1. The (normalized) Lennard-Jones potential

\[ V(x) = \frac{1}{12x^{12}} - \frac{1}{6x^6} \]

provides a simple model for the interaction between two molecules separated by a distance \( x > 0 \). Graph the potential \( V(x) \) and sketch the \((x, x_t)\)-phase plane of the ODE in \( x > 0 \) for a particle moving in this potential

\[ x_{tt} - \frac{1}{x^{13}} + \frac{1}{x^7} = 0. \]

Solution

- We have \( V(x) \to \infty \) as \( x \to 0^+ \) and \( V(x) \to 0 \) as \( x \to \infty \). The potential has a unique, non-degenerate minimum at \( x = 1 \) with \( V(1) = -1/12 \). The corresponding equilibrium \((x, x_t) = (1, 0)\) is therefore a center.

- The trajectories are

\[ \frac{1}{2} x_t^2 + V(x) = E \]

If \( E = -1/12 \), this is the equilibrium. If \(-1/12 < E < 0\) this is a periodic orbit (corresponding to a ‘bound’ state of the particles). If \( E \geq 0 \), the trajectory comes in from infinity, turns around and goes out to \( \infty \) (corresponding to a ‘scattered’ state). In that case, since \( V(x) \to 0 \) as \( x \to \infty \), the velocity of the particle approaches the constant values \( x_t \to \pm \sqrt{2E} \) as \( t \to \pm \infty \).

Remark. The force between the particles \(-V'(x)\) is zero at the equilibrium \( x = 1 \), repulsive for \( x < 1 \), and attractive for \( x > 1 \). The attractive force approaches zero as \( x \to \infty \). The strong short-range repulsion is due, for example, to the Pauli exclusion of the molecules’ electron shells, while the weak long range attraction is due, for example, to van der Waals forces.

In the problem, we assume that the particles move along a straight line; in general, the particles would move in three space dimensions with positions \( \vec{x}_1(t), \vec{x}_2(t) \in \mathbb{R}^3 \) in the central potential \( V(|\vec{x}_1 - \vec{x}_2|) \), analogous to the Kepler problem for planetary motion (where the potential would be the inverse square attractive potential \( V = -1/|\vec{x}|^2 \)).
2. Find and classify the equilibria of the system
\[ x_t = x^2 - y - 1, \]
\[ y_t = (x - 2) y. \]
Sketch the phase plane.

**Solution**

- From the second equation, we have \( x = 2 \) or \( y = 0 \) at an equilibrium. Using these values and solving the first equation, we find that there are three equilibria
  \[ (x, y) = (-1, 0), \quad (1, 0), \quad (2, 3). \]
  The derivative of the vector field \( \vec{f}(x, y) = (x^2 - y - 1, (x - 2)y)^T \) is
  \[ D\vec{f} = \begin{pmatrix} 2x & -1 \\ y & x - 2 \end{pmatrix}. \]
- Linearizing around \((-1, 0)\), we get
  \[ \begin{pmatrix} x \\ y \end{pmatrix}_t = \begin{pmatrix} -2 & -1 \\ 0 & -3 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}. \]
  The eigenvalues are \( \lambda = -2, -3 \) so this is a stable node. The ‘slow’ direction, corresponding to \( \lambda = -2 \) is \( \vec{r} = (1, 0)^T \).
- Linearizing around \((1, 0)\), we get
  \[ \begin{pmatrix} x \\ y \end{pmatrix}_t = \begin{pmatrix} 2 & -1 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}. \]
  The eigenvalues are \( \lambda = 2, -1 \) so this is a saddle. The unstable direction \( \vec{r}_1 \), corresponding to \( \lambda = 2 \), and the stable direction \( \vec{r}_2 \), corresponding to \( \lambda = -1 \), are given by
  \[ \vec{r}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \vec{r}_2 = \begin{pmatrix} 1 \\ 3 \end{pmatrix}. \]
• Linearizing around \((2, 3)\), we get
\[
\begin{pmatrix} x \\ y \end{pmatrix}_t = \begin{pmatrix} 4 & -1 \\ 3 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}.
\]
The eigenvalues are 
\[
\lambda = 1, \ 3,
\]
so this is an unstable node. The ‘slow’ direction, corresponding to 
\[
\lambda = 1, \text{ is } \vec{r} = (1, 3)^T.
\]

• The system has no periodic orbits. There are unique heteroclinic orbits
from the unstable node to the saddle and the saddle to the stable node,
and a one-parameter family of heteroclinic orbits from the unstable to
the stable node.

