A Short Introduction to Hamiltonian Mechanics

Robin Leroy (eggrobin)

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In this post I shall assume understanding of the concepts described in chapter 4 (Conservation of Energy), chapter 8 (Motion) as well as sections 11–4 and 11–5 (Vectors and Vector algebra) of chapter 11 of Richard Feynmann's *Lectures on Physics*.

It is the continuation of my *Introduction to Runge-Kutta Integrators*, but it does not rely on the concepts described in that post.

1 Motivation

We have previously seen how to compute the evolution of physical systems while keeping the buildup of error in check. However, the error will still build up over time. We would like to ensure that fundamental properties of the physical system are preserved. For instance, we'd like a low strongly-bound orbit not to turn into an escape trajectory (or a reentry) over time: we need conservation of energy.

In order to make an integrator that conserves energy, it is helpful to look at physics from a viewpoint where the conservation of energy is the fundamental hypothesis, rather than a consequence of the application of some forces.

2 Gravitation from a Hamiltonian viewpoint

We consider a system of N bodies 1 through N, with masses m_1 through m_N. The state of the system is defined by the *positions* and *momenta* of those bodies. For each body j, the position $\boldsymbol{Q}_j$ and the momentum $\boldsymbol{P}_j$ are 3-dimensional vectors, so the state of the entire system lies in a $6N$-dimensional space, the *classical*[1] *phase space*. We can write the state as $(\boldsymbol{q}, \boldsymbol{p})$, where $\boldsymbol{q} = (q_1, \dots, q_{3N})$ and $\boldsymbol{p} = (p_1, \dots, p_{3N})$ are $3N$-dimensional.

The total energy $\mathcal{H}$, the *Hamiltonian*, is a function of the state of the system, the energy of a given state being $\mathcal{H}(\boldsymbol{q}, \boldsymbol{p})$.

The evolution of the state $(\boldsymbol{q}, \boldsymbol{p})$ is defined[2] for each dimension $i \in \{1, \dots, 3N\}$, by the *equations of motion*

$$\begin{cases} \frac{\mathrm{d}\, q_i}{\mathrm{d}\, t} &= \frac{\mathrm{d}\, \mathcal{H}}{\mathrm{d}\, p_i} \\ \frac{\mathrm{d}\, p_i}{\mathrm{d}\, t} &= -\frac{\mathrm{d}\, \mathcal{H}}{\mathrm{d}\, q_i} \end{cases}$$

This can be written[3] as

$$\begin{cases} \frac{\mathrm{d}\, \boldsymbol{q}}{\mathrm{d}\, t} &= \frac{\mathrm{d}\, \mathcal{H}}{\mathrm{d}\, \boldsymbol{p}} \\ \frac{\mathrm{d}\, \boldsymbol{p}}{\mathrm{d}\, t} &= -\frac{\mathrm{d}\, \mathcal{H}}{\mathrm{d}\, \boldsymbol{q}} \end{cases}$$

Where for a function $f(\boldsymbol{x}, \boldsymbol{y})$, we define[4] $\frac{\mathrm{d}\, f}{\mathrm{d}\, \boldsymbol{x}} \coloneqq \left(\frac{\mathrm{d}\, f}{\mathrm{d}\, x_1}, \frac{\mathrm{d}\, f}{\mathrm{d}\, x_2}, \dots, \frac{\mathrm{d}\, f}{\mathrm{d}\, x_n}\right)$. In this way, we

[1] A similar formalism exists for quantum mechanics, in which case we talk about the *quantum* phase space.

[2] The interested reader may wish to refer to *Wikipedia* (`http://goo.gl/NiXJY4`) or any classical mechanics book for a derivation from Lagrangian mechanics. We shall take the Hamiltonian formulation as an axiom.

[3] Readers familiar with multivariate calculus might prefer the notations $\frac{\mathrm{d}\, \boldsymbol{q}}{\mathrm{d}\, t} = \boldsymbol{\nabla}_{\boldsymbol{p}} \mathcal{H}$, $\frac{\mathrm{d}\, \boldsymbol{p}}{\mathrm{d}\, t} = -\boldsymbol{\nabla}_{\boldsymbol{q}} \mathcal{H}$, or $\frac{\mathrm{d}}{\mathrm{d}\, t}\begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{p} \end{pmatrix} = \begin{pmatrix} \boldsymbol{0} & \mathbb{1} \\ -\mathbb{1} & \boldsymbol{0} \end{pmatrix} \boldsymbol{\nabla} \mathcal{H}$.

