11	Fri., 11/14	**8.1-.2** WKB Approximation & Tunneling	**Daily 11.F**
12	Mon., 11/17 Tues. 11/18	**6.1** Time-independent Perturbation, non-degenerate	**Daily 12.M** **Weekly 12**

Daily: Kyle Jacob Spencer Gigja Anton Jessica Sean Antwain Jonathan Casey Jeremy Mark Connor Brad

Equipment

- Griffith's text

Check dailies

Announcements

Daily 11.W Wednesday 11/12

1. *Math*: Griffiths 5.15
2. *Starting Weekly HW*: Griffith 5.16
3. *Starting Weekly HW*: Griffiths 5.18

These next few days, we'll be looking at ways to get approximate solutions to problems that are too difficult to exactly solve.

8. WKB Approximation

The first approximation technique that we'll look at is WKB's. The idea starts out rather similar to a trick we've played twice now – when solving Schrodinger's equation, factor limiting behavior out of your solution. We did this when tackling the Harmonic Oscillator the second time – factoring out the behavior as r goes to 0 and as r goes to infinity, so we could then focus on the simpler equation that governs the in between undulations. We did it again when tackling the radial equation for a central potential in 3-D (and you did it on the test when tackling the radial equation in 2-D).

The inspiration is that, if the potential varies on large length scale, then on the small length scale, the solution should look a lot like it would for a constant potential:

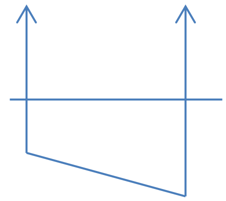
$$\psi(x) = Ae^{\pm ikx} \quad \text{for E > V,} \quad k = \sqrt{2m(E-V)}/\hbar \quad \textit{classically allowed region}$$
$$\psi(x) = Ae^{\pm \kappa x} \quad \text{for E < V,} \quad \kappa = \sqrt{2m(V-E)}/\hbar \quad \textit{classically forbidden region}$$

Of course, over the long length scale, the potential does vary, so the amplitude and the wavenumber or decay constant vary with *x*.

Conceptual Exercise

Given a potential, sketch a plausible wavefunction (amplitude and wavelength / decay length grow where |E-V| is small)

To get rigorous about this, we look at the two regions separately.



Does the WKB approximation mean we can solve quite a bit that was too complex before we had this?" [Casey P](#)

Yes, it's useful for potentials that won't yield exact, analytical solutions or if you just want a quick ball-park value. It's one of three approximation methods that the text introduces, two of which we'll looking at. They, along with computational approaches like we took early in the semester, are tools for tackling potentials that would be too difficult to tackle exactly.

"Could we instead talk about an average potential and treat the problem like the ones we did in Chapter 2 rather than assume the potential varies slowly? Would the results differ greatly?"
Spencer

That certainly would be the first and simplest approximation. For some questions, it might be good enough. What it wouldn't catch is spatial variation in the wavefunction (how its amplitude and wavelength might grow or shrink). I particularly expect that it would work well/poorly for states for whom the variation in energy is insignificant/significant compared with the states' energies.

8.1 The "Classical" Region

For

$$E\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi \quad \text{or} \quad -\hbar^2\frac{\partial^2\psi}{\partial x^2} = 2m(E - V(x))\psi \equiv p^2(x)\psi$$

We'll guess a solution of the form

$$\psi(x) = A(x)e^{i\phi(x)}$$

with both A(x) and ϕ(x) real to help tease apart the undulations and the modulations. Note: this guess is not an approximation, it's a perfectly valid way of expressing a complex function, but we're hoping it will prove a *useful* way for the cases we're interested in – short-scale undulations and long-scale modulation.

Plugging in,

$$\frac{\partial^2}{\partial x^2}\left(A(x)e^{i\phi(x)}\right)=-\frac{p^2(x)\psi}{\hbar^2}$$
$$\frac{\partial}{\partial x}\left(iA(x)e^{i\phi(x)}\frac{\partial\phi(x)}{\partial x}+\frac{\partial A(x)}{\partial x}e^{i\phi(x)}\right)$$

Or using the prime-ing notation to indicate differentiation with respect to *x*,

$$\frac{\partial}{\partial x}\left(i\phi' A e^{i\phi}+A' e^{i\phi}\right)=i\phi'' A e^{i\phi}+i\phi' A' e^{i\phi}-(\phi')^2 A e^{i\phi}+A'' e^{i\phi}+i\phi' A' e^{i\phi}$$
$$\left[i(\phi'' A+2\phi' A')+\left(A''-(\phi')^2 A\right)\right]e^{i\phi}=-\frac{p^2(x)}{\hbar^2}Ae^{i\phi}$$

