PHY662, Spring 2004, Feb. 26, 2004

26th February 2004

1 Miscellaneous

1. HWK #7 is due Tues., Mar. 2.
2. I am out of town on Mon., Mar. 1 - so I encourage you to start early on the homework. Office hours Friday? 3-4?
3. Continue to read Ch. 17 Shankar (or Griffiths Ch. 6).
4. Today: WKB final wrapup, intro to perturbation theory in physics, do start non-degenerate time-independent perturbation theory.
5. Use `maple` along the way.

2 Intro to `maple`

Computer symbolic manipulation, numerical methods, and plotting routines can make your life a whole lot easier, allowing you to focus on the physics. You need to know how to do things by hand, but automation can reduce errors and improve your work.

1. Basic introduction: a sequence of input prompts and outputs. Define functions, apply `fsolve`, etc. See "Basic Tasks" for a reference sheet. Read the New User Tour for a better background.
2. How can we normalize (numerically) the radial wavefunction $U(r) = \frac{\sin^2(\frac{\Pi r}{2})}{\sinh(\Pi r)}$?

3 WKB - just a little more.

1. Discuss tunneling out of a box: to get the *rate* of escape, multiply tunneling probability by "attempt rate".
   (a) The "attempt rate" is also a semi-classical approximation: frequency of classical oscillation within the potential.

(b) Note that this frequency is constant for a harmonic potential (just ω) and is $2L/v$, with $v = \sqrt{2E/m}$ for a square well potential.

(c) The tunneling probability is $2 \int \kappa(x)\, dx$, where $\kappa(x) = \sqrt{2m[V(x) - E]}$ and the integral is over the forbidden region.

2. The trickiest part of the WKB approximation is where the classical momentum vanishes. This is where the oscillating solution needs to be connected to the exponential solution. Derive, for example, the quantization condition $2 \int_{x_1}^{x_2} dx \sqrt{2m(E - V)} = (n + \frac{1}{2})h$ for a bound state with classical turning points x_1 and x_2, by matching the $\exp(\pm i \int k(x)\, dx)$ with $\exp(-\int \kappa(x)\, dx)$ parts of the WKB solution, using an Airy function where each of these functions breaks down.

Note the asymptotic forms

$$Ai(z) \sim (2\sqrt{\pi} z^{1/4})^{-1} e^{-\frac{2}{3} z^{3/2}} \qquad z \gg 0$$
$$Ai(z) \sim [(\sqrt{\pi}(-z)^{1/4}]^{-1} \sin\left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right] \qquad z \ll 0\,.$$

Apply this to connection formula, following Griffiths. The term $e^{i\int k\, dx}$, $e^{-i\int k\, dx}$ can be written as a $\sin()$ with a phase shift (the wave function can be chosen to be real). By changing coordinates $z = \alpha(x - x_r)$, $\alpha = \left[\frac{2mV'(x_r)}{\hbar^2}\right]^{1/3}$, near the classical turning point $x = x_r$, one gets the equation

$$\frac{d^2\psi}{dz^2} = z\psi\,,$$

for small z. The result from matching with $aAi(z) = aAi(\alpha x)$, with is (choosing $a = D\sqrt{\frac{4\pi}{\alpha\hbar}}$)

$$\psi(x) \quad \approx \quad \begin{cases} \frac{2D}{\sqrt{k(x)}} \sin[\int_x^{x_r} k(x')\, dx'], & \text{if } x < x_r \\ \frac{D}{\sqrt{k(x)}} e^{-\hbar^{-1}\int_{x_r}^{x} |k(x')|\, dx'}, & \text{if } x > x_r. \end{cases}$$

This means that the function

$$D\sqrt{\frac{4\pi}{\alpha\hbar}} Ai[\alpha(x - x_r)]$$

is the patching function between the two WKB solutions. For an infinite wall at $x = 0$, this gives a quantization condition:

$$\int_0^{x_r} k(x)\, dx = (n - \frac{1}{4})\pi, \quad n = 1, 2, \ldots\,.$$

If the left turning point at x_l is also "soft", one gets the quantization condition

$$\int_{x_l}^{x_r} k(x)\, dx = (n - \frac{1}{2})\pi, \quad n = 1, 2, \ldots\,.$$

4 Perturbation theory

Again, lots of problems are not exactly solvable. The step after an attempt at an exact solution is often perturbation theory, which means looking for a nearby solution to a known solution.

