ODE's

PHYSICS 598 CPA : Problem Set 6

Ricky Chue

1 Nonlinear dynamics and chaos

1.1 (q, b, ω_0) = (0.5, 0.9, 2/3)

For Figs. 1 and 2, we see there are about 10.5 periods from $t = 0$ to $t = 100$ for 1000 time steps. Each period is about 9.5 time units. The motion is approximately sinusoidal, but deviation is demonstrated in the first oscillation in those two figures.

The fact that the motion is not sinusoidal is more obvious when we view Fig. 3. If the motion were sinusoidal, the phase diagram should have looked like an ellipse. The deviation of the first oscillation to the other oscillations is reflected by the loop on the right in Fig. 3. After the first oscillation, the oscillation becomes periodic as the phase diagram later on traces out the same curve. The fact that the oscillation is periodic is checked by setting time goes from 0 to 1000, and time steps increases to 10000 (Fig. 4). The same curve is traced out in the phase diagram.

1.2 (q, b, ω_0) = (0.5, 1.15, 2/3)

For the driving force being increased in this case, the motion looks "chaotic", at the first glance of Figs. 5 and 6. In fact it is not "chaotic" and this is reviewed in Fig. 7, where time goes from 0 to 500, with 1000 time steps. The pattern in the phase diagram is not periodic, apparently, yet it is not random either. To investigate further, in Fig. 8 the same plot is shown with time going from 0 to 5000, and 10000 time steps. The patterns extend in the x-axis, and they are not random.

To see why such change is obtained, let's investigate the dimensionless quantity $f_d^0/(ml/\omega_0^2)$, which is basically b. Note that (ml/ω_0^2) is the characteristic force scale at natural frequency ω_0. Now, the fact that b changes from 0.9 to 1.15 implies that resonance occurred at the later case.

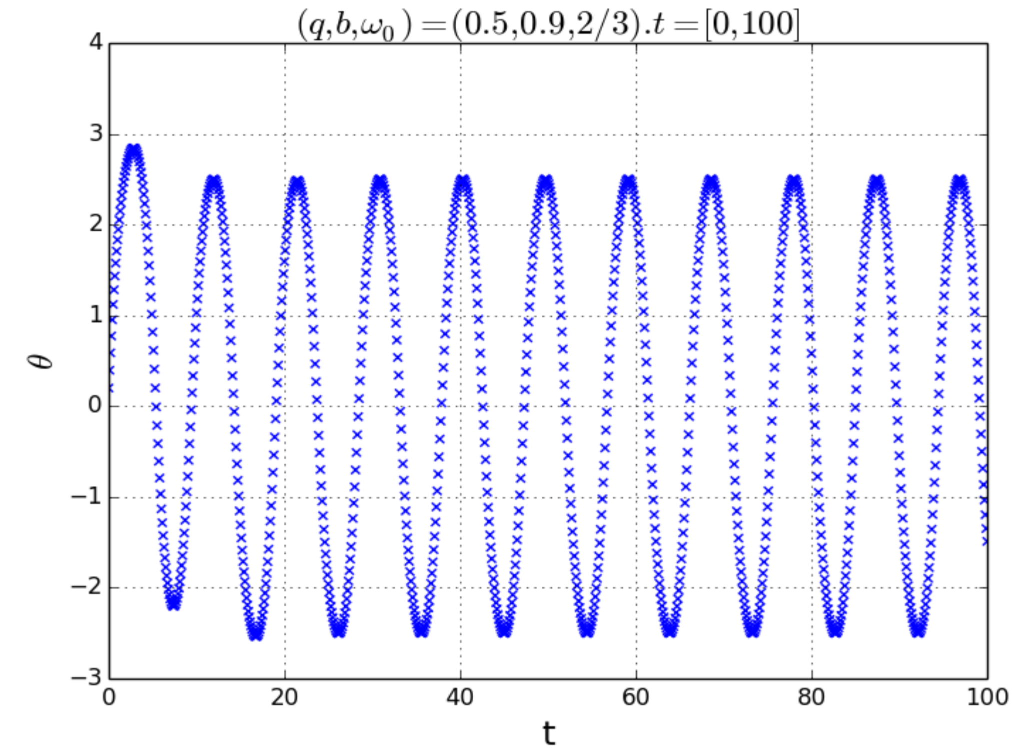

Figure 1: θ $vs.$ t for $t = [0, 100]$ for 1000 time steps.