Or getting all terms on the same side,

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

Now, since A and f are real, we have two completely independent terms that don't have a prayer of canceling each other – everything in the first brackets and multiplied by *i*, and everything in the second brackets. Yet they add up to 0, which tells us that each of these two terms must themselves be 0.

$$\phi'' A+2\phi' A'=0 \quad \text{and} \quad A''-(\phi')^2 A+\frac{p^2(x)}{\hbar^2}A=0$$

The former can be stepped back a pace with the differentiation to read

$$\frac{\partial}{\partial x}\left(A^2\phi'\right)=0$$

Which requires that $A^2\phi' = B$, some constant. Or $A=\sqrt{\dfrac{B}{\phi'}}$

Now, Griffiths has C^2 in place of my *B*, and so implies, and then asserts that C is real; however, we've not earned that assertion – for all we know at this point, ϕ' is negative.

Now it's time for the approximation. Looking at the other equation,

$$\frac{A''}{A}-(\phi')^2+\frac{p^2(x)}{\hbar^2}=0$$

Assume that A"/A << than the other terms. Qualitatively, that is assuming that the length scale over which this amplitude varies is much larger than the length scale over which the phase varies or of the wavelength.

$$(\phi')^2\approx\frac{p^2(x)}{\hbar^2}$$

$\phi'\approx\pm\dfrac{p(x)}{\hbar}$ so, $\phi(x)\approx\pm\dfrac{\int_{x_o}^{x}p(x')dx'}{\hbar}$ which, of course, introduces one arbitrary constant since we've only constrained the function's derivative.

Then returning to $A = \sqrt{\frac{B}{\phi'}}$, we have

$$A \approx \sqrt{\frac{B\hbar}{\pm p(x)}}$$

Now, we'd defined our function in the first place with A real, so B must have the same sign as we choose in the denominator.

$A \approx \sqrt{\frac{|B|\hbar}{p(x)}}$ or defining C to adsorb the constant h-bar and the rooting, $A \approx \frac{C}{\sqrt{p(x)}}$

So, the solution is

$$\psi(x) = A(x)e^{i\phi(x)} \approx \frac{C}{\sqrt{p(x)}} e^{\pm i \int_{x_o}^{x} p(x')dx'/\hbar}$$

$$|\psi(x)|^2 \approx \frac{C^2}{p(x)}$$

Griffiths points out that this backs up the intuitive rule of thumb we'd been using when sketching wavefunctions: the probability of finding the particle at a location is inversely proportional to its momentum, thus how fast it's going at that location.

Example 8.1 Bumpy-bottomed infinite-square well

$$V(x) = \begin{cases} V_{in}(x) & \text{in box} \\ \infty & \text{out of box} \end{cases}$$

Guess solution of

$$\psi(x) \approx \frac{1}{\sqrt{p(x)}}\left(C_+ e^{+i\phi(x)} + C_- e^{-i\phi(x)}\right)$$

Now, since the function for $\phi(x) \approx \pm \int_{x_o}^{x} p(x')dx'/\hbar$ introduces an arbitrary constant in the exponent, and that's equivalent to introducing one in the multiplicative constant C-, we can consider it adsorbed into C-. So we're free to choose the obvious starting point for our integral in this case,

$$\phi(x) \approx \int_0^x p(x')dx'/\hbar \text{, which means } \phi(0) \approx \int_0^0 p(x')dx'/\hbar = 0$$

For that matter, we can rewrite our guess in the form

$$\psi(x) \approx \frac{1}{\sqrt{p(x)}}\left(C_s \sin(\phi(x)) + C_c \cos(\phi(x))\right)$$

Boundary Conditions

$\psi(0) = \psi(a) = 0$

Where our requirement that $\psi(0) = 0$ means, like always, $\psi(0) \approx \frac{1}{\sqrt{p(0)}}(C_c) = 0$ so $C_c = 0$.

$$\psi(x) \approx \frac{C_s \sin(\phi(x))}{\sqrt{p(x)}}$$

Similarly, our requirement that

$$\psi(a) \approx \frac{C_s \sin(\phi(a))}{\sqrt{p(a)}} = 0$$

Means that

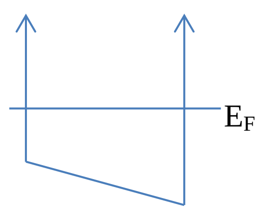
$$\phi(a) \approx \int_0^a p(x')dx'/\hbar = n\pi$$

Example 1.b

Solid conductor with voltage applied across it. Picking up where the free-electron model left off, say we apply a voltage across a conductor to make a current flow. What would the wavefunction and energies be?