• For this system, all the lines through the equilibria are invariant. This
clear for the \(x\)-axis \(y = 0\). For the others, note that
\[
\frac{d}{dt} [y - (x + 1)] = y_t - x_t = (x - 2)y - x^2 + y + 1 = (x - 1)[y - (x + 1)].
\]
Hence if \(y - (x + 1) = 0\) initially, which is the equation of the line
through \((-1, 0)\) and \((2, 3)\), then it remains zero for all \(t\). Similarly, for
the line through \((1, 0)\) and \((2, 3)\),
\[
\frac{d}{dt} [y - 3(x - 1)] = y_t - 3x_t = (x - 2)y - 3(x^2 - y - 1) = (x + 1)[y - 3(x - 1)].
\]

• In sketching the phase plane, it is also useful to look at the isoclines
where
\[
\frac{dy}{dx} = \frac{(x - 2) y}{x^2 - y - 1} = \text{constant}.
\]
In particular, the trajectories are horizontal on the lines \(x = 2\) and
\(y = 0\) where \(y_t = 0\), and vertical on the parabola \(y = x^2 - 1\) where
\(x_t = 0\). See the attached figures for the phase plane.
3. Consider the scalar ODE

\[ x_t = (x + 1)(\mu + x - x^2) \]

where \( \mu \in \mathbb{R} \) is a parameter.

(a) Find the equilibria and determine their stability.

(b) Draw a bifurcation diagram. What bifurcations occur as \( \mu \) is varied?

(c) Sketch phase lines for qualitatively different values of \( \mu \).

(d) How would the bifurcation diagram from (b) be perturbed in a generic imperfect bifurcation for this ODE?

Solution

- The equilibria are

  \[ x = -1 \]

  and, for \( \mu \geq -1/4 \),

  \[ x = \frac{1 \pm \sqrt{1 + 4\mu}}{2}. \]  

  (1)

- Writing

  \[ f(x; \mu) = (x + 1)(\mu + x - x^2) \]

  \[ = \mu + (1 + \mu)x - x^3, \]

  we have

  \[ f_x(x; \mu) = 1 + \mu - 3x^2. \]

- For \( x = -1 \), we have

  \[ f_x(-1, \mu) = \mu - 2 \]

  so the equilibrium is asymptotically stable \( (f_x < 0) \) if \( \mu < 2 \) and unstable \( (f_x > 0) \) if \( \mu > 2 \).

- For the equilibria in (1), we find that

  \[ f_x \left( (1 \pm \sqrt{1 + 4\mu})/2; \mu \right) = \mp \frac{1}{2} \sqrt{1 + 4\mu} \left[ 3 \pm \sqrt{1 + 4\mu} \right]. \]

    Thus, the plus equilibrium is asymptotically stable \( (f_x < 0) \) for all \( \mu > -1/4 \). The minus equilibrium is unstable for \( -1/4 < \mu < 2 \),
when $3 - \sqrt{1 + 4\mu} > 0$, and asymptotically stable for $\mu > 2$, when $3 - \sqrt{1 + 4\mu} < 0$. Note that the minus solution branch in (1) crosses the solution branch $x = -1$ at $\mu = 2$ when this change of stability occurs.

- There is a saddle-node bifurcation at

$$(x, \mu) = \left(\frac{1}{2}, -\frac{1}{4}\right)$$

and a transcritical bifurcation at

$$(x, \mu) = (-1, 2)$$

The bifurcation diagram and phase lines are shown in the attached figures.

- A generic perturbation of this system will destroy the transcritical bifurcation or split it into a pair of saddle-node bifurcations (see the attached figures).
4. Consider the system

\[ \begin{align*}
    x_t &= y, \\
    y_t &= -x + y \left(1 - x^2 - 2y^2\right).
\end{align*} \]

(a) Let \( V(x, y) = x^2 + y^2 \) Compute \( V_t \) on trajectories. Show that \( V \) is increasing with \( t \) (\( V_t \geq 0 \)) if \( r^2 < 1/2 \) and decreasing (\( V_t \leq 0 \)) if \( r^2 > 1 \), where \( r = \sqrt{x^2 + y^2} \) is the distance from the origin.

(b) Deduce that there is a periodic orbit of the system in the annulus \( 1/2 < r^2 < 1 \).

Solution

• (a) We have

\[ V_t = 2xx_t + 2yy_t \]

\[ = 2xy + 2y \left[-x + y \left(1 - x^2 - 2y^2\right)\right] \]

\[ = 2y^2 \left(1 - x^2 - 2y^2\right). \]

• If \( x^2 + y^2 > 1 \), then

\[ 1 - x^2 - 2y^2 \leq 1 - x^2 - y^2 < 0 \]

so \( V \) is decreasing (in fact, strictly decreasing unless \( y = 0 \)).

• If \( x^2 + y^2 < 1/2 \), then

\[ 1 - x^2 - 2y^2 \geq 1 - 2x^2 - 2y^2 > 0 \]

so \( V \) is increasing (in fact, strictly increasing unless \( y = 0 \)).

