Quantum Physics III (8.06) — Spring 2018

Assignment 4

Posted: Thursday, March 1, 2018

Readings

- Griffiths Chapter 8 on WKB approximation
- Shankar Section 16.2.

Problem Set 4

1. **The equation satisfied by the approximate WKB solution (10 points)**

   In trying to solve the equation

   $$-\hbar^2\psi'' \;=\; p^2(x)\psi\,, \tag{1}$$

   we wrote the approximate solution $\psi_a(x)$ given by

   $$\psi_a(x) \;=\; \frac{1}{\sqrt{p(x)}}\exp\Big(\frac{i}{\hbar}\int^x p(x')dx'\Big)\,.$$

   (a) Find the exact differential equation satisfied by the approximate solution and show it can be written as

   $$-\hbar^2\psi_a'' \;=\; \Big[\;p^2(x) + \;\cdots\;\Big]\psi_a\,,$$

   where the dots represent extra terms not present in (1) that you must determine and are functions of $p(x)$ and its derivatives.

   (b) Consider the extra terms you found and explore the condition that each one is much smaller than $p^2(x)$. Express the resulting conditions as constraints on the local de Broglie wavelength $\lambda(x)$ and its derivatives.

2. **Airy functions and bound states in linear potentials (10 points)**

   Consider the Schrödinger equation for a particle of mass m in a potential

   $$V(x) = \begin{cases} gx\,, & \text{for } x > 0 \\ \infty\,, & \text{for } x \leq 0 \end{cases} \tag{1}$$

   Here $g > 0$ is a constant.

(a) Remove the units from the Schrödinger equation by letting $x = L\tilde{u}$, with $\tilde{u}$ unit free and L a length scale constructed as

$$L^3 = \frac{\hbar^2}{2mg}\,.$$

With a further transformation to a variable u, also unit free, reduce the differential equation to the form

$$\frac{d^2\psi}{du^2} \;=\; u\,\psi\,. \tag{2}$$

(b) The Schrodinger equation (2), extended to $u \in (-\infty, \infty)$, is tailored for a solution in momentum space! Using a unit-free momentum variable k we write

$$\tilde{\psi}(k) \;=\; \int_{-\infty}^{\infty} e^{-iku}\psi(u)du\,,$$

which goes together with the inverse relation

$$\psi(u) \;=\; \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{iku}\tilde{\psi}(k)dk\,.$$

Find the differential equation satisfied by $\tilde{\psi}(k)$ and solve it choosing $\tilde{\psi}(0) = 1$. Write your answer for $\psi(u)$ in terms of an integral

$$\psi(u) \;=\; \frac{1}{\pi}\int_{0}^{\infty} dk\,\cos\Big(\,\cdots\,\Big)\,,$$

where the dots represent some function of k and u that you should determine. The result is an integral representation for the Airy function: $\psi(u) = \mathrm{Ai}(u)$. [As a check on your result, confirm that your (numerical) integral gives $\mathrm{Ai}(1) = 0.135292$] One can use the integral representation to show that the Airy function $\mathrm{Ai}(u)$ decays quickly for large positive u and is oscillatory for $u < 0$.

(c) Determine the first two zeroes of the Airy function. Use those to give the values of the energies E for the lowest two energy eigenstates of the original potential (1) with a wall at $x = 0$. Express your answers as

$$E = \#\left(\frac{\hbar^2 g^2}{2m}\right)^{1/3},$$

where # are pure numbers.

3. **Quantum Mechanics of a Bouncing Ball (10 points)**

The semiclassical approximation can also be used to estimate the energy eigenvalues and eigenstates for potentials that cannot be treated exactly so easily. This problem is loosely based on Griffiths 8.6.

Consider the quantum mechanical analogue to the classical problem of a ball of mass m bouncing elastically on the floor, under the influence of a gravitational potential which gives it a constant acceleration g.

(a) Find the semiclassical approximation to the allowed energies E_n, in terms of m, g, and $\hbar$.

(b) Estimate the zero point energy of a neutron "at rest" (i.e. in the quantum mechanical ground state) on a horizontal surface in the earth's gravitational field. Express your answer in eV. [This may sound artificial to you, but the experiment has been done. See V. V. Nesvizhevsky *et al.*, Nature **415**, 297 (2002) and arXiv:hep-ph/0306198 for an experimental measurement of the quantum mechanical ground state energy for neutrons bouncing on a horizontal surface in the earth's gravitational field. This experiment got a lot of press at the time, because it involves both gravity and quantum mechanics, which made for an eye catching press release. It of course has *nothing* to do with quantum gravity.]

(c) Now imagine dropping a ball of mass 1 gram from rest from a height of 1 meter, and letting it bounce. Do the 8.01 "calculation" of the classical energy of the ball. The quantum mechanical state corresponding to a ball following this classical trajectory must be a coherent superposition of energy eigenstates, with mean energy equal to the classical energy. How large is the mean value of the quantum number n in this state?