The simplest model is an infinite square well with a sloped bottom.

$$V(x) = \begin{cases} \infty & \text{outside} \\ -eV\dfrac{x}{a} & \text{inside} \end{cases}$$



Let's say that

Let's say that $V(x) = \frac{1}{2}m\omega^2 x^2$, what's the approximate solution?

We need $p(x) = \sqrt{2m(E - V(x))}$ for the amplitude, $\phi(x) \approx \int_0^x p(x')dx'/\hbar$ for the phase, and $\phi(a) \approx \int_0^a p(x')dx'/\hbar = n\pi$ for setting a condition on the energy.

$$p(x) = \sqrt{2m\left(E - \frac{1}{2}m\omega^2 x^2\right)}$$

So $\phi(x) \approx \int_0^x \sqrt{2m\left(E - \frac{1}{2}m\omega^2 x'^2\right)}dx'/\hbar = \sqrt{2mE}/\hbar \int_0^x \sqrt{\left(1 - \frac{m\omega^2 x'^2}{2E}\right)}dx'$

Define $u = \sqrt{\frac{m}{2E}}\omega x' \Rightarrow x' = u\frac{1}{\omega}\sqrt{\frac{2E}{m}}$

$$\phi(x) \approx \sqrt{2mE}/\hbar \int_0^x \sqrt{\left(1-u^2\right)}du \frac{1}{\omega}\sqrt{\frac{2E}{m}} = \frac{2E}{\hbar\omega}\int_0^{u=\sqrt{\frac{m}{2E}}\omega x} \sqrt{\left(1-u^2\right)}du$$

$$\frac{2E}{\hbar\omega}\frac{1}{2}\left[\sqrt{1-\frac{m}{2E}\omega^2 x^2}\sqrt{\frac{m}{2E}}\omega x + \sin^{-1}\left(\sqrt{\frac{m}{2E}}\omega x\right)\right]$$

And the condition

$$\frac{2E}{\hbar\omega}\int_0^{u=\sqrt{\frac{m}{2E}}\omega a} \sqrt{\left(1-u^2\right)}du$$

Now,

$$\phi(a) \approx \int_0^a p(x')dx'/\hbar = n\pi$$

Means

$$\frac{E}{\hbar\omega}\left[\sqrt{1-\frac{m}{2E}\omega^2 a^2}\sqrt{\frac{m}{2E}}\omega a + \sin^{-1}\left(\sqrt{\frac{m}{2E}}\omega a\right)\right] = n\pi$$

$$\frac{1}{\hbar}\left[\sqrt{\frac{mE}{2}a^2 - \left(\frac{m}{2}\right)^2\omega^2 a^4} + \frac{E}{\hbar\omega}\sin^{-1}\left(\sqrt{\frac{m}{2E}}\omega a\right)\right] = n\pi$$

Not pretty. Transendental relation that sets the allowed E values.

8.2 Tunneling

When V > E, we could run through the same argument, but then pop on the world at the end that, oops, V > E, so

$$p(x) = \sqrt{2m(E - V(x))} = i\sqrt{2m(V(x) - E)}$$

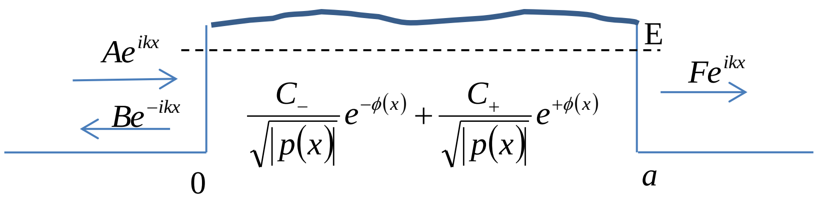
Then we'd have the same basic argument but we'd adsorb the *i* in the constant C out front and cancel the i in the exponent to have

$$\psi(x) \approx \frac{C}{\sqrt{|p(x)|}} e^{\pm\int_{x_o}^{x}|p(x')|dx'/\hbar}$$

Griffiths warns that one part of our derivation would have trouble, but I suspect that if we were careful, the same basic argument would be applicable since experience tells me you can safely hold off on ‘fixing’ the sign under the root until the end of your argument.