• (b) It follows from (a) that the annulus \( 1/2 \leq r^2 \leq 1 \) is a trapping region for the flow, since trajectories enter the region but cannot leave. The only equilibrium of the system is the origin \((x, y) = (0, 0)\), so there are no equilibria inside the annulus. The Poincaré-Bendixson theorem then implies that there must be a limit cycle inside the annulus.
5. Consider the expanding map $E : \mathbb{T} \to \mathbb{T}$ on the circle defined by

$$E(\theta) = 2\theta \pmod{2\pi}$$

for $\theta \in \mathbb{T}$, with the associated discrete dynamical system

$$\theta_{n+1} = 2\theta_n \pmod{2\pi}, \quad n \in \mathbb{N}.$$

(a) Is the map $E$ invertible? What is its fixed point?
(b) What are the points of period two (fixed points of $E^2$)?
(c) If $k \in \mathbb{N}$ is any positive integer, how many points of period $k$ (fixed points of $E^k$) are there?
(d) Does $E$ have non-periodic orbits? If so, what do you think the orbits look like? How do nearby points typically behave under successive iterations of $E$?

**Solution**

- (a) The map is not invertible since it is two-to-one *e.g.* both 0 and $\pi$ map to 0. The map stretches the circle by a factor of 2 and then wraps it around itself twice. (Think of doing this with an elastic band.) Thus, $E$ maps both of the half-circles $[0, \pi)$ and $[\pi, 2\pi)$ one-to-one and onto the whole circle. The origin $\theta = 0$ is the only fixed point of the map. Note that it is unstable since $E'(0) = 2 > 1$.

- (b) The origin $\theta = 0$ has period two (and minimal period one). In addition there is an orbit with minimal period two consisting of the points $\theta = 2\pi/3, 4\pi/3$ *e.g.* modulo $2\pi$:

$$E^2 \left(\frac{2\pi}{3}\right) = E \left(\frac{4\pi}{3}\right) = \frac{8\pi}{3} = \frac{2\pi}{3}.$$

Thus, there are three points with period two

$$\left\{0, \frac{2\pi}{3}, \frac{4\pi}{3}\right\},$$

two of which have minimal period two.

- (c) There are $2^k - 1$ points with period $k$ (see below).
• (d) Only countably many points lie on periodic orbits, so $E$ certainly has non-periodic orbits since $T$ is uncountable. ‘Typical’ orbits are dense in $T$. (In fact, one can show that the set of points with dense orbits form a set of full Lebesgue measure $2\pi$ in $T$.) The distance between nearby points doubles each iteration under the action of $E$, until the points separate by an angle of more than $\pi/2$, so there is sensitive dependence on initial conditions.

Remark. This expanding map is one of the simplest example of a chaotic map. The clearest way to understand its behavior is through the method of symbolic dynamics. Represent an angle $\theta = 2\pi x$ on the circle by a binary expansion of $0 \leq x \leq 1$:

$$x = 0.x_1x_2x_3x_4\ldots$$

where $x_i = 0$ or $x_i = 1$. This representation is not quite unique, since for example $0.00000\ldots$ and $0.11111\ldots$ both represent the angle $\theta = 0$ or equivalently $\theta = 2\pi$, and similarly for other binary expansions terminating in 1’s. (This is the binary analog of $1 = 0.9999\ldots$.) If $\Sigma$ denotes the sequence space of these binary expansions, then the expanding map $E : T \to T$ corresponds to a left shift $\sigma : \Sigma \to \Sigma$ of the sequence space

$$\sigma(0.x_1x_2x_3x_4\ldots) = 0.x_2x_3x_4\ldots.$$ 

Points which eventually map to zero correspond to expansions that terminate in all 0’s (or all 1’s). Period $k$ points correspond to binary expansions of rational numbers with blocks of $k$ repeating digits. There are $2^k$ such expansions, which gives $2^k - 1$ points of period $k$ for $E$ since the expansions $0.0000\ldots$ and $0.1111\ldots$ correspond to the same point of $T$. To construct a sequence with dense orbit, under $\sigma$, list all finite sequences of length 1, 2, 3, \ldots and string them together. The results is a sequence whose digits agree to an arbitrarily large finite number of terms with any other given sequence after sufficiently many shifts.

More formally, we define the sequence space $\Sigma = \{0, 1\}^\mathbb{N}$ of sequences $(x_1, x_2, x_3, \ldots)$ of zeros and ones $x_i \in \{0, 1\}$, the left shift $\sigma : \Sigma \to \Sigma$ by

$$\sigma((x_1, x_2, x_3, \ldots)) = (x_2, x_3, \ldots),$$

and the map $\psi : \Sigma \to T$ by

$$\psi(x_1, x_2, x_3, \ldots) = 2\pi(0.x_1x_2x_3\ldots).$$
Then

\[ E \circ \psi = \psi \circ \sigma \]

meaning that \( E \) is topologically semi-conjugate to \( \sigma \). (It is only semi-conjugate because the map \( \psi \) is not one-to-one, so it is not invertible.) We can therefore analyze the dynamics of \( E \) in terms of the easier to understand shift-map \( \sigma \). Similar ideas can be used to analyze the dynamics of other chaotic dynamical systems such as the logistic map, Smale horseshoes, and homoclinic tangles.