4. **Semi-classical approximation of the potential $V(x) = \alpha x^4$ (10 points)**

Consider the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \alpha x^4 \psi = E\psi.$$

Let the energies be $E_0 < E_1 < \ldots$ and define the dimensionless energies $e_n = \frac{E_n}{\gamma}$ where

$$\gamma \equiv \left(\frac{\hbar^4 \alpha}{m^2}\right)^{1/3}.$$

In an 8.05 problem set we explored numerical solutions of this potential and found that the first few energies were

$$\begin{aligned}
e_0 &= 0.667986 \\
e_1 &= 2.39364 \\
e_2 &= 4.69680 \\
e_3 &= 7.33573 \\
e_4 &= 10.2443 \\
e_5 &= 13.3793
\end{aligned}$$

In this problem we will show how to estimate these energies using semiclassical methods.

(a) Assume that the turning points are at $-x_0, x_0$ with $x_0 > 0$. Express the energy E in terms of α and x_0.

(b) Use the connection formulae to show (assuming the WKB approximation is valid) that

$$\frac{1}{\hbar}\int_{-x_0}^{x_0}\sqrt{2m(E_n - V(x))}dx = \left(n+\frac{1}{2}\right)\pi \tag{1}$$

for $n = 0, 1, 2, \ldots$.

(c) In what follows, we will use $\tilde{E}_n$ to denote the estimate of the n^{th} energy that is obtained from (1) while E_n represents the true energy. Compute the integral in (1) to obtain a formula for $\tilde{e}_n \equiv \tilde{E}_n/\gamma$ in terms of n. The answer should be of the form $\tilde{e}_n = \beta(n+\delta)^{\epsilon}$ for β, δ, ϵ constants to be determined. You may find the following expression useful:

$$\int_0^1 \sqrt{1-t^4}dt = \frac{\sqrt{\pi}\Gamma(\frac{1}{4})}{8\Gamma(\frac{7}{4})} \approx 0.874019.$$

Write down $\tilde{e}_0, \tilde{e}_1, \tilde{e}_2, \tilde{e}_3, \tilde{e}_4, \tilde{e}_5$ and the relative errors $\left|\frac{\tilde{e}_0 - e_0}{e_0}\right|$, $\left|\frac{\tilde{e}_2 - e_2}{e_2}\right|$ and $\left|\frac{\tilde{e}_5 - e_5}{e_5}\right|$.

5. **Application of the Semiclassical Method to the Double Well Potential (20 points)**

Do Griffiths Problem 8.15.

This is not as difficult a problem as its length would indicate. Griffiths leads you through all the steps. This is an instructive problem in quantum dynamics. You should recall that this is the potential that we used to describe the physics of the ammonia molecule, early in 8.05. Back then, we had to wave our hands a little when we talked about tunneling splitting the degeneracy between the even and odd states. Now, you can do this calculation for real.

Hint for (a) and (b): The steps suggested by Griffiths are: work out the wave function ψ_1 in region (i); from ψ_1 use the connection formulae at x_2 to obtain the wave function ψ_2 in regions (ii); use ψ_2 and the connection formulae at x_1 to obtain the wave function ψ_3 in region (iii). Equation (8.59) can be found by requiring that ψ_3 should satisfy $\psi_3(0) = 0$ or $\psi_3'(0) = 0$ at $x = 0$.

It is a bit easier (and more transparent) to use a slightly different approach from what Griffiths suggests. Given that the wave function should be an even or odd function of x, the wave function in region (iii) can be written down immediately. For example in the even case,

$$\psi(x) = \frac{C}{\sqrt{\kappa(x)}}\cosh\left[\frac{1}{\hbar}\int_0^x dy\,\kappa(y)\right], \qquad -x_1 < x < x_1 \tag{2}$$

using our standard notations. (2) is an example where by symmetry, the exponentially small piece in a classically forbidden region is known exactly. The wave function ψ_2 in region (ii) then can be obtained using two ways: from ψ_1 in region (i) via connection formulae at x_2, or from ψ_3 in region (iii) via connection formulae at x_1. The consistency of two wave functions leads to equation (8.59) of Griffiths.

6. **Tunneling from perturbation theory (20 points)** A key feature of tunneling is that the rate is suppressed exponentially by an amount that scales with the width of the barrier and the square root of the height of the barrier. We will see in this problem how exponential suppression can arise from high-order degenerate perturbation theory.

   In this problem we consider a particle localized on a line with a potential equal to zero at the endpoints and a potential barrier of height V_0 and width W in the middle. Thus the WKB transmission coefficient (or tunneling probability) for particle with energy much smaller than V_0 is $\exp(-2W\sqrt{2mV_0}/\hbar)$.

   (a) First suppose the positon of the particle is restricted to sites $0, 1, \ldots, N$. The Hamiltonian consists of two terms. There is a "barrier" term H_0 which is a potential of height V_0 on all sites except 0 and N; i.e.

$$H_0 = V_0 \sum_{x=1}^{N-1} |x\rangle\langle x|, \tag{3}$$

   and a "hopping" term

$$\delta H = -\lambda \sum_{x=1}^{N} |x-1\rangle\langle x| + |x\rangle\langle x-1|. \tag{4}$$

   Assume that $\lambda \ll V_0$.