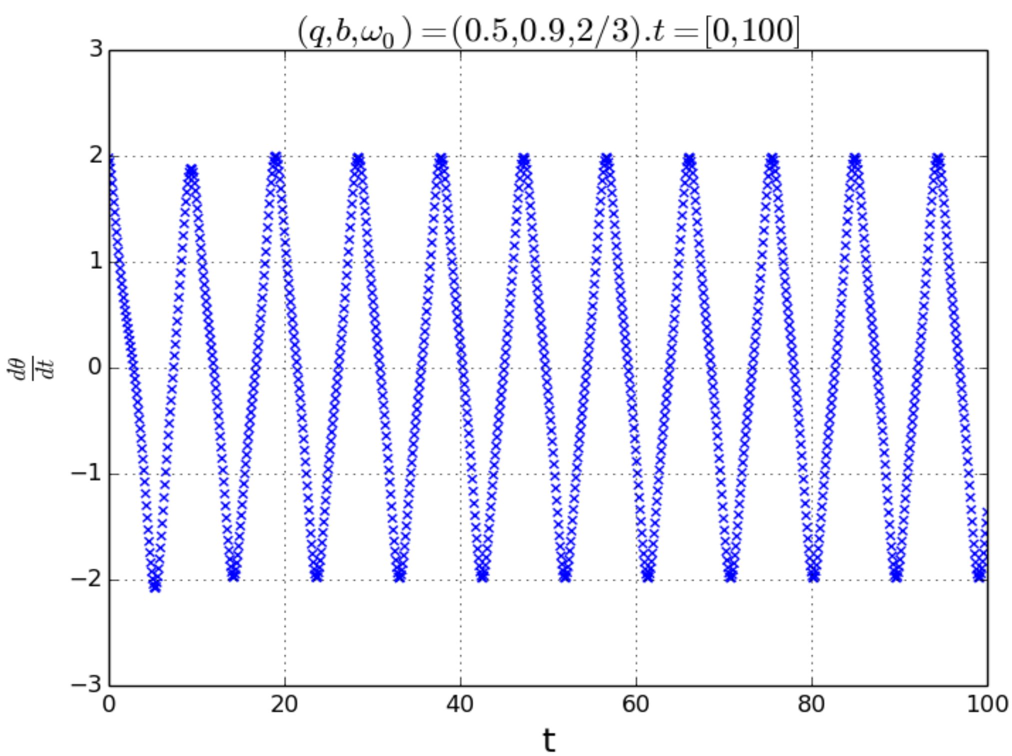

Figure 2: $\frac{d\theta}{dt}$ $vs.$ t for $t = [0, 100]$ for 1000 time steps.

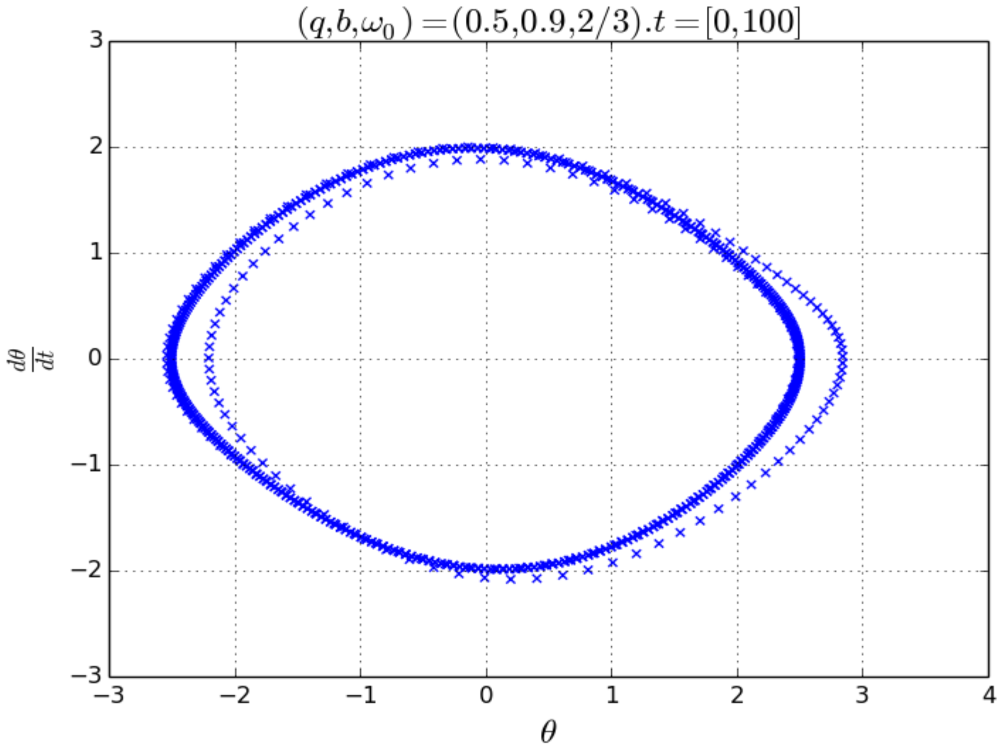

Figure 3: $\frac{d\theta}{dt}$ $vs.$ θ for $t = [0, 100]$ for 1000 time steps.

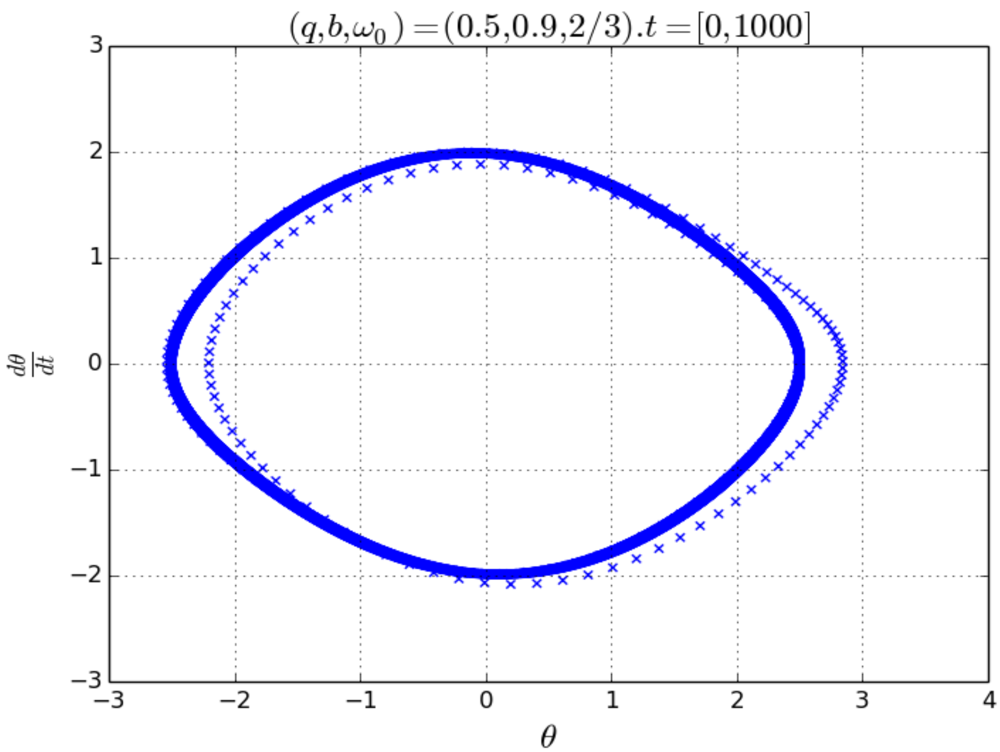

Figure 4: $\frac{d\theta}{dt}$ $vs.$ θ for $t = [0, 1000]$ for 10000 time steps.

