Laboratory 4

Due Wednesday, November 6, 2013

PHY4140 students can choose any one of the two problems. The total number of points for the chosen problem will be considered as 100%. The students will be awarded bonus points for any parts of the other problem they do. **PHY5340 students need to do both problems.**

Problem 1

As in Lab 2, consider a quantum particle of mass m moving in the potential

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

In Problem 2 of Lab 2, the quantum energy levels of this system were calculated using the WKB approximation. In this lab, you will find the energy levels of this system by solving the Schrödinger equation directly and compare them to those obtained using the WKB approximation in Lab 2. I am providing a file (`WKB_levels.dat`) that you can use in your comparisons. But if you have done that problem (more or less) correctly, you will need to compare to *both* your data and the provided file, as described below. The description of `WKB_levels.dat` and some background information are given in a separate document, `WKB_descr.pdf`. In brief, the first column of `WKB_levels.dat` is the number of the energy level; the second column is the corresponding energy calculated "exactly" within the WKB approximation; and the third column is based on integrating the period $T(A)$ using the trapezoidal rule, as in questions 2–4 of Problem 2 of Lab 2, which for brevity will be called the "trapezoidal estimate" or the "trapezoidal approximation". If you have done questions 2–4 of Problem 2 of Lab 2, your results may differ from these a bit (or a lot): perhaps you have used a different integration method, or perhaps your $T(A)$ was not accurate, or maybe you have made some mistake. In any case, in this lab you will need to estimate the accuracy of both the results in `WKB_levels.dat` and of you own results, if you do have them.

1. (4 pts.) Write down the time-independent Schrödinger equation for a particle of mass m in potential (1). Write a program solving this equation

to find a single energy level and the corresponding wave function $\psi(x)$ **normalized correctly**, i.e., $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$. Also, make sure that $\psi(x)$ is real and that at $x = 0$, $\psi(x) > 0$ (if the function is even) or $d\psi(x)/dx > 0$ (if it is odd). The input to the program should be the initial guess for the energy (either as a single number or as an interval — the choice is up to you) and, optionally, the parity of the expected wave function (even or odd). Test your program by finding the following energy levels and the corresponding wave functions for the *harmonic* oscillator ($m = 2$, $\alpha = 1$, $\beta = 0$, $\hbar = 0.1$): $n = 0, 1, 2, 3, 5, 10, 23$. In all cases, the relative accuracy should be at least 10^{-4} for the energy and at least 10^{-3} for the wave function relative to its maximum value. In this question you can use the known energies and wave functions for the harmonic oscillator to both obtain the initial guess for the energy and estimate your accuracy (but please choose your initial guess a bit away from the known exact value of the energy to test your code properly). Describe in detail the procedure that allowed you to reach the required accuracy, including all relevant parameters of your program (separately for each n, if they differ for different n). Plot your wave functions. In at least the first four cases, also plot the error compared to the exact analytical expression for the wave function.

2. (3 pts.) Using either the program from Problem 1.1 above (suitably modified if necessary) or a separate program, find **all** energy levels of the anharmonic oscillator ($m = 2$, $\alpha = 1$, $\beta = 1$, $\hbar = 0.1$) between $E = 0$ and $E = 5$ and output them to a file. (If you do modify the program from 1.1, save the modified program separately from the original one.) You do not need to find the wave functions in this question. You may use the energies from `WKB_levels.dat` as your initial guesses, but you still need to explain why you think you have not missed any levels (assume that you cannot be sure if `WKB_levels.dat` really lists all the levels, albeit approximately). Your accuracy has to be at least an order of magnitude better than the difference between the calculated energy level and the corresponding entry in the second column of `WKB_levels.dat` (this will ensure that your estimates of the accuracy of the WKB approximation can be trusted). Explain why you think you have achieved that accuracy.

3. (3 pts.) Using your results from Problem 1.2, study the accuracy of the WKB approximation, of the "trapezoidal approximation" to the WKB approximation given in column 3 of `WKB_levels.dat` and of your own approximation (if you have done it).

Answer the following questions, both qualitatively and quantitatively:

(a) Is the WKB approximation accurate? How accurate is it for high levels? For low levels?

(b) Does the WKB approximation give a useful prediction of the deviation from the levels of the harmonic oscillator for low levels? For high levels? How accurate is it?

(c) Is the additional error of the “trapezoidal estimate” significant compared to the error already inherent in the WKB approximation?

(d) Same as in (c), for your own approximation.

Some useful quantities that you may want to calculate to answer these questions are listed in file `quantities.pdf`. You are not obliged to calculate all of them and you may choose to calculate some that are not listed. Output all quantities you calculate to one or several files and describe them in your report or `README`.

