Presentation Problem 1

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1 Problem (as given in assignment)

Problem 5. A very common type of toy potential across physics is the "W" potential: a quartic potential with a negative quadratic term. Because the potential is quartic, many things cannot be said about it analytically, but some can, and it is also a fruitful venue for numerical analysis.

Let's consider a mass m moving in the potential

$$U(x) = U_0 \left(\frac{x^4}{4a^4} - \frac{x^3}{3a^3} - \frac{x^2}{a^2} \right)$$

for some length a and constant U_0 with dimensions of energy.

a) Show that this potential has two minima, and determine the approximate form of the potential (up to second order) around each minimum.

b) What are the angular frequencies associated with each of the minima above?

c) Write down a first order ODE for the mass based on energy conservation, assuming its initial position x_0 and velocity v_0 are known. Non-dimensionalize this equation using a as a reference length, m as a reference mass, and mv_0^2 as a reference energy.

d) Make a contour plot of the non-dimensionalized total energy as a function of non-dimensionalized position and non-dimensionalized velocity. Explain in your contour plot where you can "see" trajectories in which the mass is trapped in one or the other of the two potential wells.

e) Another possible type of trajectory is one in which the mass oscillates back and forth through both of the potential wells. Indicate where in your contour plot you can "see" this type of trajectory.

f) Choose a set of initial conditions and numerically solve the differential equation above. Show the trajectory of the mass on your contour plot.

2 Presentation

We have mass m moving in the quartic potential

$$U(x) = U_0 \left(\frac{x^4}{4a^4} - \frac{x^3}{3a^3} - \frac{x^2}{a^2} \right), \tag{1}$$

where a and U_0 are constant with units of length and energy, respectively. To find the potential energy minima, first set $U'(x)$ equal to zero

$$U'(x) = U_0 \left(\frac{x^3}{a^4} - \frac{x^2}{a^3} - \frac{2x}{a^2} \right),$$

$$0 = \left(\frac{x^2}{a^2} - \frac{x}{a} - 2 \right) x.$$

Therefore one extrema is at $x = 0$ and the others can be found with the quadratic formula

$$x = \frac{a^{-1} \pm \sqrt{a^{-2} + 8a^{-2}}}{2a^{-2}},$$

$$x = \frac{a^2}{2} \left(\frac{1}{a} \pm \frac{3}{a} \right).$$

So we have extrema at

$$x = 2a, -a, 0. \tag{2}$$

To find out which of these extrema are minima, take the second derivative of $U(x)$ and plug in each extremum:

$$U''(x) = U_0 \left(\frac{3x^2}{a^4} - \frac{2x}{a^3} - \frac{2}{a^2} \right), \tag{3}$$

$$U''(0) = \frac{-2U_0}{a^2},\ U''(-a) = \frac{4}{a^2},\ U''(2a) = \frac{6}{a^2}.$$

So the minima are at $x = 2a$ and $x = -a$.

To approximate the potential around each minima, Taylor expand $U(x)$ about $x = 2a$ and $x = -a$

$$U(-a + \Delta x) \approx U_0 \left(-\frac{5}{12} + \frac{3(\Delta x + a)^2}{2a^2} \right), \tag{4}$$

$$U(-2a + \Delta x) \approx U_0 \left(-\frac{8}{3} + \frac{3(\Delta x - 2a)^2}{2a^2} \right). \tag{5}$$

The period of oscillation around each minima is given by

$$T = 2\pi \sqrt{\frac{m}{U''(x_{min})}}, \tag{6}$$

so the angular frequencies of oscillation about the minima are

$$\omega_{2a} = \sqrt{\frac{6u_0}{ma^2}},\ \omega_{-a} = \sqrt{\frac{4u_0}{ma^2}}. \tag{7}$$

By applying conservation of energy, we can find the first order ODE that describes the motion mass m moving in potential $U(x)$. Assuming that $x(0) = x_0$ and $\dot{x}(0) = v_0$,

$$U(x_0) + \frac{1}{2}mv_0^2 = U(x) + \frac{1}{2}m\dot{x}^2. \tag{8}$$

To non-dimensionalize (8), let $E_{\text{ref}} = mv_0^2$, $\ell_{\text{ref}} = a$, and $t_{\text{ref}} = \frac{a}{v_0}$. Let $\xi = \frac{x}{\ell_{\text{ref}}}$, $\nu_0 = \frac{U_0}{E_{\text{ref}}}$, and $\tau = \frac{t}{t_{\text{ref}}}$. Taking the derivative of x with respect to t,

$$\frac{dx}{dt} = \frac{d(\ell_{\text{ref}}\xi)}{dt} = \ell_{\text{ref}}\frac{d\xi}{d\tau}\frac{d\tau}{dt}.$$