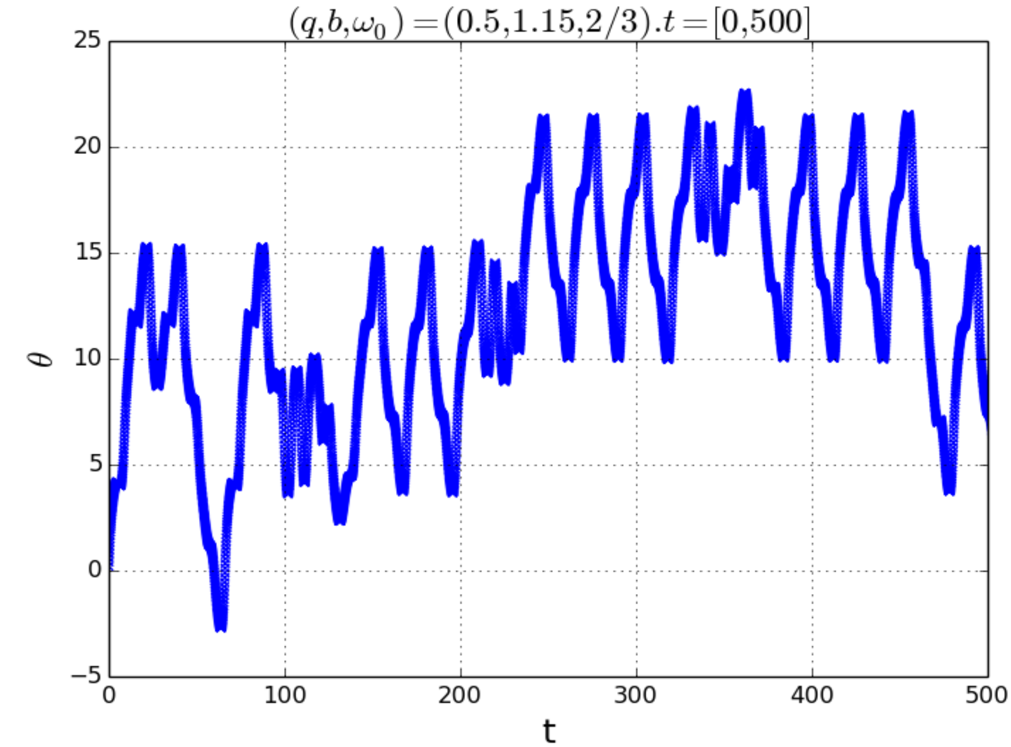

Figure 5: θ $vs.$ t for $t = [0, 500]$ for 1000 time steps.

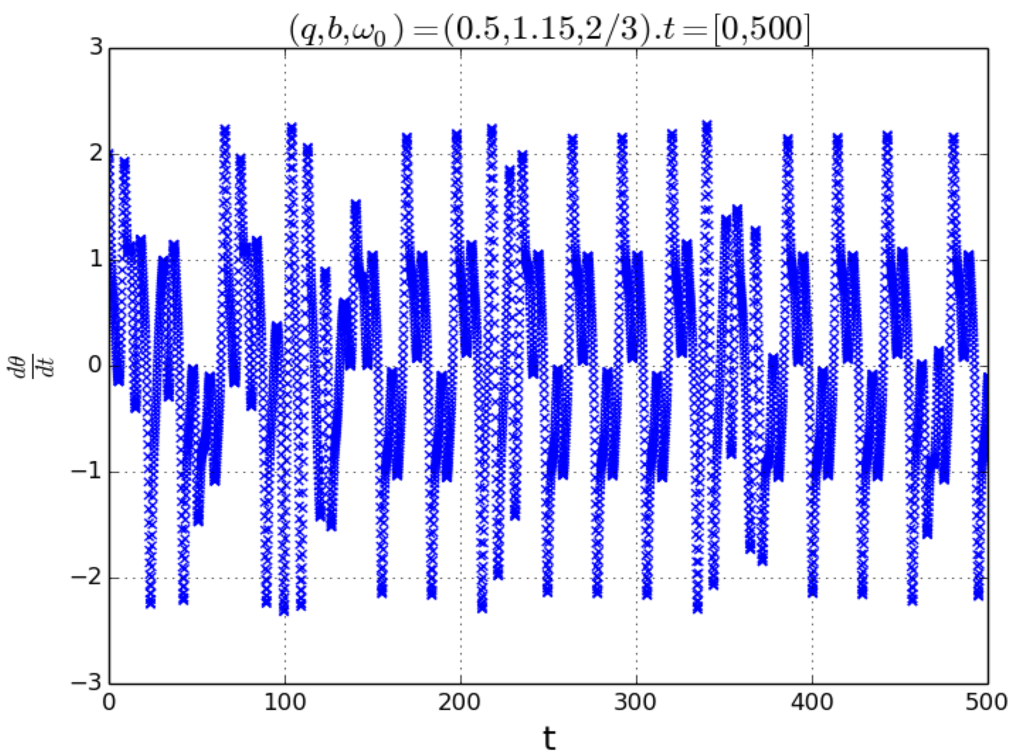

Figure 6: $\frac{d\theta}{dt}$ $vs.$ t for $t = [0, 500]$ for 1000 time steps.

