Laboratory 2

Due Monday, September 23, 2013

Save the results of this lab — you may need them for future labs!

Problem 1

Consider a point particle of mass m oscillating without any damping in a 1D potential

$$U(x) = \alpha x^2 + \beta x^4, \tag{1}$$

where $\alpha > 0$ and $\beta \geq 0$ are constants. From energy conservation, it is possible to express the period of the oscillations T as

$$T(A) \propto \int \frac{dx}{\sqrt{E(A) - U(x)}}, \tag{2}$$

where $E(A)$ is the total energy of the particle oscillating with amplitude A.

1. (1 pt) Derive Eq. (2) with the proper proportionality factor and integration limits.

2. (2 pts) Express the period for some arbitrary m, α and β in terms of that for $m = 2$, $\alpha = 1$ and $\beta = 1$ (perhaps for a different energy). Your equation should have the following form:

$$T(E; m, \alpha, \beta) = C_1 T(C_2 E; 2, 1, 1), \tag{3}$$

where C_1 and C_2 are some functions of m, α and β. Given Eq. (3), it is sufficient to study the case $m = 2$, $\alpha = 1$, $\beta = 1$ and then obtain the results for other values by scaling.

3. (5 pts)

(a) Write a program calculating the period $T(A)$ for a given range of amplitudes for $m = 2$, $\alpha = 1$, $\beta = 1$ by integrating Eq. (2) numerically. The goal is to calculate the period with the relative accuracy $|\delta T|/T < 10^{-6}$. Choose an appropriate integration method. Estimate the error explicitly or argue that it is below 10^{-6}.

(b) Justify your choice of the method comparing it to other alternatives. Justifications can include efficiency, ease of use, etc.

4. (2 pts)

(a) Using your program, calculate the period for A between 0 and 5 with the step of 0.01. The result should be a file, in which the first column is the amplitude, the second column is the period and the third (optional) column is the error estimate.

(b) Plot your results. Describe them qualitatively.

5. (3 pts) For small A, the period can be approximated with

$$T(A) \approx T(0) - CA^n. \tag{4}$$

Based on your numerical results from 4(a), find constants $T(0)$, C, n. Theoretically, what should the value of $T(0)$ be? Do your results agree with this? **Two bonus points**, if you calculate C and n theoretically as well.

6. **(Optional for PHY4140 students)** (5 pts) (a) Calculate the period theoretically in the limit of large A. Hint: reduce the integral in this limit to that for the beta function:

$$B(a,b) = \int_0^1 x^{a-1}(1-x)^{b-1}dx. \tag{5}$$

You will need to get the numerical value for one particular pair $\{a,b\}$. If you don't have software to do that, just go to `www.wolframalpha.com` and type `Beta[a,b]`, where `a` and `b` are your values.

(b) Find numerically how large A should be for the exact values to agree with the large-A approximation you have obtained with the relative error below 10^{-5}. (No need to give a very precise answer.)

(c) Use your program to calculate the period for A between 5 and the value found in 6(b). Choose an appropriate step of A.

(d) Plot your result from 6(c) together with that from 4(a) and the theoretical dependences from 5 and 6(a). Include the fit from item 7 below if you choose to do it. You may have to do several plots to show all the important features. You are free to choose the appropriate scales for the axes (linear, logarithmic) as necessary.

7. **(Optional - 3 bonus points)** Based on the results obtained so far, find a fitting formula approximating $T(A)$ to within 1-2% for **all** A. The simpler the formula the better.

Problem 2

Now consider a **quantum** particle with $m = 2$ moving in the same potential [Eq. (1)] with $\alpha = 1$, $\beta = 1$. Your goal is to find the energy levels E_n of the particle. While to solve the problem exactly one needs to solve the Schrödinger equation (which you'll learn to do numerically later in the course), the approximate semiclassical result based on the WKB approximation is that E_n are the solutions of

$$S(E_n) = 2\int_{-A(E_n)}^{A(E_n)} |p(x; E_n)|dx = 2\pi\hbar(n + 1/2), \tag{6}$$

where $p(x; E)$ is the momentum of the classical particle with coordinate x and total energy E and $n = 0, 1, 2, \ldots$. The quantity $S(E)$ is sometimes called the *abbreviated action*. You can find a detailed explanation of this in many quantum mechanics textbooks, e.g., Bransden & Joachain, Quantum Mechanics, Sec. 8.4. While the semiclassical approximation is in general valid for large n, it also happens to be exact for the harmonic oscillator, and therefore one can expect that the low energy levels (for which the anharmonic x^4 term is small) are reproduced reasonably accurately as well.

1. (1 pt) Prove theoretically that

$$S(E) \propto \int_0^E T(E')dE', \tag{7}$$

where $T(E)$ is the period of the classical oscillator.

2. (3 pts) Calculate $S(E)$ for E from 0 to 10 by integrating numerically the $T(A)$ dependence you've obtained in Problem 1 [keep in mind it's $T(A)$, not $T(E)$!] Use your output files from Problem 1 as the input for this problem. Your $S(E)$ does not have to be very accurate [after all, Eq. (6) is approximate itself!], but do estimate your numerical error. Your output should be a file with E in the first column, $S(E)$ in the second and the error estimate in the third. As always, it is better to overestimate your error than to underestimate it.

3. (1 pt) Write down an equation giving the energy levels of the harmonic oscillator with $m = 2$, $\alpha = 1$ and $\beta = 0$.

3. (3 pts) Using your $S(E)$ result and putting $\hbar = 0.1$, find all energy levels between $E = 0$ and $E = 5$. Your output should be a file with n in the first column, E_n in the second, the error estimate in the third, **and the**

corresponding levels for the harmonic oscillator in the fourth column. Describe your results qualitatively comparing to the harmonic oscillator. **Up to two bonus points** for a nice graphical presentation of your results.

4. (2 pts) Justify the choice of the methods you have used in items 2 and 3.

5. **(Optional - 5 bonus points)** Now, solve the problem "properly" by writing a program that does the integral (6) directly and couples the calculation of the integral to a root-finding procedure. Find E_n for a few different n covering the energy range from $E = 0$ to 5 and compare to what you have obtained above using a different method. Do your results agree within the error that you have claimed?