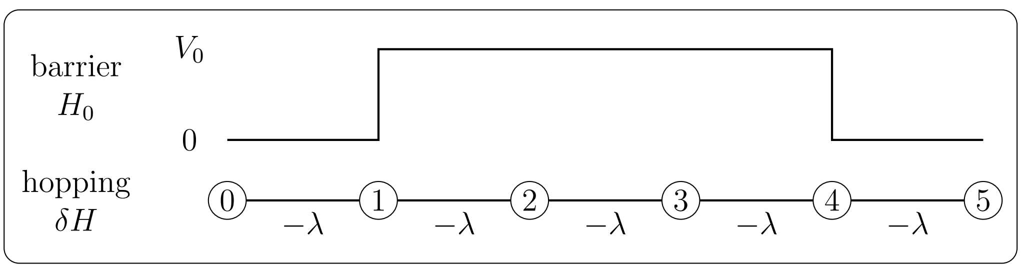

Figure 1: A particle is constrained to occupy one of $N+1$ nodes (here $N = 5$) with a barrier potential H_0 from (3) and a hopping term δH from (4).

   If there were no hopping term, there would be a two-dimensional space of zero-energy degenerate ground states spanned by $|0\rangle$ and $|N\rangle$, or by the more useful linear combinations

$$|g_+\rangle = \frac{|0\rangle + |N\rangle}{\sqrt{2}} \qquad \text{and} \qquad |g_-\rangle = \frac{|0\rangle - |N\rangle}{\sqrt{2}}.$$

   In the absence of hopping, the other states $|1\rangle, \ldots |N-1\rangle$ are also degenerate with energy V_0.

   At sufficiently high order of perturbation theory the hopping term will lift the degeneracy between the ground states so that: $E_{g_+} \neq E_{g_-}$. The formula for the

k^{th}-order correction to the energy of the $|g_\pm\rangle$ states is

$$E_{g\pm}^{(k)} = \sum_{m_1} \cdots \sum_{m_{k-1}} \frac{\delta H_{g\pm,m_{k-1}} \cdots \delta H_{m_2,m_1} \delta H_{m_1,g\pm}}{(E_{g\pm}^0 - E_{m_1}^0) \cdots (E_{g\pm}^0 - E_{m_{k-1}}^0)} + \text{other terms.} \tag{5}$$

Here $m_1, \ldots, m_{k-1}$ range over all states outside the degenerate subspace $|g_\pm\rangle$ and we have used the fact that a similar term does not couple $|g_+\rangle$ to $|g_-\rangle$.

What is the smallest value of k for which $E_{g_-}^k - E_{g_+}^k$ is nonzero? It turns out that the other terms not shown begin to contribute only for higher values of k, and one may ignore them for the purposes of this problem.

Evaluate the energy splitting for this value of k. Your answer should decrease exponentially with N, since N is analogous to W, but the scaling with V_0 will not look like the WKB case.

(b) Now suppose that the discrete approximation above came from a 1-D Hamiltonian in which we discretized space and replaced the $p^2/2m$ with a finite difference operator. If the lattice spacing is ℓ then the finite-difference operator corresponding to $\frac{d^2}{dx^2}$ is

$$D_\ell^2 = \frac{1}{\ell^2} \sum_x -2|x\rangle\langle x| + |x\rangle\langle x+1| + |x\rangle\langle x-1|.$$

If we ignore the diagonal part, the kinetic energy term $\frac{p^2}{2m}$ is equivalent to δH from (4). What is the corresponding value of λ?

Suppose that the potential term is a square barrier of width W and take $\ell = W/N$ so this corresponds to N lattice sites.

We see that as we reduce ℓ the energy splitting in (a) goes down since $N = W/\ell$ increases as $\ell \to 0$. This is an artifact of our approximation scheme since the physics of the system should not depend on the "regulator" ℓ that we hope to take to zero. But we cannot make ℓ arbitrarily small because λ would diverge and we could not keep the ratio λ/V_0 small, spoiling the perturbation-theory argument. Let us impose the perturbation condition explicitly by setting

$$\frac{\lambda}{V_0} = \epsilon \ll 1$$

with ϵ a *fixed* small constant. Verify that this means that $\ell^2 V_0$ is kept constant as $\ell \to 0$. Eliminate ℓ to estimate the energy splitting as a function of ϵ, W, V_0, m and $\hbar$.

(c) Part (a) and (b) have given estimates of the splitting in energies of $|g_\pm\rangle$ but have not directly addressed tunneling. In this part, suppose that the Hamiltonian is simply

$$H = E_+|g_+\rangle\langle g_+| + E_-|g_-\rangle\langle g_-|$$

and define $\Delta = E_- - E_+$. Suppose that we begin at time 0 in the state $|0\rangle$, and after time t we measure whether the particle is in state $|0\rangle$ or $|N\rangle$. At what time t will we find the state in position N with probability 1? Using the energy splitting from (b) above, give the tunneling rate (tunneling probability per unit time) and find how it scales with W and V_0. How does your answer compare with the WKB prediction?