THE WKB APPROXIMATION

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Note 1. *The following notes are largely adapted from (physics) lecture notes for a course at UC Berkeley and are available at* `http://hitoshi.berkeley.edu/221A/WKB.pdf`.

In this document we provide a brief introduction to the WKB approximation for one-dimensional Schrödinger operators. We focus primarily on the example of the harmonic oscillator. We also include a discussion of the stationary phase approximation in one dimension. These notes are the basis for my lectures at the undergraduate conference *Quantization and Mathematics*, held at Northwestern University during the weeks of June 18-30, 2012.

For a different perspective on the WKB method for the one-dimensional Schrödinger equation (from the point of view of the stationary phase approximation), see the book review by Marsden and Weinstein of the book *Geometric asymptotics* by Guillemin and Sternberg. It appeared in the Bulletin of the AMS in May 1979.

The main goal of these lectures is to provide a motivation for the construction of approximate solutions. Our second goal is to show that there are discrete energy levels for which the quantum harmonic oscillator admits static solutions. We do this by constructing approximations of solutions of the one-dimensional static Schrödinger equation away from classical turning points and then match them up using Airy functions. Our approach will not be particularly rigorous, but most of the work done can be made rigorous relatively easily (see me if you are interested in making it rigorous!). There is one step, however, where making our argument rigorous is more difficult, namely, when we declare that the approximate energy levels we find are actually approximations of the energy levels for the problem. We do not address this issue in these notes.

We use the notation $O(h^k)$ to denote the product of h^k and a bounded function.

1. The one-dimensional Schrödinger equation

For a given potential $V(x)$ (that grows at infinity in a way we will not make precise), the one-dimensional Schrödinger equation seeks a wave function $\Psi(t,x)$ satisfying

$$ih\frac{\partial \Psi}{\partial t} = -\frac{h^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi = \left[-\frac{h^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(t,x) \tag{1}$$

Here h is Planck's constant and m is a mass. For the purposes of these lectures, we always adopt the convention that $m = 1$. (If you like, we can choose units so that this is true.)

We seek *static* solutions of this equation, i.e., those so that $\Psi(t,x) = e^{-iEt/h}\psi(x)$ for some other function ψ, which is independent of t. One should think of E as an energy level. The equation (1) then becomes

$$\left[-\frac{h^2}{2}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\psi(x). \tag{2}$$

Note 2. *We always assume that E is a* regular value *of $V(x)$. In other words, we assume that the set of points where $V(x) = E$ is discrete and that $V'(x)$ does not vanish at these points. We assume additionally that the set of points where $V(x) = E$ is in fact finite.*

As the operator $-\frac{h^2}{2}\frac{\partial^2}{\partial x^2} + V(x)$ plays such an important role, let us give it the name L, i.e.,

$$(L\psi)(x) = -\frac{h^2}{2}\psi''(x) + V(x)\psi(x). \tag{3}$$

We may thus rewrite our equation (2) as

$$L\psi - E\psi = 0. \tag{4}$$

The typical example we use is the *quantum harmonic oscillator*, which is the above problem with $V(x) = \frac{1}{2}\omega^2 x^2$. (Typically there is a factor of m as well, but we are assuming $m = 1$.)

2. Classical mechanics

In the Hamiltonian formulation of classical mechanics, one begins with a *Hamiltonian* function $H(x, p)$, which should be thought of as an expression for energy. H is a function of position x and momentum p, and the positions and momenta of classical particles evolve according to the Hamilton flow of H. In particular, if $(x(t), p(t))$ is the trajectory of the particle, then

$$\begin{aligned} \dot{x}(t) &= \frac{\partial H}{\partial p} \\ \dot{p}(t) &= -\frac{\partial H}{\partial x}. \end{aligned} \tag{5}$$

For such trajectories (x, p), the Hamiltonian is conserved, i.e.,

$$H(x(t), p(t)) \text{ is independent of } t.$$

Exercise 1. *("Conservation of energy") Show that the Hamiltonian is conserved by differentiating it in time and using the equations* (5).