4. (3 pts.) Using the program you have developed in 1.1, calculate the wave functions for the energy levels of the anharmonic oscillator ($m = 2$, $\alpha = 1$, $\beta = 1$, $\hbar = 0.1$) given below. In all cases, your accuracy should be better than 10^{-3} relative to the maximum.

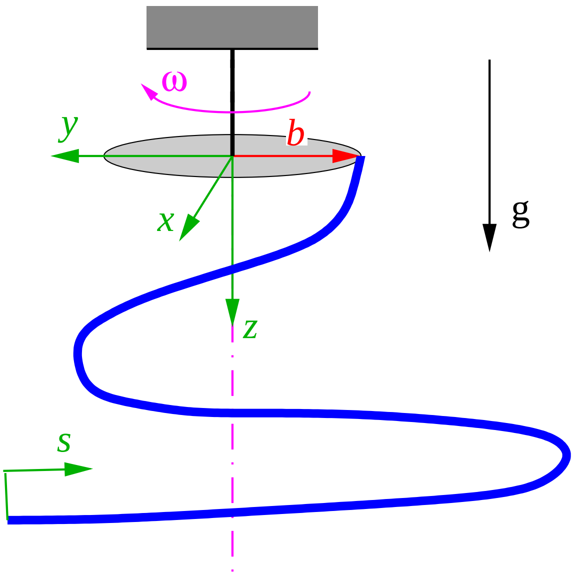
(a) For $n = 0, 1, 2, 3, 5, 10, 23$, compare to the corresponding wave functions of the harmonic oscillator calculated in 1.1. For each n, do a comparison plot. In addition, for $n = 10$ and 23 also compare *rescaled* wavefunctions $\sqrt{A}\psi(Ax)$, where A is the amplitude of the classical oscillator with the same α, β and energy, again, doing a comparison plot. This rescaling matches the oscillation ranges, but also preserves the normalization of the wave functions.

(b) Consider again the $n = 10$ and 23 levels of the *harmonic* oscillator. For each, find the energy level of the *anharmonic* oscillator closest in energy and do a comparison plot plotting $\sqrt{A}\psi(x)$.

Describe the results of (a) and (b) qualitatively.

Problem 2

Consider a fully flexible and inextensible string of length L and constant linear mass density ρ (so the total mass is ρL). One end of the string is forced to move in a horizontal circle of radius b with angular velocity ω and the other end is free (see the picture). We are interested in the steady-state motion of the string such that at all times the string is in a vertical plane



rotating with angular velocity ω and is stationary in this rotating frame. In other words, for a point on the string that is at distance s (measured along the string) from its free endpoint ($0 \le s \le L$), the coordinates of this point in the lab frame are

$$\begin{aligned} x(s,t) &= r(s)\cos(\omega t), \\ y(s,t) &= r(s)\sin(\omega t), \\ z(s,t) &= z(s) \text{ (is } t\text{−independent).} \end{aligned} \tag{2}$$

Note $r(s)$ can be both positive and negative (the string can cross the rotation axis).

1. (3 pts.) Introducing the position-dependent tension in the string, $T(s)$, take an infinitesimal element of the string and by considering the forces acting on it, write down two differential equations relating $r(s)$, $z(s)$ and $T(s)$, one equation for the radial component of the force and the other for the vertical component (the tangential component is automatically zero). **Do not** assume that any of the quantities are small. Adding to this an inextensibility condition of the form $f(r'(s), z'(s)) = 0$, you will end up with a set of three differential equations for the three unknown functions, $r(s)$, $z(s)$ and $T(s)$. Transform these equations into a form convenient for solving

numerically, e.g.,

$$\begin{aligned} r''(s) &= f_1(r'(s), r(s), T(s)), \\ T'(s) &= f_2(r'(s), r(s), T(s)), \\ z'(s) &= f_3(r'(s)). \end{aligned} \tag{3}$$

Since you have one equation of second order and two of first order, you will need $2+1+1=4$ **boundary conditions** – derive these as well. Nondimensionalize the equations by introducing $\tilde{s} = s/L$, $\tilde{r} = r/L$, $\tilde{z} = z/L$, $\tilde{T} = T/\rho g L$. This makes the problem dependent on two dimensionless parameters,

$$\alpha = \omega\sqrt{\frac{L}{g}} \tag{4}$$

and

$$\beta = \frac{b}{L}. \tag{5}$$

Note that since the equations are nonlinear, even with four boundary conditions specified there may still be multiple solutions for particular α and β.