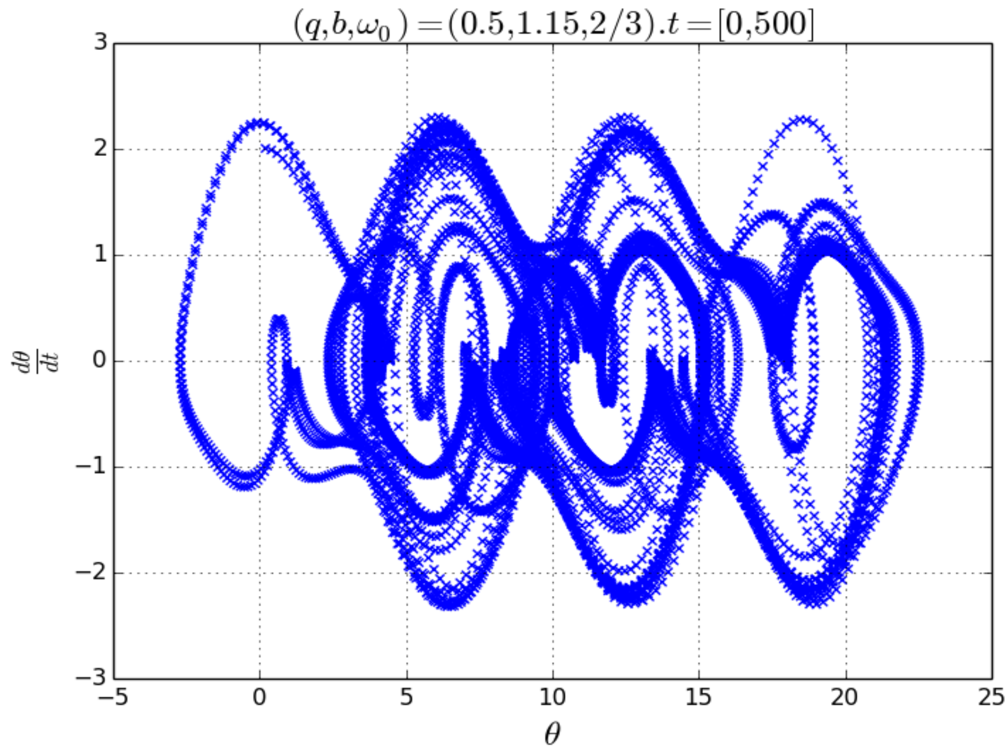

Figure 7: $\frac{d\theta}{dt}$ $vs.$ θ for $t = [0, 500]$ for 1000 time steps.

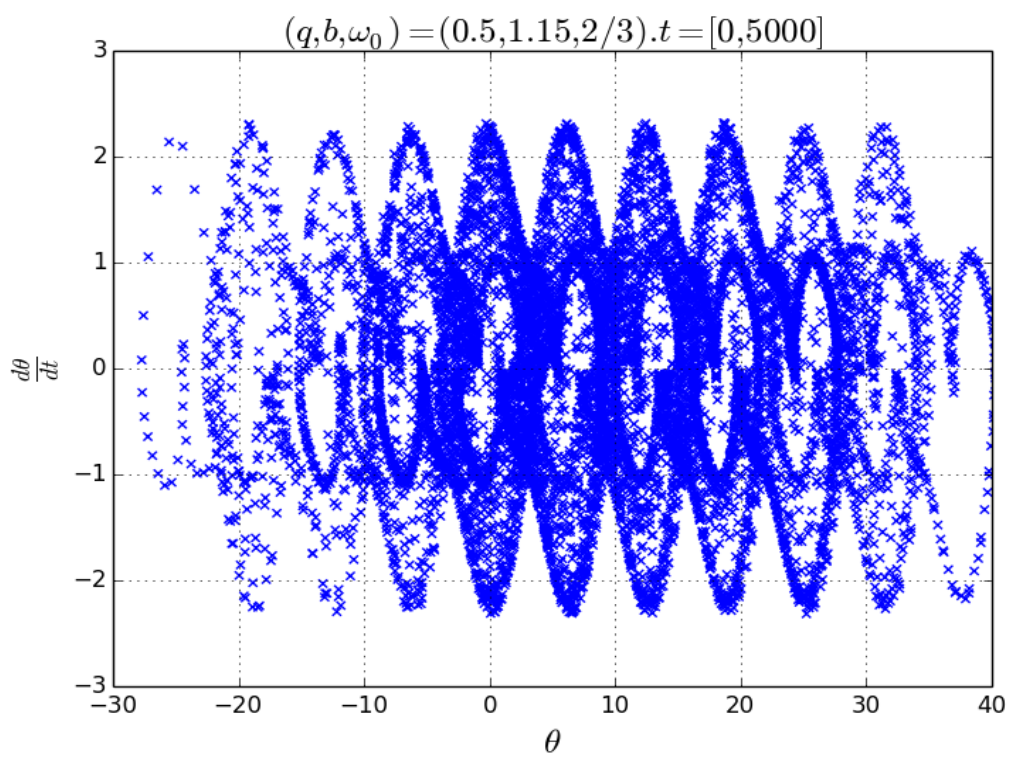

Figure 8: $\frac{d\theta}{dt}$ $vs.$ θ for $t = [0, 5000]$ for 10000 time steps.

2 Stiff system of equations

2.1 4^{th}-order Runge-Kutta scheme

The system of differential equations were integrated by the RK scheme from $x = 0$ to $x = 100$, yet the solution blows up in the first few steps. It is not a stable scheme to integrate these set of stiff system of equations.

2.2 Stiff ODE integrator

If the system is integrated implicitly, using the codes provided in the Numerical Recipes, the "blow-up" problem can be solved. The system is integrated from $x = 0$ to $x = 1000$.

Fig. 9 shows the plots of $y_1(x)$, $y_2(x)$ and $y_3(x)$ using steps of x: $\Delta x = 0.05$, with tolerance $\epsilon = 0.05$. The step size of the integration will be adjusted by the code as it proceeds. To confirm convergence, Fig. 10 shows the same numerical solutions, but with initial steps $\Delta x = 0.005$ and tolerance $\epsilon = 0.005$.

3 2-point boundary value problem by shooting

The equations were integrated using the shooting method by the 4^{th}-order RK method, from $x = 0$ to $x = 1$ with 1000 times steps.

To solve the differential equation, we replace the boundary conditions by two initial conditions, *i.e.*:

$$y_1(0) = 0 \quad \text{and} \quad y_2(0) = \delta$$

where δ was picked randomly initially such that the numerical solution satisfies $y_1(0) = 0$ and $y_1(1)$ in proximity to 1. After several trials, it was found that δ lies within the interval [0.0, 5.0]. Then the value of δ is iterated in this interval by the bisection method to the relative tolerance of 10^{-8}, where δ is found to be 3.1415926.