For the systems considered here, the Hamiltonian can be written

$$H(x, p) = \frac{1}{2}p^2 + V(x). \tag{6}$$

We think of the first term as representing kinetic energy and the second term as potential energy.

Note 3. *Often the Schrödinger equation* (2) *above is called the* quantization *of this Hamiltonian.*

Let us seek functions $x(t)$ and $p(t)$ of a special form. Indeed, let's assume that $\dot{x} = p$ and $p(t) = S'(x(t))$.

Proposition 4. *If $\dot{x} = p$ and $p = S'(x)$, then if x and p satisfy Hamilton's equations* (5) *for a non-zero value of the Hamiltonian, then S satisfies the* Hamilton-Jacobi equation

$$\frac{1}{2}\left(S'(x)\right)^2 + V(x) = E \tag{7}$$

for some energy E.

Proof. Suppose that x and p satisfy Hamilton's equations and let $E = H(x(0), p(0))$. Note that $E \neq 0$ by assumption. We know from Exercise 1 that $H(x(t), p(t)) = E$ for all t. Plugging in the form of p then finishes the proof. □

Note 5. *One thing to note about this is the occurrence of classical "turning points" where the classical particle changes direction. These occur when $p = 0$, i.e., when $V(x) = E$ and $S'(x) = 0$. The region where the total energy E is less than $V(x)$ is referred to as the* classically forbidden region.

One may solve the Hamilton-Jacobi equation above relatively explicitly, as we have

$$S'(x) = \pm\sqrt{2(E - V(x))}$$

and so S is an antiderivative of this function. Note that in the classically forbidden region, $S'(x)$ (and so $S(x)$) is imaginary. For the harmonic oscillator, this takes the form

$$S'(x) = \pm\sqrt{2E - \omega^2 x^2}.$$

3. The WKB approximation

In this section our aim is to construct *approximate solutions* of the static Schrödinger equation (4). We want our solutions to decay at infinity and so we expect that the family of allowable energies E should *quantize*, i.e., there should be only a discrete set of allowed energies.

In constructing our approximations, we treat h as a small (positive) parameter and keep track of terms up to order h. The idea is that if h is small enough then the approximation we build will be close to a true solution.

We proceed in three steps. We first construct approximate solutions away from the turning points (where $V(x) = E$). Next we construct approximate solutions near the turning points using a linear approximation of the potential, which involves understanding *Airy functions*. We finally piece these together, which will give us a condition on the allowable energies E.

3.1. Away from the turning points.

Because the set of turning points is finite, it divides the real line into regions where either $V(x) > E$ or $V(x) < E$. On each of these regions, we seek an approximation of the form

$$\psi(x) = e^{iS(x)/h}, \tag{8}$$

where $S(x)$ also depends nicely on h, i.e., $S(x) = S_0(x) + hS_1(x) + O(h^2)$. (Although we only want to keep track of ψ up to order h, this requires that we keep track of S up to order h^2, as we are dividing it by h.) The ansatz (guess) (8) is often referred to as *the WKB ansatz*.

Plugging our guess into the equation (4) yields

$$L\psi - E\psi = \left(\frac{1}{2}(S'(x))^2 + V(x) - E - \frac{ih}{2}S''(x)\right)\psi(x). \tag{9}$$

Plugging in $S(x) = S_0(x) + hS_1(x) + O(h^2)$ and grouping terms of the same order in h then yields

$$L\psi - E\psi = \left(\left(\frac{1}{2}(S_0'(x))^2 + V(x) - E\right) + h\left(S_1'(x)S_0'(x) - \frac{i}{2}S_0''(x)\right)\right)\psi + O(h^2). \tag{10}$$

Note that the term of the form $h^2(S_1'(x))^2$ was absorbed into the $O(h^2)$ term.

