Notes for Lecture 10

The WKB approximation

Here, we study an important approximation that appeals especially to *us*, classical objects. This approximation deals with the opposite end of the energy spectrum in comparison to the variational principle. The variational principle is concerned with the lowest energy state, or the first few excited states if circumstances allow. In contrast, the WKB approximation starts from the "semi-classical limit," i.e. the limit of the high quantum number and, correspondingly, the limit of high energy.

10.1 Semi-classical view

As a popular saying goes, nobody really understands quantum mechanics. Of course, this saying does not mean nobody aced in a quantum mechanical course/exam! I hope dearly that everyone will be successful in my course. What this saying means is something quite different than doing well or not in a quantum mechanics course, though. Even if you do very well in this course, and all other subsequent advanced quantum courses, something about quantum mechanics may "always feel kind of wrong or unfamiliar." And this *always* refers to the contrast between quantum mechanics and classical mechanics. We know mathematics of quantum mechanics and what it implies in terms of measurable consequences, but we just cannot *feel* why the quantum mechanical laws work the way they do. However, any one who tried to catch a fly ball (and got a black eye) really "feels" the classical mechanics: i.e. $\vec{F} = m\vec{a}$. In contrast, the "wave function", the "spin," the "uncertainty principle," "identical particles," and the "quantum entanglement" etc. are easy to state in the quantum mechanical formalism, but none of these "make sense" in our classical world, since the classical particles that live in our classical world do not operate by these weird rules. We "know" that microscopic worlds have this clockwork machine that we call

quantum mechanics, and we also know that from it all of the classical phenomena (somewhat miraculously) emerge, but in truth "a real understanding" of the way that this microscopic machine works seems to us as tantalizing as any other outstanding mysteries of physics and beyond.

For this reason, people tend to look constantly for ways to understand quantum mechanics in "semi-classical terms." When this is successful, it brings us a great joy! We get a sense that things do not seem so weird after all! For instance, the original Bohr theory of atoms provided such a semi-classical view. The WKB (Wentzel, Kramers, Brillouin) approximation can be viewed as a systematic way to justify the original Bohr view. Not only is this satisfying, or pleasing, to "our intuition," it also predicts very useful formulae; for example, the WKB approximation is central in explaining quantum mechanical tunneling (as in STM, etc.), alpha decay, and cold emission. However, please be warned – one must be aware of the limit of this approximation, like any other approximate methods. Use it with joy when it is quantitatively applicable (at high energy) and *for qualitatively thinking certain aspects of quantum mechanics* (at any energy), but do not be surprised if it becomes quite incorrect when you "push it" to the quantum limit, as you might be tempted to do. Even when the WKB approximation is very useful and very correct, the quantum limit may be "just around the corner" in your mind, as that limit is, not surprisingly, often of the central concern in quantum mechanics!

10.2 The WKB expansion

Let us consider a familiar form of the TISE, Eq. 3.1 or 3.3 in the real space representation. Specifically, let us consider a particle in one dimension.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) \;=\; E\psi(x) \tag{10.1}$$

How might one consider a semi-classical approximation of this equation? The following points are worth recalling.

1. The semi-classical limit is approached for high quantum number (and thus high energy).

2. At high quantum number, $\psi(x)$ oscillates very rapidly.

3. This means that the de Broglie wavelength is much smaller than the length scale of the problem determined by $V(x)$ (and the energy value).

4. Also, at high quantum number, the energy level spacing $\sim \hbar\omega$ where ω is the characteristic angular frequency of the system, becomes much smaller than the energy itself. In this sense, the effect of $\hbar$ becomes negligible.

5. If the effect of $\hbar$ becomes negligible, then the canonical commutation relations $[\hat{q}, \hat{p}_q] = i\hbar$ (q is a generalized coordinate and p_q its canonical conjugate momentum) and the angular momentum commutation relations $[\hat{J}_j, \hat{J}_k] = i\hbar\epsilon_{jkl}\hat{J}_l$ become unimportant, allowing for the classical mechanical behaviors to emerge.

With these points in mind, let us consider a solution of the form

$$\psi(x) = A\exp\left(i\frac{S(x)}{\hbar}\right) \tag{10.2}$$

where A is a normalization constant. Trivially, *any* wave function $\psi(x)$ can be expressed this way: $S(x) = -i\hbar\log\psi$ with $A = 1$ will do, or $S(x) = -i\hbar\log\psi(x) + i\hbar\log\psi(x_0)$ with $A = \psi(x_0)$ at some chosen value of x_0 will do. In this general view, note that $S(x)$ is a complex function, and *completely* replaces $\psi(x)$.