Let primes denote derivatives with respect to τ. Then $\dot{x}$ is

$$\dot{x} = \frac{\ell_{\text{ref}}}{t_{\text{ref}}}\xi'. \tag{9}$$

Returning to (8) and substituting in ξ for x/ℓ_{ref} and $\xi' = \frac{t_{\text{ref}}}{\ell_{\text{ref}}}\dot{x}$,

$$U_0\left(\frac{\xi_0^4}{4} - \frac{\xi_0^3}{3} - \xi_0^2\right) + \frac{1}{2}mv_0^2 = U_0\left(\frac{\xi^4}{4} - \frac{\xi^3}{3} - \xi^2\right) + \frac{m}{2}\frac{\xi'^2}{t_{ref}^2}\ell_{\text{ref}}^2. \tag{10}$$

Dividing both sides by E_{ref},

$$\nu_0\left(\frac{\xi_0^4}{4} - \frac{\xi_0^3}{3} - \xi_0^2\right) + \frac{1}{2} = \nu_0\left(\frac{\xi^4}{4} - \frac{\xi^3}{3} - \xi^2\right) + \frac{1}{2}\xi'^2.$$

Isolating ξ' yields the dimensionless first order ODE,

$$\xi' = \sqrt{2\nu_0\left(\frac{\xi_0^4 - \xi^4}{4} - \frac{\xi_0^3 - \xi^3}{3} - (\xi_0^2 - \xi^2)\right) + 1}. \tag{11}$$

Let non-dimensionalized total energy $E_{tot}/E_{\text{ref}} = \varepsilon$. The right hand side of Eq. (10) is the non-dimensionalized total energy, so ε is given by

$$\varepsilon = \nu_0\left(\frac{\xi^4}{4} - \frac{\xi^3}{3} - \xi^2\right) + \frac{1}{2}\xi'^2. \tag{12}$$

By making a contour plot of ε versus ξ and ξ', we can visualize the potential energy wells around each minima.

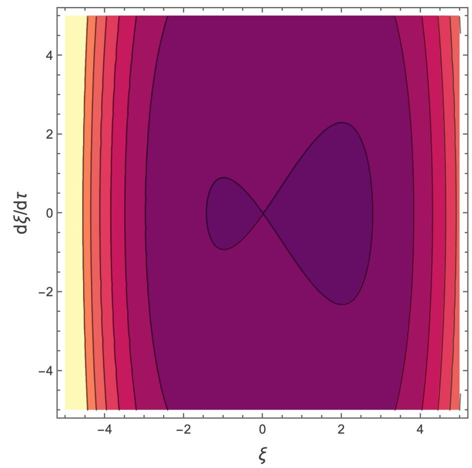


Figure 1: Contour plot of total non-dimensionalized energy ε versus non-dimensionalized position ξ and non-dimensionalized velocity ξ'. The potential wells are around the non-dimensionalized minima of $U(x)$ as expected.

From the contour plot in Fig. 1, we can see that if we have an initial non-dimensionalized position ξ_0 near a minima and small enough initial non-dimensionalized velocity ξ_0', the trajectory of the mass m will circle around the minima. Because the potential wells are touching we also know that the mass can move between both potential wells. We can demonstrate these three cases by numerically solving the equation of motion and making the right choices of initial conditions.