In Fig. 11, the numerical and analytic solutions of the differential equation are plotted from $x = 0$ to $x = 1$. Figs. 12 and 13 show the error of the numerical solution. At the first few steps, the relative error of the numerical solution is relatively large, but then it converges to less than 10^{-6}, as shown in Fig. 13.

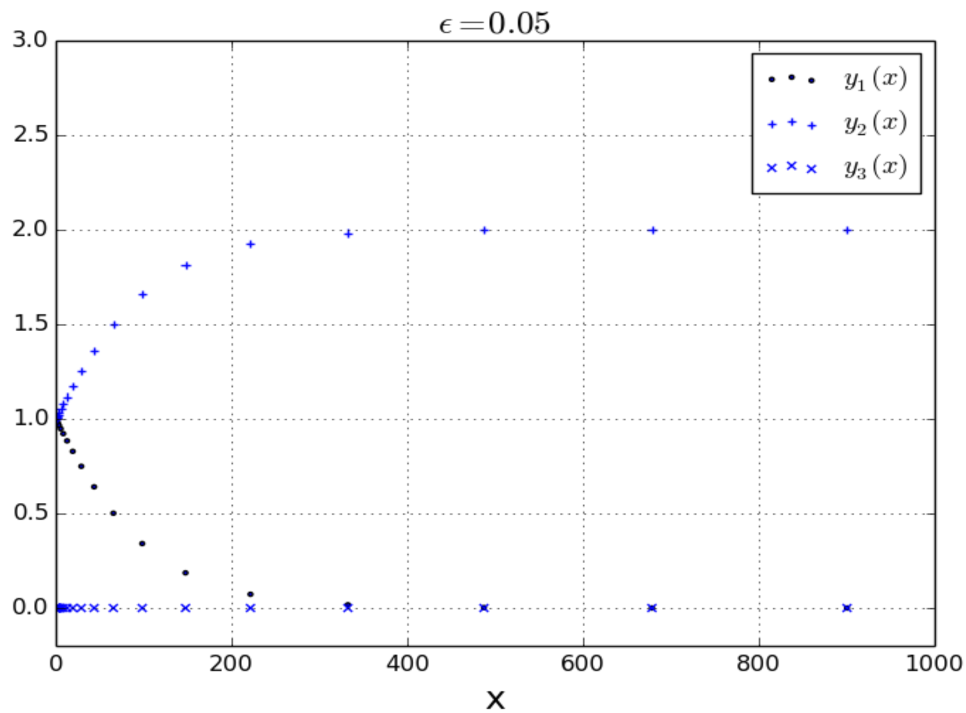

Figure 9: $y_1(x)$, $y_2(x)$ and $y_3(x) vs. x$, from $x = 0$ to $x = 1000$, with initial step $\Delta x = 0.05$ and tolerance $\epsilon = 0.05$.

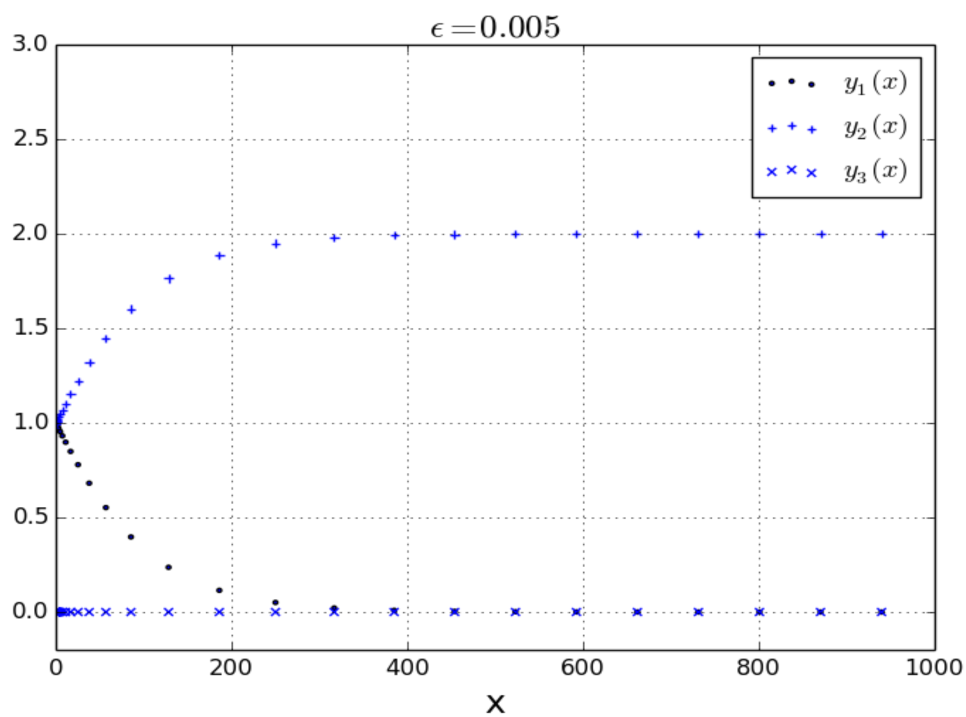

Figure 10: $y_1(x)$, $y_2(x)$ and $y_3(x) vs. x$, from $x = 0$ to $x = 1000$, with initial step $\Delta x = 0.005$ and tolerance $\epsilon = 0.005$.