Now, this is useful for thinking how a wavefunction would propagate through a ‘classically forbidden’ region, where E <V.

He sets us up for a particular scenario:



Now, we *can* use the WKB approach to find an expression for the wavefunction within the barrier. However, Griffiths uses it to give a ballpark approximation for the particular question of tunneling through a barrier. His argument is that, as we know, the transmission coefficient is

$$T=\left|\frac{A}{F}\right|^2$$

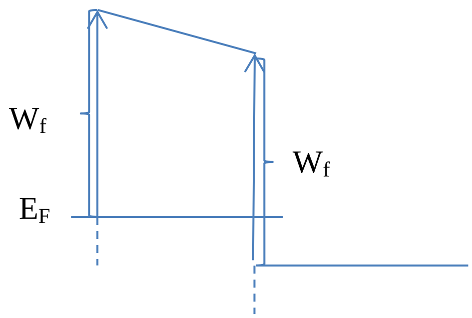
Then he argues that A is roughly the amplitude of the wave on the left of the barrier, while F is the amplitude on the right, and if the barrier is large compared with the decay length, then $C_+\approx 0$, so it’s $\frac{C_-}{\sqrt{|p(x)|}}e^{-\phi(x)}$ that connects the dots between A and F. That is

$$T=\left|\frac{F}{A}\right|^2\approx\left|\frac{\frac{C_-}{\sqrt{|p(a)|}}e^{-\phi(a)}}{\frac{C_-}{\sqrt{|p(0)|}}e^{-\phi(0)}}\right|^2=\left|\frac{\sqrt{|p(0)|}}{\sqrt{|p(a)|}}e^{-(\phi(a)-\phi(0))}\right|^2=\frac{|p(0)|}{|p(a)|}e^{-2(\phi(0)-\phi(a))}=\sqrt{\left(\frac{V(0)-E}{V(a)-E}\right)}e^{-2\int_0^a|p(x')|dx'/\hbar}$$

Griffiths ignores the prefactor (indeed, it would cause real trouble in example 8.2), and focuses just on the exponential.

Example 2.b

The converse of our conductor with a voltage applied across it is a capacitor with a voltage applied across it. The barrier for an electron escaping a material into free space, akin to the ionization energy, is known as the "Work function"; you may vaguely remember that from the photo-electric effect in which photons had to deliver that much energy to free electrons.



$$V(x) = \left(W_f + E_F\right) - eV\frac{x}{a}$$

What would be the transmission probability?

Note: this is a rather simple model for electrons tunneling between a sharp metal tip and conducting sample in STMs.

In scanning tunneling microscopy, the electric field between tip and sample translates into a roughly linear voltage / potential. $V(x) = V(0) - bx$.

$$\int_0^a |\, p(x')|\, dx'/\hbar$$

$$\int_0^a |p(x)| dx = \int_0^a \left|\sqrt{2m(V(x)-E)}\right| dx = \int_0^a \left|\sqrt{2m(V(0)-bx-E)}\right| dx = \sqrt{2mb}\int_0^a \left|\sqrt{\left(\frac{V(0)-E}{b} - x\right)}\right| dx$$

$$-\frac{2}{3}\sqrt{2mb}\left(\frac{V(0)-E}{b} - x\right)^{3/2}\Bigg|_0^a = -\frac{2}{3}\sqrt{2mb}\left(\left(\frac{V(0)-E}{b} - a\right)^{3/2} - \left(\frac{V(0)-E}{b}\right)^{3/2}\right)$$

Since this appears in the exponent, this shows the exponential dependence on the separation of tip and sample, a.

Example 8.2 Gamow's theory of Alpha Decay

"Can we go over example 8.2 i got lost in this example?"

Jessica Hide responses Post a response

Admin

Yes I think that it would be good to go over example 8.2. It looks like p(x)=E-E here and I am no sure why.

Kyle B,

No, it's still V(r) – E, but he happened to note that, at the turning point, r_2, where p = 0, $V(r_2) = E$

I would also like this.

Gigja

I would also like for us to go over this example as well; as for the p(x) function, I don't recall seeing it in the example.

Jeremy, Redlands, CA