Our aim is to choose S_0 and S_1 so that $L\psi - E\psi = O(h^2)$. To do this we just arrange that the $O(1)$ and $O(h)$ terms both vanish, i.e., we arrange that

$$\frac{1}{2}(S_0'(x))^2 + V(x) - E = 0$$
$$S_1'(x)S_0'(x) - \frac{i}{2}S_0''(x) = 0.$$

The first of these equations is none other than the Hamilton-Jacobi equation that popped up in Section 2, so we know that $S_0'(x)$ satisfies

$$S_0'(x) = \begin{cases} \pm\sqrt{2(E - V(x))} & E > V(x) \\ \pm i\sqrt{2(V(x) - E)} & V(x) > E \end{cases}$$

We may thus choose S_0 to be an antiderivative of this quantity. Using the second equation now implies that

$$S_1' = \frac{i}{2}\frac{S_0''}{S_0'},$$

i.e., the derivative of S_1 is fixed once we fix our choice of S_0'. We may solve this to conclude that

$$S_1(x) = \frac{i}{2}\log|S_0'(x)| + C$$

for some constant C.

Plugging this into our guess shows that

$$\psi(x) = c\,|S_0'(x)|^{-1/2}\, e^{iS_0(x)/h} + O(h)$$

and that such ψ satisfy $L\psi - E\psi = O(h^2)$.

Exercise 2. *Show that by keeping track of more terms in the series for S you may construct a better approximate solution. In other words, show that if you keep track of S up to order h^k then you may arrange that $L\psi - E\psi = O(h^k)$.*

Returning to our example of the harmonic oscillator, we have that $V(x) = \frac{1}{2}\omega^2x^2$, and the turning points are given by $x = \pm\frac{\sqrt{2E}}{\omega}$. Let us label these two points x_L and x_R, for "left" and "right". The classically forbidden region ($V(x) > E$) is given by $x > x_R$ or $x < x_L$. We know that $S_0'(x)$ is imaginary in this region, so $iS_0(x)$ has a non-zero real part. Because we want to guarantee that our solutions do not grow exponentially at infinity, we are forced to choose the sign of S_0' to pick the decaying solution. This corresponds to choosing

$$S_0'(x) = \begin{cases} i\sqrt{\omega^2x^2 - 2E} & x > x_R \\ i\sqrt{\omega^2x^2 - 2E} & x < x_L \end{cases}$$

For concreteness, let us call the first case $S_{0,R}$ and the second case $S_{0,L}$. In the classically allowed region (where $V(x) < E$), we have two different options corresponding to our choice of sign, and we call these $S_{0,\pm}$. Observe that all have the same magnitude, $\sqrt{|\omega^2x^2 - E|}$.

We may thus write

$$\psi(x) = \begin{cases} \frac{c_L}{(2\cdot|V(x)-E|)^{1/4}}e^{iS_{0,L}(x)/h} + O(h) & x < x_L \\ \frac{c_-}{(2\cdot|E-V(x)|)^{1/4}}e^{iS_{0,-}(x)/h} + \frac{c_+}{(2\cdot|E-V(x)|)^{1/4}}e^{iS_{0,+}(x)/h} + O(h) & x_L < x < x_R \\ \frac{c_R}{(2\cdot|V(x)-E|)^{1/4}}e^{iS_{0,R}(x)/h} + O(h) & x > x_R \end{cases} \tag{11}$$

Note that we have the freedom to choose our constants c_L, c_R, and $c_\pm$, but we have no guarantees that these match up.

3.2. **Near the turning points.** Near the turning points, the approximation above breaks down. Perhaps the easiest way to see this is that the denominators all tend to 0! A more careful analysis would also show that our expansion for S also breaks down, i.e., hS_1 is no longer much smaller than S_0.