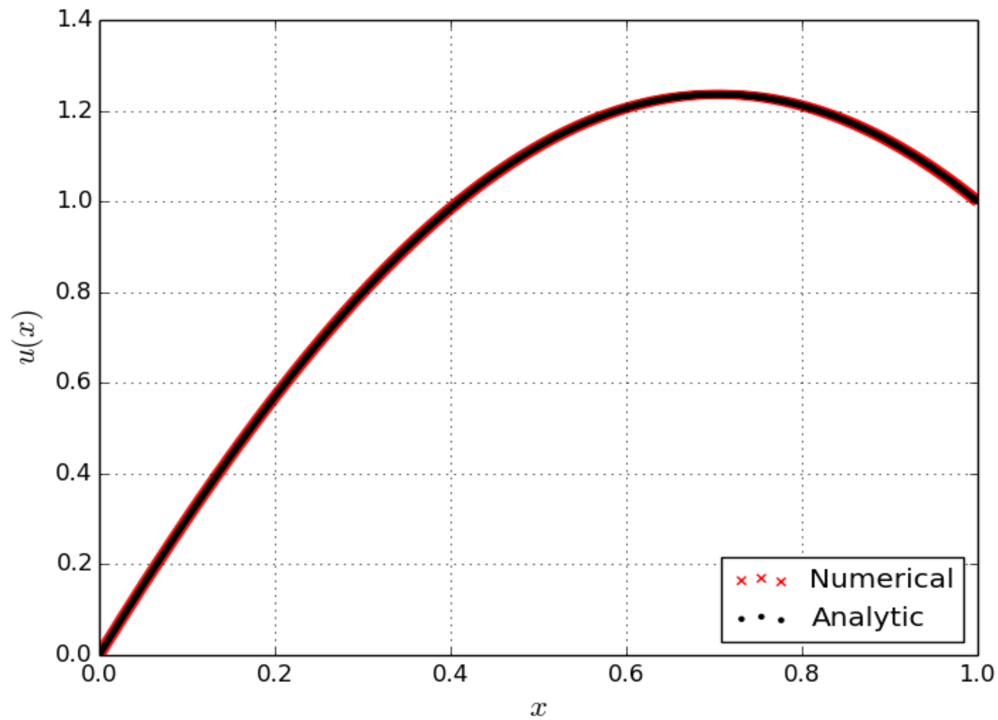

Figure 11: $u(x) vs. x$, from $x = 0$ to $x = 1$.

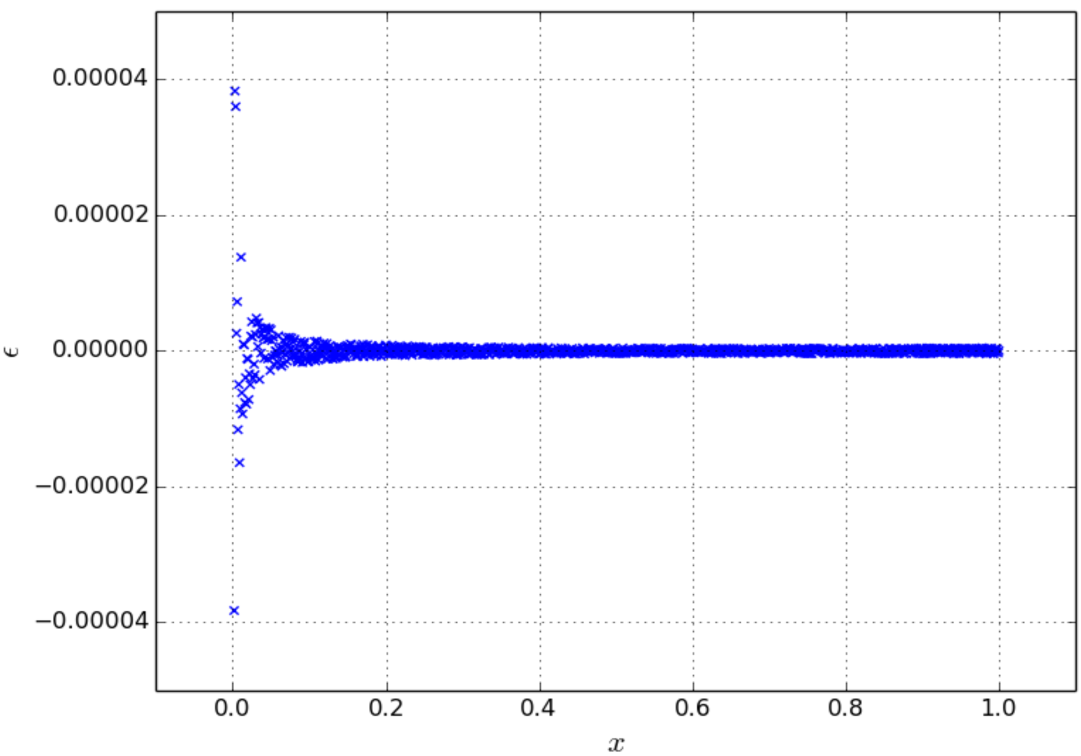

Figure 12: Relative error of the numerical solution to the analytic solution, as a function of x.