In the semi-classical limit, we expect $S(x)$ to oscillate rapidly in comparison to the length scale of $V(x)$. I.e., $S(x)$ is expected to behave like kx, *locally*, i.e. on a short length scale over which $V(x)$ does not change appreciably.

With this expectation in mind, let us plug Eq. 10.2 into Eq. 10.1, obtaining a differential equation for $S(x)$[1].

$$-\frac{\hbar^2}{2m}\left(\frac{i}{\hbar}\frac{d^2S}{dx^2} - \frac{1}{\hbar^2}\left(\frac{dS}{dx}\right)^2\right)\psi(x) = (E - V(x))\,\psi(x)$$

$$\left(\frac{dS}{dx}\right)^2 - i\hbar\frac{d^2S}{dx^2} = p^2(x) \qquad p(x) \equiv \sqrt{2m(E-V(x))} \tag{10.3}$$

$$\left(\frac{dS}{dx}\right)^2 - p^2(x) = i\hbar\frac{d^2S}{dx^2} \qquad \text{RHS: perturbation term} \tag{10.4}$$

So far, we have been treating the TISE exactly. However, in the last form, the perturbation expansion with $\hbar$ as a perturbation parameter is suggested, thereby giving **the WKB expansion**. It is in this sense that the WKB approximation is a semi-classical approximation. If $\hbar$ goes to zero, we lose the quantization of angular momentum, the quantization of energy, and the commutator algebra, as we explained above. This is indeed the limit that we like to explore. So, let us work out a leading

[1] The real part of this is the *action* that you are familiar with from classical mechanics, as in "the least action principle." To learn more about quantum mechanics from the action point of view, you can read, in your leisure time, one of the books by Feynman, e.g. "Quantum Mechanics and Path Integrals."

order perturbation solution on Eq. 10.4, treating $\hbar$ as a perturbation parameter (for more discussion, see the next section).

$$\left(\frac{dS^{(0)}}{dx}\right)^2 - p^2(x) = 0 \qquad \text{0th order eq.} \quad (10.5)$$

$$S^{(0)}(x) = \pm\int^x dx\, p(x) \qquad \text{0th order sol.} \quad (10.6)$$

$$\left(\frac{dS^{(0)}}{dx} + \frac{dS^{(1)}}{dx} + ...\right)^2 - p^2(x) = i\hbar\frac{d^2S^{(0)}}{dx^2} \qquad \text{plug } S^{(0)} \text{ into the RHS of Eq. 10.4}$$

$$\pm 2p(x)\frac{dS^{(1)}}{dx} = \pm i\hbar p'(x) \qquad \text{keep } O(\hbar) \text{ terms only} \rightarrow \text{1st order eq.} \quad (10.7)$$

$$S^{(1)}(x) = i\frac{\hbar}{2}\log p(x) \qquad \text{1st order sol.} \quad (10.8)$$

where in the last step an integration constant is omitted, since it can be absorbed into the constant A in Eq. 10.2.

The third step above may be potentially a bit confusing. Why do we use both $S^{(0)}$ and $S^{(1)}$ on the LHS? Recall from the perturbation theory (LN 3, page 4, box, step 3) that what we need to do is to solve $L = R_{j+1}$ with $j = 0$. In this expression, formally and only formally, L can be thought to contain the solution to all orders, starting from the zeroth order. What is crucial, of course, is to note that the solution of the approximate equation $L = R_{j+1}$ is valid only up to the $(j+1)$-th order (point 4 of the same box), where the only new information that we get is the $(j+1)$-th order correction. Remembering this, we are using the expansion $S = S^{(0)} + S^{(1)} + ...$ on the LHS, to isolate the first order term there. The isolated first order term is the LHS of the next equation ($\pm 2p(x)\frac{dS^{(1)}}{dx}$), which is equated to the first order term of the RHS (which is just itself at this step of the perturbation). Note that, compared to the $\psi(x)$ form or the Schrödinger equation, which is *linear* in $\psi(x)$, the above equation for $S(x)$ is *non-linear*. This is the reason why plugging in only $S^{(1)}$ to the LHS of Eq. 10.4 will not do.