Our assumption on the turning points ($V(x) = E$) implies that at each turning point x_0, we have $V'(x_0) \neq 0$. We use the linear approximation of V near these turning points, i.e.,

$$V(x) = V(x_0) + V'(x_0)(x - x_0) + O((x - x_0)^2).$$

Note that $V(x_0) = E$ by assumption. Plugging this approximation into the equation (2) yields

$$-\frac{h^2}{2}\frac{d^2}{dx^2}\psi(x) + \big(E + V'(x_0)(x - x_0) + O((x - x_0)^2) - E\big)\,\psi(x) = 0.$$

In other words,

$$-\frac{h^2}{2}\frac{d^2}{dx^2}\psi + V'(x_0)(x - x_0)\psi = O((x - x_0)^2).$$

We now use the change of variables given by

$$u = \left(\frac{2V'(x_0)}{h^2}\right)^{1/3}(x - x_0).$$

(Note that in this change of variables, we have that $O((x - x_0)^2) = O(h^{4/3}u^2)$.) Using the chain rule, we have that

$$\frac{d^2}{dx^2}\psi = \left(\frac{2V'(x_0)}{h^2}\right)^{2/3}\frac{d^2}{du^2}\psi,$$

and so the equation becomes

$$\begin{aligned}
0 &= -\frac{h^2}{2}\left(\frac{2V'(x_0)}{h^2}\right)^{2/3}\frac{d^2}{du^2}\psi + V'(x_0)(x - x_0)\psi + O((x - x_0)^2) \\
&= -\left(h^{2/3}2^{-1/3}V'(x_0)^{2/3}\right)\left(\frac{d^2}{du^2}\psi - V'(x_0)^{1/3}h^{-2/3}2^{1/3}(x - x_0)\psi + O(h^{-2/3}(x - x_0)^2)\right) \\
&= -\left(h^{2/3}2^{-1/3}V'(x_0)^{2/3}\right)\left(\frac{d^2}{du^2}\psi - u\psi + O(h^{2/3}u^2)\right).
\end{aligned}$$

We treat the $O(h^{2/3}u^2)$ as negligible and solve the related equation

$$\left(\frac{d^2}{du^2} - u\right)\psi = 0. \tag{12}$$

This is called the Airy equation and has two linearly independent solutions. One of these solutions is called the Airy function and is given by an integral expression:

$$\mathrm{Ai}(u) = \frac{1}{\pi}\int_0^\infty \cos\left(\frac{1}{3}t^3 + ut\right)dt \tag{13}$$

Exercise 3. *Verify that* $\mathrm{Ai}(u)$ *indeed solves the Airy equation* (12). *Hint: You can write it as an integral of a derivative; you then need to check that the boundary terms vanish. The boundary term at infinity is tricky, so you should consider what happens over a small interval when* t *is large. Part of this exercise is to determine why this integral even converges! You can check this with an informal argument regarding the oscillations, by a clever application of integration by parts, or by using complex analysis.*

As u goes to $\pm\infty$, the Airy function has the following behavior[1]:

$$\mathrm{Ai}(u) \sim \begin{cases} \frac{1}{2\sqrt{\pi}} u^{-1/4} \exp\left(-\frac{2}{3}u^{3/2}\right) & u \to \infty \\ \frac{1}{\sqrt{\pi}}(-u)^{-1/4} \cos\left(\frac{2}{3}u\sqrt{-u} + \frac{\pi}{4}\right) & u \to -\infty \end{cases}$$

Here the asymptotic behavior means that $\mathrm{Ai}(u)$ is equal to the claimed function plus terms that decay faster than the given function. (In fact, it has a sort of "Taylor series" at infinity, but we don't necessarily need this here.) For the purposes of these lectures, we'll take the above formula as a "black box".

Undoing the change of coordinates tells us that

$$\psi(x) = c_{x_0} \,\mathrm{Ai}\left(\left(\frac{2V'(x_0)}{h^2}\right)^{1/3} (x - x_0)\right) \tag{14}$$

is a solution of equation (2) up to order $(x - x_0)^2$ near x_0.