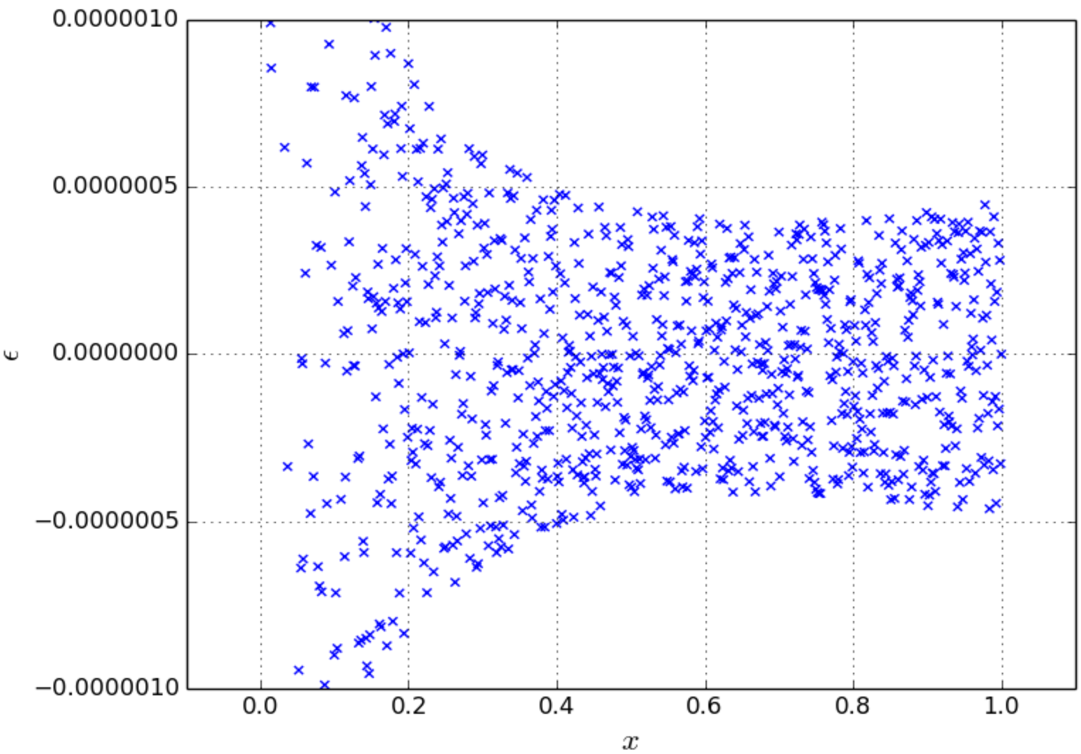

Figure 13: Similar to Fig. 12, with y-axis enlarged.

4 1-D Shrödinger Equation

With constants $\hbar = m = 1$, and $\alpha = 1$ and $\lambda = 4$, the Shrödinger equation becomes:

$$u''(x) + 2\left[E - V(x)\right]u(x) = 0, \quad \text{where} \quad V(x) = 6\left[\frac{1}{2} - \frac{1}{\cosh^2 x}\right]$$

Note, for classical turning points, they are given by:

$$V(x) = E$$
$$\Rightarrow \cosh x = \sqrt{\frac{6}{3-E}}$$

To have an intelligent initial guess for the ground state energy, let's expand $V(x)$ close to $x = 0$.

$$V(x) \simeq 6\left[\frac{1}{2} - \frac{1}{1+\frac{1}{2}x^2}\right] \simeq 6\left[\frac{1}{2} - \left(1 - \frac{1}{2}x^2\right)\right] = 3\left(x^2 - 1\right)$$

Compare this to the harmonic oscillator $\frac{1}{2}kx^2 + C$, the equivalent spring constant is $k = 6$. Also, $V(x)$ obtains its lowest point at $x = 0$, where $V(0) = -3$. So, the suggested initial guess of the ground state energy would be:

$$E_{0,guess} = \frac{1}{2}\hbar\omega_0 + V(0) = \frac{1}{2}\hbar\sqrt{\frac{k}{m}} - 3 \simeq -1.77$$

We can also expect the excited states to be separated by the energy difference of $\hbar\omega_0 \simeq 2.44$, which just serves as an indicator for the initial guesses of the other two excited states.

One of the sanity checks for the numerical solution is to check if $u(x) \to 0$ as $|x| \to \infty$. Physically it makes sense since the wavefunction far away from the potential barrier will have a value close to 0.

The numerical solution is obtained by the following procedures.

a. Make an initial guess on E_n.

b. Denote the classical turning points be $\pm x_0$, where $x_0(E) > 0$. The domain of the computation is taken to be $[x_l, x_r] = [x_0 - 10x_0, x_0 + 10x_0]$.

c. The boundary conditions can be taken as:

$$u(x_l) = 0,\ u'(x_l) = 1,\ u(x_r) = 0,\ u'(x_r) = \delta$$

Take $\delta = 1$ (Bear in mind, in general $u'(x_l) \neq u'(x_r)$. The solution obtained by the boundary condition can be matched to the solution with a simple normalization factor, if energy E is chosen correctly.) The equation is integrated twice, firstly from the left to the right, from $x = x_l$ to $x = x_0$. The next time from the right to the left, from $x = x_r$ to $x = x_0$, in 1000 steps respectively.

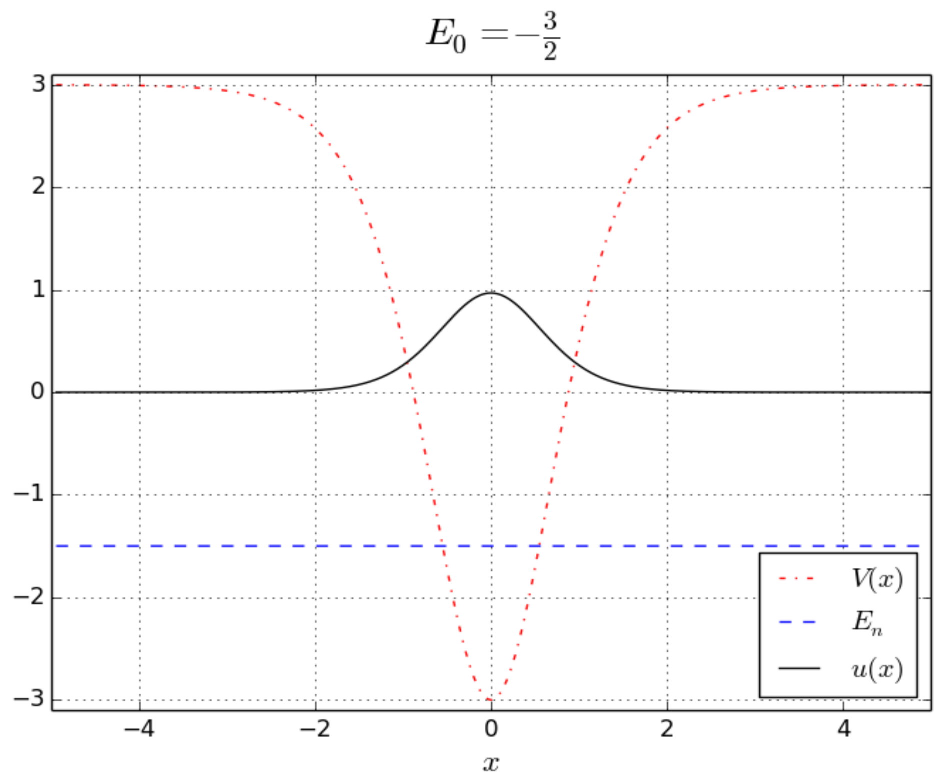

Figure 14: 1-D Shrödinger Equation for $E_0 = -\frac{3}{2}$.

d. The quantity:

$$r \equiv \frac{u_r'(x_r)}{u_r(x_r)} - \frac{u_l'(x_r)}{u_l(x_r)}$$

is computed. If the exact solution is obtained (with consistent boundary conditions), then r should be exactly 0, independent of the choice of δ. The range of E is iterated until $r < 10^{-5}$, then we obtain the eigenstate.