It turns out that numerical solvers can handle the second order ODE formulation of this problem much easier than the first order ODE form we found in Eq. (11). To find the non-dimensionalized second order ODE describing the motion of mass m moving in potential $U(x)$, we start by using the fact that

$$F = -\nabla U \tag{13}$$

together with Newton's Second Law, which gives

$$m\ddot{x} = -U_0 \left(\frac{x^3}{a^4} - \frac{x^2}{a^3} - \frac{2x}{a^2} \right). \tag{14}$$

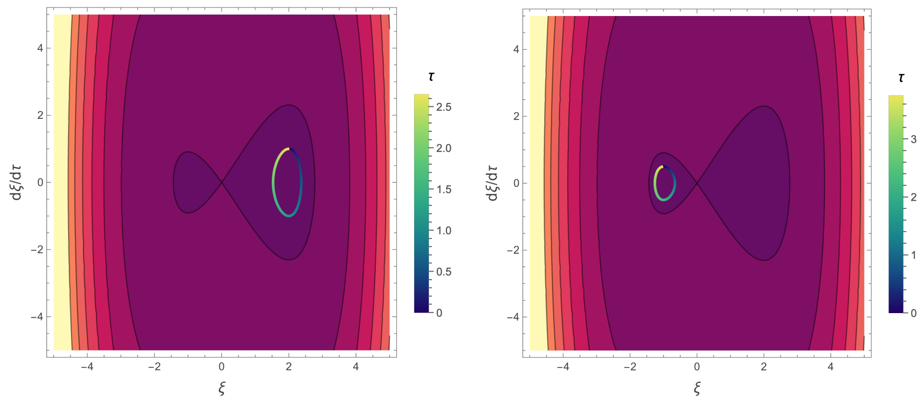
From Eq. (9), we have that $\dot{x} = \ell_{\text{ref}}\, \xi'/t_{\text{ref}}$, so

$$\ddot{x} = \frac{d(\ell_{\text{ref}}\xi'/t_{\text{ref}})}{dt} = \frac{\ell_{\text{ref}}}{t_{\text{ref}}} \frac{d\xi'}{d\tau} \frac{d\tau}{dt} = \frac{\ell_{\text{ref}}}{t_{\text{ref}}^2} \xi''. \tag{15}$$

Substituting into Eq. (14) and dividing by E_{ref}, we find the non-dimensionalized second order ODE

$$\xi'' = -\nu_0 \left(\xi^3 - \xi^2 - 2\xi \right), \tag{16}$$

which is much easier for Mathematica's `NDSolve` to handle than Eq. (11).



(a) $\xi_0 = 2$, $\xi_0' = 1$. (b) $\xi_0 = -1$, $\xi_0' = 0.5$.

Figure 2: Trajectory for mass m moving under potential $U(x)$ for one period of oscillation, for two different choices of initial conditions. Dimensionless time τ displayed on a blue-green-yellow scale.

Starting off at $\xi_0 = 0$ with $\xi_0' = 0.01$, the mass moves along the contour line that encloses both minima.

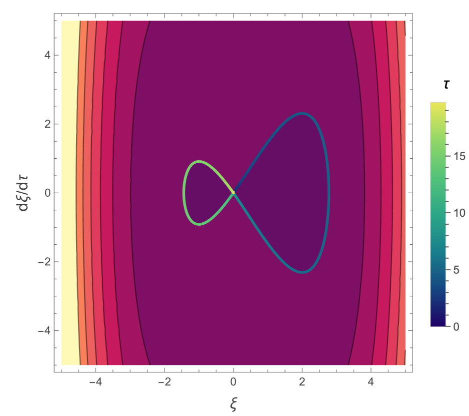


Figure 3: Trajectory where the mass oscillates between both potential wells, with initial conditions $\xi_0 = 0$ and $\xi_0' = 0.01$. Dimensionless time τ is displayed on a blue-green-yellow scale.

With numerical solutions in hand, we can check that we found the correct angular frequencies in Eq. (7).

By the definition of ξ',

$$\xi' = \frac{d\xi}{d\tau}. \tag{17}$$

Let $\Delta\tau = \tau_f - \tau_i$. Then rearranging and integrating both sides,

$$\Delta\tau = \int_{\xi_i}^{\xi_f} \frac{d\xi}{\xi'}. \tag{18}$$

If we set ξ_i and ξ_f equal to the minimum and ξ_f equal to the maximum of the non-dimensionalized position we solved for numerically, then

$$\frac{T}{2} = \int_{\xi_i}^{\xi_f} \frac{d\xi}{\xi'}, \tag{19}$$

where T is the period of oscillation. From (11),

$$\frac{T}{2} = \int_{\xi_i}^{\xi_f} \frac{d\xi}{\sqrt{2\nu_0\left(\frac{\xi_0^4-\xi^4}{4} - \frac{\xi_0^3-\xi^3}{3} - (\xi_0^2 - \xi^2)\right) + 1}}. \tag{20}$$

