and only if it contains fractional powers of $E - V$. Note also that differentiation with respect to x cannot convert a fractional power of $E - V$ into an integer power and vice versa. Hence, if S'_n is real (or imaginary) at some x, so does its derivative S''_n.

Now we prove that all *even* terms S'_{2n} contain just fractional powers of $E - V$, while all *odd* terms S'_{2n+1} contain only integer powers of $E - V$. Schematically,

$$S'_{2n} \not\supset \{(E-V)^{-k}\ ,\ k \in \mathbb{N}\}\ , \quad S'_{2n+1} \not\supset \{(E-V)^{-k+\frac{1}{2}}\ ,\ k \in \mathbb{N}\}\ . \tag{38}$$

The proof is by induction. For the pair S'_1, S'_2 the statement is obviously true. Let it be true for all pairs up to S'_{2n-1}, S'_{2n}. Then we show that it also holds for the pair S'_{2n+1}, S'_{2n+2}. Consider first the odd term S'_{2n+1}. The recurrent expression (36) is rewritten as

$$S'_{2n+1} = -\frac{1}{2S'_0}(S''_{2n} + S'_1 S'_{2n} + S'_2 S'_{2n-1} + \ldots + S'_{2n} S'_1)\ . \tag{39}$$

By the induction hypothesis, S''_{2n} has only fractional powers of $E - V$. The subsequent series consists of the products of an odd and an even terms, hence all occurrences of $(E-V)$ in the series are also supplemented with the half-integer powers. Finally, multiplying by $S_0^{'-1}$ reduces the powers of all $(E - V)$-terms by one half, thus making them all integer. We conclude that the second statement in (38) is true.

Let us move to the even term, S'_{2n+2}. We have,

$$S'_{2n+2} = -\frac{1}{2S'_0}(S''_{2n+1} + S'_1 S'_{2n+1} + S'_2 S'_{2n} + \ldots + S'_{2n+1} S'_1)\ . \tag{40}$$

By what has been just proved, $S''_{2n+1} \not\supset \{(E-V)^{-k+\frac{1}{2}}\ ,\ k \in \mathbb{N}\}$. The series next to S''_{2n+1} contains the products of two odd or two even terms. All such products are also free of the fractional powers of $E - V$. Indeed, in the odd terms there are no such powers by the induction hypothesis, while all inclusions of $E - V$ in the products of even terms are of the form

$$(E-V)^{-\frac{a}{2}} \cdot (E-V)^{-\frac{b}{2}} = (E-V)^{-\frac{a+b}{2}}\ . \tag{41}$$

Since, by the induction hypothesis, a and b are odd, their sum $a + b$ is even, so the r.h.s. of eq. (41) is an integer power of $E - V$. Multiplying the expression in parenthesis in eq. (40) by $S_0^{'-1}$ converts all powers of $E - V$ into half-integers. Thus, the first statement in (38) is also true, and this completes the proof.

We conclude that the odd terms S'_{2n+1} do not contain any square roots of $E - V$ and, hence, they are all real. Meanwhile, we have also proved a perhaps somewhat nontrivial fact that, at a given point x, all S'_{2n}-terms can be either simultaneously real or simultaneously imaginary. This means that the splitting of the wave function domain onto classically allowed and classically forbidden regions is precise in all order in $\hbar$. In particular, the turning points, computed by the means of the LO WKB approximation, cannot shift when more terms in the expansion (1) are taken into account.

(b) Real-valuedness of S'_{2n+1} implies that S_{2n+1} do not contribute to the phase of the wave function. So, we can rewrite eq. (1) as

$$\psi = Ae^{\frac{i}{\hbar}\tilde{S}}\ , \tag{42}$$

where all odd terms are collected into the amplitude A, while $\tilde{S}$ now contains only even terms. Plugging this form of ψ into the Schroedinger equation and extracting its real and imaginary parts, we get the system of equations for A and $\tilde{S}$,

$$\begin{cases} \tilde{S}'^2 - \hbar^2 \dfrac{A''}{A} = p^2 \ , \\ 2\tilde{S}'A' + A\tilde{S}'' = 0 \ . \end{cases} \tag{43}$$

The second of these equations is integrable with respect to A ! The answer is

$$A = \frac{C}{\sqrt{\tilde{S}'}} \tag{44}$$

with C some constant. We conclude that the amplitude of the wave function is fully determined by its phase (up to a constant multiplier). Expanding (44) with respect to $\hbar$, one can relate the terms with the odd powers of $\hbar$ to the differentials of the terms with the even powers of $\hbar$. Moreover, as all S'_{2n} are simple polynomials of p and its derivatives, the terms S_{2n+1} are expressed explicitly through p, p', p'', etc. Hence, all S'_{2n+1} are total derivatives of those expressions.