Let us now use again the linear expansion $V(x) \sim E + V'(x_0)(x - x_0)$ to conclude that

$$u = \left(\frac{2V'(x_0)}{h^2}\right)^{1/3} (x-x_0) = \left(\frac{1}{4V'(x_0)^2h^2}\right)^{1/3} 2V'(x_0)(x-x_0) \sim \left(\frac{1}{4V'(x_0)^2h^2}\right)^{1/3} 2(V(x)-E),$$

and so for $u > 0$,

$$u^{1/2} \sim \left(\frac{1}{4V'(x_0)^2h^2}\right)^{1/6} \sqrt{2(V(x) - E)}.$$

Similarly, we know that $\frac{2}{3}u^{3/2} = \int u^{1/2}du$ and so

$$\frac{2}{3}u^{3/2} \sim \frac{\operatorname{sgn} V'(x_0)}{h} \int \sqrt{2(V(x) - E)},$$

where the constants have cancelled due to the change of variables, and $\operatorname{sgn} V'(x_0)$ is 1 when $V'(x_0)$ is positive and -1 when $V'(x_0)$ is negative.

If $V'(x_0) > 0$, the function ψ has asymptotics given by

$$\psi(x) = \begin{cases} \frac{c_{x_0}}{2}\left(\frac{h(2V'(x_0))^{1/3}}{h^{2/3}\pi\sqrt{2(V(x)-E)}}\right)^{1/2} \exp\left(-\frac{1}{h}\int_{x_0}^{x}\sqrt{2(V(x') - E)}dx'\right) & x > x_0 \\ c_{x_0}\left(\frac{h(2V'(x_0))^{1/3}}{h^{2/3}\pi\sqrt{2(E-V(x))}}\right)^{1/2} \cos\left(\frac{1}{h}\int_{x_0}^{x}\sqrt{2(E - V(x'))}dx' + \frac{\pi}{4}\right) & x < x_0 \end{cases} \tag{15}$$

[1] One thing that is nice about special functions is that they've been studied for a very long time, so you don't have to derive formulae like these on your own!

Similarly, if $V'(x_0) < 0$, then the classically allowed region is to the right of the turning point and ψ has asymptotics given by

$$\psi(x) = \begin{cases} \frac{c_{x_0}}{2}\left(\frac{h(2|V'(x_0)|)^{1/3}}{h^{2/3}\pi\sqrt{2(V(x)-E)}}\right)^{1/2} \exp\left(\frac{1}{h}\int_{x_0}^{x}\sqrt{2(V(x')-E)}dx'\right) & x < x_0 \\ c_{x_0}\left(\frac{h(2|V'(x_0)|)^{1/3}}{h^{2/3}\pi\sqrt{2(E-V(x))}}\right)^{1/2} \cos\left(\frac{1}{h}\int_{x_0}^{x}\sqrt{2(E-V(x'))}dx' - \frac{\pi}{4}\right) & x > x_0 \end{cases}$$

In the case of the harmonic oscillator, the expressions above do not simplify much, but one has that $V'(x_L) = 2\omega^2 x_L = -2\omega\sqrt{2E}$ and $V'(x_R) = 2\omega\sqrt{2E}$.

3.3. **Piecing the approximate solution together.** We now have approximate solutions away from the turning points and approximate solutions near the turning points. Our aim is to determine when we can piece them together. In this section we consider only the example of the harmonic oscillator, though other specific examples are not too bad, either.

We have three regions of interest and two points where they must meet. Consider first the right turning point $x_R = \frac{\sqrt{2E}}{\omega}$. To the right of x_R, $S_{0,R} = i\int\sqrt{2(V(x)-E)}$, and so our solution must behave as

$$\frac{c_R}{2^{1/4}|V(x)-E|^{1/4}}e^{-\frac{1}{h}\int\sqrt{2(V(x)-E)}}$$

and we want this to match the Airy function found in the previous section, whose asymptotics are given by

$$\frac{h^{1/6}c_{x_R}|V'(x_R)|^{1/6}}{2^{5/6}}|2(V(x)-E)|^{-1/4}\exp\left(\frac{1}{h}\int\sqrt{2(V(x)-E)}\right),$$

and so we must have $c_{x_R} = h^{-1/6}\tilde{c}_{x_R}$, where $\tilde{c}_{x_R}$ is a constant multiple of c_R, determined by the matching condition.