This approach has been very successful for lots of problems. Here are two drawbacks:

1. You need a small parameter. Without an expansion in some variable that is "small", you are lost.
2. Many expansions are only asymptotically correct. So you require some more information or techniques to get good approximations.

Physicists have been very creative in finding expansion parameters. Here are some:

- Ratios of energies: the interaction between the magnetic dipoles in an H atom are much smaller than the Coulombic energies.
- Ratios of length scales: for example, in WKB, the length scale over which the wavelength changes is taken to be much longer than the wavelength itself.
- Dimensionality: an ϵ-expansion is often used, where the dimensionality is, say, $4-\epsilon$ or $2+\epsilon$, as many theories are solvable in 2 or 4 dimensions (how inconvenient it is that we have three space dimensions).
- Magnitude of dimensionless constants: e.g., $\alpha \approx 137.04^{-1}$.

Here is an example of point 2 above: let's compute an expansion in λ for

$$C(\lambda) = \int_{-\infty}^{\infty} e^{-x^2-\lambda x^4} \; .$$

The answer we will arrive at is

$$C(\lambda) = \sqrt{\pi} \sum_{k=0}^{\infty} \frac{(2k+1)!!}{k!} \left(\frac{\lambda}{4}\right)^k \; .$$

How does this series behave?

It is well behaved only in the limit $\lambda \to 0$. (Look at the coefficients of λ^k.) (There is a clue to a problem here: when $\lambda < 0$, $C(\lambda)$ diverges.)

5 Non-degenerate Time-Independent Perturbation Theory

Follow the usual derivation - using an expansion coefficient λ (as in Griffiths) rather than Shankar's parameter-free description.

Assume we have exact eigenstates for a Hamiltonian H^0,

$$H^0 \psi_n^0 = E_n^0 \psi_n^0 \, .$$

Very important note: the assumption is that ψ_n^0 is properly normalized: $\int \psi^* \psi = 1$. We wish to find the eigenstates for the Hamiltonian $H = H^0 + \lambda H'$. We can at least formally expand the new eigenstates and eigenvalues:

$$\begin{aligned} \psi_n &= \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \ldots \\ E_n &= E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \ldots \end{aligned}$$

Writing $H\psi_n = E_n \psi_n$ gives, collecting equations to each order in λ,

$$\begin{aligned} H^0 \psi_n^0 &= E_n^0 \psi_n^0 && (0^{\text{th}} \text{ order in } \lambda) \\ H^0 \psi_n^1 + H' \psi_n^0 &= E_n^0 \psi_n^1 + E_n^1 \psi_n^0 && (1^{\text{st}} \text{ order in } \lambda) \\ H^0 \psi_n^2 + H' \psi_n^1 &= E_n^0 \psi_n^2 + E_n^1 \psi_n^1 + E_n^2 \psi_n^0 && (2^{\text{nd}} \text{ order in } \lambda) \, . \end{aligned}$$

The 0th order equation is not new. Today we will just look at the 1st order correction - this is what will be needed for homework. Take the first order equation, multiply by ψ_m^0 and integrate over the space of the wavefunction to get:

$$\langle \psi_m^0 | H^0 | \psi_n^1 \rangle + \langle \psi_m^0 | H' | \psi_n^0 \rangle = E_n^0 \langle \psi_m^0 | \psi_n^1 \rangle + E_n^1 \langle \psi_m^0 | \psi_n^0 \rangle \, .$$

Choosing $m = n$ gives

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle \, .$$

Simple application: let H_0 be the Hamiltonian for a particle in a one-dimensional box with $0 < x < a$. Let $H' = a\delta(x - a/2)$. Then $E_n^0 = \frac{\hbar^2 \pi^2 n^2}{2ma}$, $\psi_n^0 = \sqrt{\frac{2}{a}} \sin(\frac{n\pi x}{a})$, $n = 1, 2, \ldots$. This gives

$$E_n^1 = \int_0^a (\frac{2}{a}) \sin^2(\frac{n\pi x}{a}) \delta(x - \frac{a}{2}) \, dx \, .$$