Therefore, to first order, **the WKB solution** is

$$\psi(x) = \frac{A}{\sqrt{p(x)}}\exp\left(\frac{i}{\hbar}\int^x dx\, p(x)\right) + \frac{B}{\sqrt{p(x)}}\exp\left(-\frac{i}{\hbar}\int^x dx\, p(x)\right) \quad (10.9)$$

While this is a solution to the linear order in $\hbar$, it is clear that **the WKB expansion** can be carried out to higher orders, if desired. Also, note that the integral $\int^x dx\, p(x)$ means an indefinite integral of $p(x)$. The coefficient A or B and any arbitrary integration constant of the indefinite integral together define *one* coefficient: i.e. the above solution contains two independent coefficients, not four.

Note that we assumed nothing about the reality of $p(x)$ in this derivation. Indeed, $p(x)$ in Eq. 10.9 need not be real. As defined in Eq. 10.3, $p(x)$ may well be purely

imaginary if $V(x) > E$ (non-classical region or "tunneling" region), while it will be real if $E > V(x)$ (classical region).

10.3 The perturbation parameter

As is often the case, we now ask the question "what is the perturbation parameter?" *after* we have done the perturbation expansion.

In the above, we've been talking about $O(\hbar)$, but it is clear that $\hbar$ cannot be a real perturbation parameter, since it has a dimension (of angular momentum or action).

Let us look at the solution that we got in Eqs. 10.6 and 10.8

$$S(x) \;=\; \pm \int^x dx\, p(x) + i\frac{\hbar}{2} \log \frac{p(x)}{p(x_0)} + ...$$

where for this discussion we put the integration constant in the first order term explicitly. It is clear from this expression that the following conditions must hold in order for the perturbation to make sense

$$\varepsilon \;\equiv\; \frac{\hbar}{|\int dx\, p(x)|} \ll 1 \quad \text{and} \quad \left|\frac{p(x)}{p(x_0)}\right| \gtrsim 1 \tag{10.10}$$

Here, x_0 is an arbitrary/typical value of x at which the WKB approximation is valid, and $|\int dx\, p(x)|$ is *not* the magnitude of an indefinite integral but the magnitude of the integral of $p(x)$ over a characteristic length scale of the problem (e.g. the width of the potential well; see examples below).

The requirement that $|p(x)|$ is not too small (i.e. $\left|\frac{p(x)}{p(x_0)}\right| \gtrsim 1$) is necessary, since the logarithm will diverge if $|p(x)|$ is too small. Instructively, we also note that, if $|p(x)| \to 0$, then the wave function of Eq. 10.9 diverges, signaling that something is indeed wrong.

Another way to characterize the perturbation parameter is to require that the de Broglie wavelength is much smaller than the length over which the potential changes significantly. That is, we require that the potential function changes very little over one de Broglie wavelength.

$$\left|\frac{V'(x)}{V(x)}\right| \lambda \;\ll\; 1 \qquad\qquad \lambda = h/p$$

$$\left|\frac{V'(x)}{V(x)}\,\frac{2\pi\hbar}{p(x)}\right| \ll 1$$

Notice that this condition is essentially the same as the condition of $\varepsilon \ll 1$, since by argument using the mean value theorem $\int dx\, p(x) \sim p(x)a$, where a is the characteristic length scale of the problem, and $|V'(x)/V(x)| \sim 1/a$. This condition also breaks down if $p(x) \approx 0$, correctly signaling an alarm for this problematic region, which we already identified above.

10.4 Classical region

If $p(x) > 0$, in Eq. 10.9, i.e. if $E > V(x)$, then we have a classical region. The solution, of Eq. 10.9 is indeed a locally plane wave solution, since $\int^x dx p(x) \approx p(x)(x - x_0) + const.$ in the vicinity of a chosen value of x_0, where $x \approx x_0$. The factor $1/\sqrt{p(x)}$ means that the probability density to find the particle is proportional to $1/p(x)$, which makes sense in the classical limit. For a given classical particle moving in a potential, the probability to find the particle in a given interval dx is proportional to the time that the particle spends in that time interval $dt = dx/v(x)$, and so we expect that the probability distribution function to be proportional to $1/v(x) = m/p(x)$.