We now try to match the solutions in the classically allowed region ($x_L < x < x_R$) to the other end of the Airy function solution (whose coefficient has now been determined). In the classically allowed region, we have a solution whose behavior near x_R is given by

$$\frac{1}{(2|E-V(x)|)^{1/4}}\left(c_- e^{-\frac{i}{h}\int\sqrt{2(E-V(x))}} + c_+ e^{\frac{i}{h}\int\sqrt{2(E-V(x))}}\right),$$

which should match the Airy function solution, with asymptotics

$$\tilde{c}_{x_R}\left(2^{1/3}|V'(x_0)|^{1/3}\right)^{1/2}|2(E-V(x))|^{-1/4}\cos\left(\frac{1}{h}\int_{x_R}^{x}\sqrt{2(E-V(x))}+\frac{\pi}{4}\right).$$

This determines c_- and c_+ in terms of $\tilde{c}_{x_R}$ (and so in terms of c_R).

Now we match to the other turning point. We want the solution to agree with the Airy function approximation, which has asymptotics (with $\tilde{c}_{x_L} = h^{-1/6}c_{x_L}$)

$$\tilde{c}_{x_L}\left(2^{1/3}|V'(x_0)|^{1/3}\right)^{1/2}|2(E-V(x)|^{-1/4}\cos\left(\frac{1}{h}\int_{x_L}^{x}\sqrt{2(E-V(x))}dx-\frac{\pi}{4}\right).$$

Note that we no longer have the freedom to choose c_{x_L} – it should be determined by $c_\pm$. In fact, there is no guarantee that the two exponential functions above combine to give something like a cosine at x_L!

This is where we obtain a restriction on the allowed energies: We require that

$$\cos\left(\frac{1}{h}\int_{x_R}^{x}\sqrt{2(E-V(x'))}dx' + \frac{\pi}{4}\right) = \pm\cos\left(\frac{1}{h}\int_{x_L}^{x}\sqrt{2(E-V(x'))}dx' - \frac{\pi}{4}\right),$$

i.e., we require that they are constant multiples of one another. This amounts to the requirement that their arguments differ by a multiple of π, i.e.,

$$\frac{1}{h}\int_{x_R}^{x}\sqrt{2(E-V(x'))}dx' + \frac{\pi}{4} = \frac{1}{h}\int_{x_L}^{x}\sqrt{2(E-V(x'))}dx' - \frac{\pi}{4}$$

and so

$$\int_{x_L}^{x_R}\sqrt{2(E-V(x))}dx = \left(n+\frac{1}{2}\right)\pi h.$$

If this holds, then we may find c_{x_L} and then determine c_L to obtain an approximate wave function.

For our example when $V(x) = \frac{1}{2}\omega^2 x^2$, this is the requirement that

$$\int_{-\frac{\sqrt{2E}}{\omega}}^{\frac{\sqrt{2E}}{\omega}}\sqrt{2E-\omega^2x^2}dx = \left(n+\frac{1}{2}\right)\pi h$$

We may evaluate this integral directly in this case by making the substitution $x = \frac{\sqrt{2E}}{\omega}\sin\theta$ to conclude

$$\int_{-\frac{\sqrt{2E}}{\omega}}^{\frac{\sqrt{2E}}{\omega}}\sqrt{2E-\omega^2x^2}dx = \frac{2E}{\omega^2}\int_{-\pi}^{\pi}\cos^2\theta\, d\theta = \frac{E}{\omega^2},$$

so the allowable energies are (to top order) $E = \left(n+\frac{1}{2}\right)\pi\omega^2 h$. In this case they are exactly right, but the wave functions are not. You've probably discussed this example from another point of view (creation/annihilation operators) in other settings.