Since you will need the result of this part to do the rest of the problem, you are welcome to request help, but there will be a penalty. There will be a **0.25 pt penalty** if you only ask to verify the final result and it turns out to be correct; a **0.5 pt penalty** if it is wrong but you are eventually able to correct it on your own; there will be larger penalties if you need help with your derivation. Please submit your requests to verify by email - I will need to consult my notes that I may not have with me all the time.

2. **(Optional - 2 bonus points)** Linearize your equations and boundary conditions and solve the resulting system analytically obtaining an expression for $\tilde{r}(\tilde{z})$ that should contain a Bessel function. Note that unlike the full nonlinear problem, the linearized one should normally have only one solution for given α and β. What are the exceptions to this rule?

3. (4 pts.) Write a program finding one solution of the full nonlinear problem for given α, β and an initial guess for $\tilde{r}(0)$ that can be specified either as a single number or as an interval — the choice is yours. Keep in mind that the problem is singular at $\tilde{s} = 0$ — take care of that properly. Find a solution for $\alpha = 5$, $\beta = 0.05$ and $\tilde{r}(0)$ between 0.1 and 0.2. Find the actual value of $\tilde{r}(0)$, as well as $\tilde{z}(0)$, with the accuracy of 0.1%. Plot $\tilde{r}(\tilde{z})$ for this solution. **For up to 0.5 bonus points**, do a nice graphical presentation

of the result: in particular, make sure the $\tilde{z}$ axis is vertical, the orientation is such that the gravity force points downwards, and draw the rotation axis as a dashed or dotted line.

4. **(Optional - 2 bonus points)** Use the program developed in 2.3 to find two solutions for $\alpha = 5$ and $\beta = 0.01$: one with $\tilde{r}(0)$ between 0.03 and 0.05 and the other with $\tilde{r}(0)$ between 0.1 and 0.12. You now have two distinct solutions for the same α and β, but, as mentioned, the linearized problem will have only one. Which one of the two solutions of the nonlinear problem will the solution of the linear one approximate better, the first one or the second one? Why? Now check your guess by plotting either $\tilde{r}(\tilde{z})$ or $\tilde{r}(\tilde{s})$ for both nonlinear solutions and for the linear one in the same plot. You can use any software to calculate the Bessel function (in fact, some Fortran and C compilers have them as built-in functions).

5. (5 pts.) Using either the program developed in 2.3 (suitably modified if necessary) or a separate program, find **all** solutions of the full nonlinear problem for $\alpha = 8$ and $\beta = 0.01$. Plot all solutions together in two different ways. In the first graph, just plot $\tilde{r}(\tilde{z})$ for all solutions. In the second graph, shift the curves along the $\tilde{z}$ axis to align the free ends. In other words, plot $\tilde{r}(\zeta)$, where $\zeta = \tilde{z} - \tilde{z}(\tilde{s} = 0)$. To do nice plots, make sure that the scales of the axes are exactly the same; otherwise, different curves would appear to have different lengths (but remember, the length of the string is strictly constant!)

6. **(Optional - 3 bonus points)** An important issue in this problem is **stability**: obviously, we are only going to see a particular solution experimentally if it is stable with respect to small perturbations. Strictly speaking, this is not an easy problem, since we would need to consider radial, tangential and vertical perturbations of all possible shapes. While this is doable, we will opt for a simpler, if less rigorous approach. Consider a system undergoing periodic motion driven by some external influence. Suppose that due to some fluctuation, the amplitude of the periodic motion has increased. If the external influence needed to sustain that increased amplitude is *larger* than what is actually supplied, then there will not be enough energy to maintain the increased amplitude, the system will go back to its original state decreasing the amplitude of the oscillation and the periodic motion is stable. If, on the other hand, the amplitude of the external influence needed to sustain the increased amplitude is *smaller*, then there will be oversupply of energy and the system will actually increase its amplitude further, so the periodic motion will be unstable. Considering b as the measure of the external forcing and

$|r(0)|$ as the measure of the amplitude of the motion of the system, which of the solutions found in 2.5 are stable and which are not?

7. **(Optional - 5 bonus points)** Varying α between 0 and 8, plot $|s(0)|$ as a function of α for **all** solutions, for $\beta = 0.01$, $\beta = 0.02$, and $\beta \to 0$, all in a single plot (use different colours for different β for clarity). You will end up with several curves in your plot for each β. Keep in mind that solutions may appear and disappear as α changes! Based on the considerations in 2.6 and/or other arguments, what parts of the curves for $\beta = 0.01$ and 0.02 correspond to stable and unstable solutions? What values of α are approached in the limit $\beta \to 0$, $s(0) \to 0$? How are they related to the solutions of the linearized equations in 2.2?