In terms of ω, the equation above reads

$$\frac{\pi}{\omega} = \int_{\xi_i}^{\xi_f} \frac{d\xi}{\sqrt{2\nu_0\left(\frac{\xi_0^4-\xi^4}{4} - \frac{\xi_0^3-\xi^3}{3} - (\xi_0^2 - \xi^2)\right) + 1}}, \tag{21}$$

which we can solve with Mathematica's `NIntegrate` function. For our solution with initial conditions $\xi_0 = 2$ and $\xi_0' = 1$, we expect $\omega = \sqrt{6} \approx 2.4$ from Eq. (7). Dividing the `NIntegrate` output by π and raising to the power of -1 gives

$$\omega_{2a} \approx 2.4. \tag{22}$$

For our solution with initial conditions $\xi_0 = -1$ and $\xi_0' = 0.5$, we expect $\omega = 2$ from Eq. (7). Again, dividing the `NIntegrate` output by π and raising to the power of -1, we find

$$\omega_{-a} \approx 2.1. \tag{23}$$

Reassuringly, the angular frequencies found for our numerical solutions are roughly consistent with those from our expressions for angular frequencies from Eq. (7).

A Mathematica Code

Contour plot with numerical solution:

```
u0 = 1;
x0 = 0;
v0 = 0.01;
tf = 19.7;
ti = 0;

s = NDSolve[{x''[t] == -((x[t]^3) - (x[t]^2) - 2 x[t]), x[0] == x0,
    x'[0] == v0}, x, {t, ti, tf},
   Method -> {"StiffnessSwitching",
     Method -> {"ExplicitRungeKutta", Automatic}}, AccuracyGoal -> 9,
   PrecisionGoal -> 9];

x1[t_] := (x[t] /. s)[[1]];
dx[t_] := Evaluate[D[x1[t], t]];

p = ParametricPlot[
   Evaluate[{x1[\[Tau]], dx[\[Tau]]}], {\[Tau], ti, tf},
   AxesLabel -> {Style["\[Xi]", 14], Style["d\[Xi]/d\[Tau]", 14]},
   PlotRange -> {{-3, 3}, {-3, 3}},
   ColorFunction -> {Function[{x, dx, t},
      ColorData["BlueGreenYellow"][t]]}, Frame -> True,
   PlotStyle -> {Thickness -> .0075}];

Legended[p, Placed[BarLegend[{"BlueGreenYellow", {0, tf}}], Right]];
u[y_] = u0 (y^4/4 - y^3/3 - y^2);
ee[y_, v_] := u0 (y^4/4 - y^3/3 - y^2) + 1/2 v^2;
Show[ContourPlot[ee[y, v], {y, -5, 5}, {v, -5, 5},
  FrameLabel -> {Style["\[Xi]", 14], Style["d\[Xi]/d\[Tau]", 14]}],
 Legended[p,
  Placed[BarLegend[{"BlueGreenYellow", {0, tf}},
    LegendLabel -> Style["\[Tau]", 14]], Right]]]
```

Calculating angular frequency:

```
Needs["DifferentialEquations`InterpolatingFunctionAnatomy`"];

u0 = 1;
x0 = 2;
v0 = 1;
tf = 20;
ti = 0;

U[x_] := u0*((x^4)/4 - (x^3)/3 - x^2);
```

```
s = NDSolve[{x''[t] == -((x[t]^3) - (x[t]^2) - 2 x[t]), x[0] == x0,
    x'[0] == v0}, x, {t, ti, tf},
   Method -> {"StiffnessSwitching",
     Method -> {"ExplicitRungeKutta", Automatic}}, AccuracyGoal -> 9,
   PrecisionGoal -> 7];

x1 := (x /. s)[[1]];

(NIntegrate[(1 + 2 (U[x0] - u0*((x^4)/4 - (x^3)/3 - x^2)))^(-1/2), {x,
      Min[InterpolatingFunctionValuesOnGrid[x1]],
     Max[InterpolatingFunctionValuesOnGrid[x1]]}, PrecisionGoal -> 9]/
   Pi)^(-1)
```