It is often more convenient to use k instead of $p = \hbar k$. Then, the WKB wave function is given by

$$\psi(x) = \frac{A}{\sqrt{k(x)}} \exp\left(i \int^x dx\, k(x)\right) + \frac{B}{\sqrt{k(x)}} \exp\left(-i \int^x dx\, k(x)\right) \tag{10.11}$$

$$k(x) \equiv \frac{\sqrt{2m(E - V(x))}}{\hbar} \tag{10.12}$$

where A, B are arbitrary constants (not having the same values as those in Eq. 10.9).

10.5 Tunneling region

If $E < V(x)$, then $p(x) = i\hbar\kappa(x)$ where $\kappa(x) > 0$. This is the so-called non-classical region, or the tunneling region. The WKB wave function is given by

$$\psi(x) = \frac{A}{\sqrt{\kappa(x)}} \exp\left(-\int^x dx\, \kappa(x)\right) + \frac{B}{\sqrt{\kappa(x)}} \exp\left(\int^x dx\, \kappa(x)\right) \tag{10.13}$$

$$\kappa(x) = \frac{\sqrt{2m(V(x) - E)}}{\hbar} \tag{10.14}$$

where A, B are, again, arbitrary constants (not having the same values as those in Eq. 10.9).

10.6 Connection formulae

The above formulae, Eqs. 10.11 and 10.13, are well-defined approximations, as long as our assumptions discussed in Section 10.3 are valid: (1) the potential is slowly varying compared to the De Broglie wavelength and (2) $p(x)$ is not close to 0.

Condition (2) means that the above theory will break down when x is near one of the so called "turning points," i.e. those points where $E = V(x)$.

Fortunately, the problem with $E \approx V(x)$ turns out to be an easy problem to solve **if, as is often the case, the potential can be approximated as a linear function around the turning point**. This is done in Section T8.3, which is left for your reading. Here, we are interested only in the end results (Eq. T8.46, which corresponds to the third formula below; other formulae can be derived similarly): i.e. how the solution of the problem near the turning point enables us to match the *WKB wave functions* in the classical region and the non-classical region.

Materials in Section T8.3 are interesting, but they are not crucial within the spirit of this lecture and the next, except for their end results, summarized below. This is because most useful results of the WKB approximation can be obtained by inspecting the WKB wave functions away from turning points. Usually, we do not need to know what the actual wave function looks like near turning points. However, we do need to know how WKB wave functions studied above, piecewise valid in the classical region and in the tunneling region, are connected up correctly through a turning point.

Let us assume that we have a classical region well inside two turning points x_1, x_2. Please refer to the first page of LN 11, for the diagram of the two turning points. Note the sign of the slope of the potential at each turning point. For x well on the right side of x_2, we have a non-classical region, as we also do for x well on the left hand side of x_1. Then, the connection formulae at x_1 are given by

$$\frac{1}{\sqrt{\kappa}} \exp\left(-\int_x^{x_1} dx\, \kappa(x)\right) \quad \Longleftrightarrow \quad \frac{2}{\sqrt{k}} \sin\left(\int_{x_1}^{x} dx\, k(x) + \frac{\pi}{4}\right) \tag{10.15}$$

$$-\frac{1}{\sqrt{\kappa}} \exp\left(\int_x^{x_1} dx\, \kappa(x)\right) \quad \Longleftrightarrow \quad \frac{1}{\sqrt{k}} \sin\left(\int_{x_1}^{x} dx\, k(x) - \frac{\pi}{4}\right) \tag{10.16}$$

while the connection formulae at x_2 are given by

$$\frac{2}{\sqrt{k}} \sin\left(\int_x^{x_2} dx\, k(x) + \frac{\pi}{4}\right) \quad \Longleftrightarrow \quad \frac{1}{\sqrt{\kappa}} \exp\left(-\int_{x_2}^{x} dx\, \kappa(x)\right) \tag{10.17}$$

$$\frac{1}{\sqrt{k}} \sin\left(\int_x^{x_2} dx\, k(x) - \frac{\pi}{4}\right) \quad \Longleftrightarrow \quad -\frac{1}{\sqrt{\kappa}} \exp\left(\int_{x_2}^{x} dx\, \kappa(x)\right) \tag{10.18}$$

where the sinusoidal solutions apply in the classical region and the exponential solutions apply in the non-classical, tunneling, region. The symbol $\Longleftrightarrow$ means "connects with."