After computing the wavefunctions $u(x)$, the normalization factor A is obtained by the trapezoidal rule:

$$A^2 = \int_{-\infty}^{\infty} |u(x)|^2 dx$$

The exact solutions for the eigenvalues are $E_n = -\frac{3}{2}$, 1 and $\frac{5}{2}$. The numerical solutions (Figs. 14, 15, 16) agree with the analytic solutions, and at the boundaries, the wavefunctions are indeed almost zero.

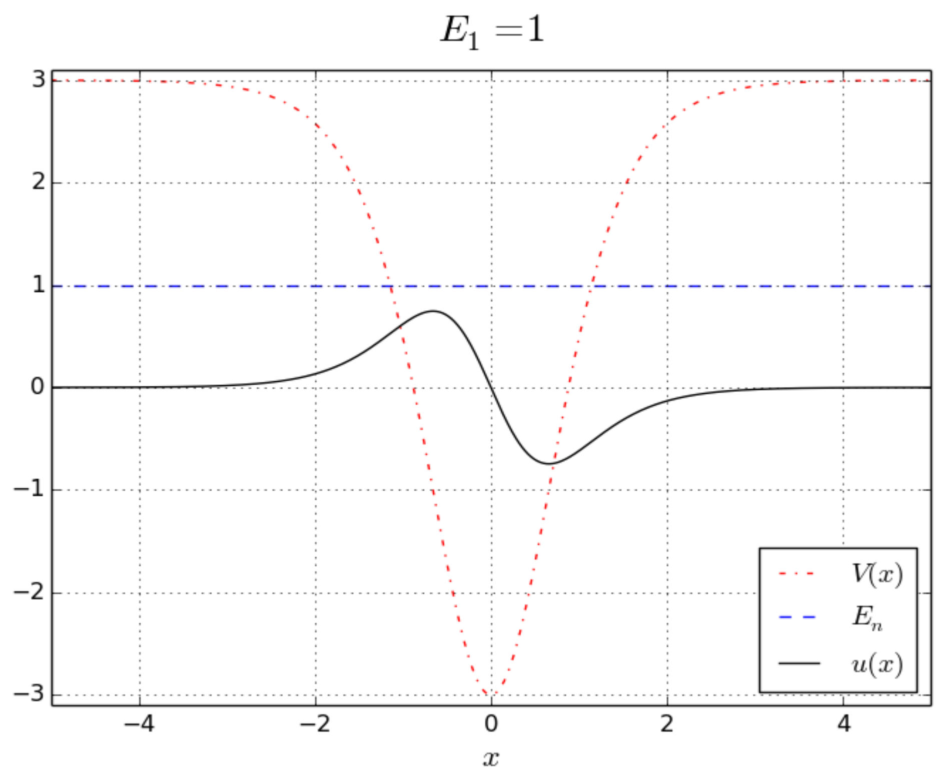

Figure 15: 1-D Shrödinger Equation for $E_1 = 1$.

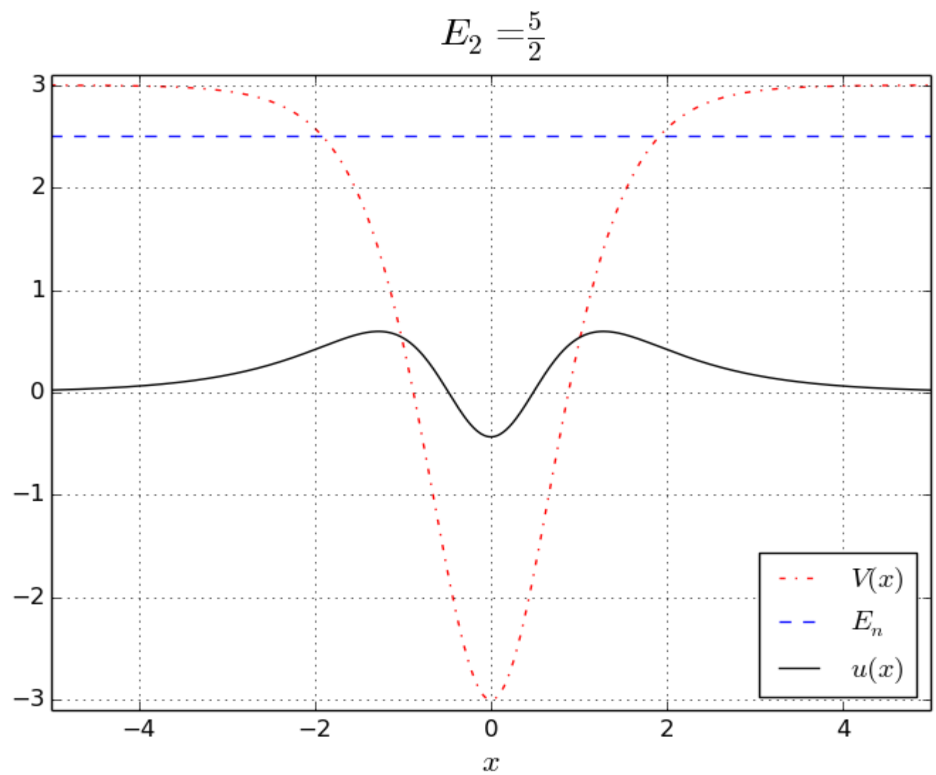

Figure 16: 1-D Shrödinger Equation for $E_2 = \frac{5}{2}$.