[4] Note to the pedantic reader: while this notation is nonstandard, and one might expect partial derivatives here, it *does* makes sense, since no matter whether the derivative is partial or total, the notations $\frac{\partial f}{\partial x}$ and $\frac{\mathrm{d}\, g}{\mathrm{d}\, t}$ both mean the projection of the differential form $\mathrm{d}\, f$ (respectively $\mathrm{d}\, g$) on the corresponding subspace. For clarity and in order not to introduce more prerequisites we shall use only straight ds, and define $\frac{\mathrm{d}\, f}{\mathrm{d}\, \boldsymbol{x}}$ as the projection of $\mathrm{d}\, f$ onto the subspace on which $\mathrm{d}\, \boldsymbol{x}$ acts as the identity.

have *defined* the change in position and momentum as a function of time, and thus completely described how the system will evolve from an initial state $(\boldsymbol{q}_0, \boldsymbol{p}_0)$.

From this formulation it immediately follows that energy is conserved: indeed,

$$\begin{aligned}\frac{\mathrm{d}\,\mathcal{H}(\boldsymbol{p},\boldsymbol{q})}{\mathrm{d}\,t} &= \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{q}} \cdot \frac{\mathrm{d}\,\boldsymbol{q}}{\mathrm{d}\,t} + \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{p}} \cdot \frac{\mathrm{d}\,\boldsymbol{p}}{\mathrm{d}\,t} \\ &= \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{q}} \cdot \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{p}} - \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{p}} \cdot \frac{\mathrm{d}\,\mathcal{H}}{\mathrm{d}\,\boldsymbol{q}} = 0.\end{aligned}$$

Here the energy is $\mathcal{H} = T+V$, where T is the kinetic energy and V is the gravitational potential energy. Since T only depends on the momenta $\boldsymbol{p}$ (recall that for body j, $T_j = \frac{1}{2} m_j v_j^2$ and $\boldsymbol{P}_j = m_j \boldsymbol{v}_j$) and V only depends on the positions $\boldsymbol{q}$, we get:

$$\mathcal{H}(\boldsymbol{p},\boldsymbol{q}) = T(\boldsymbol{p}) + V(\boldsymbol{q})$$

so the equations of motion become

$$\begin{cases} \frac{\mathrm{d}\,\boldsymbol{q}}{\mathrm{d}\,t} &= \frac{\mathrm{d}\,T}{\mathrm{d}\,\boldsymbol{p}} \\ \frac{\mathrm{d}\,\boldsymbol{p}}{\mathrm{d}\,t} &= -\frac{\mathrm{d}\,V}{\mathrm{d}\,\boldsymbol{q}} \end{cases}.$$

For a single body j, this gives us

$$\begin{cases} \frac{\mathrm{d}\,\boldsymbol{Q}_j}{\mathrm{d}\,t} &= \frac{\mathrm{d}\,T}{\mathrm{d}\,\boldsymbol{P}_j} = \frac{\mathrm{d}}{\mathrm{d}\,\boldsymbol{P}_j} \frac{1}{2} m_j v_j^2 = v \\ \frac{\mathrm{d}\,\boldsymbol{P}_j}{\mathrm{d}\,t} &= -\frac{\mathrm{d}\,V}{\mathrm{d}\,\boldsymbol{q}} \end{cases}.$$

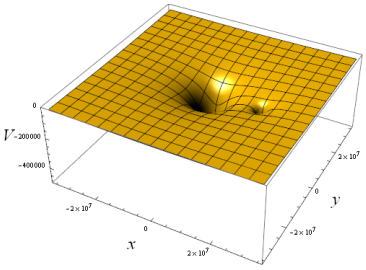

Figure 1. The potential V generated by Pluto and Charon, as a function of the position (x, y) of a 1 kg body sharing their orbital plane. V in Joules, x and y in metres.

In other words, the change in position is the velocity, and the change in momentum (the force) is in the direction which decreases the potential. It helps to visualise the potential for a two-dimensional problem, where the position of a body j is given by x_j and y_j. One can plot the potential $V(x_j, y_j)$ as a hilly landscape, where wells are created by the other bodies. The force on j (the change in its momentum) is then directed downhill and its magnitude is proportional to the slope of the hill, as if j were a ball rolling atop those hills. See for instance the potential created by Pluto and Charon in the margin. A one-dimensional example can be seen at `https://xkcd.com/681_large/`.

From this formulation of the equation of motions, it is possible to deduce properties of the trajectories just from the initial energy, even when the trajectories are very convoluted. Indeed, since the energy is conserved and since the kinetic energy (equal to $\frac{1}{2} m_j v_j^2$ for each body j) is never negative (at worst it is 0 for an unmoving body), the system cannot reach a position $\boldsymbol{q}$ where the potential $V(\boldsymbol{q})$ is greater than the initial energy.

Again, this is best seen on a 2-dimensional example with a single body moving in a fixed potential. If we plot the landscape of the potential, and a waterline at the level of the initial energy, we know that the body cannot be found on dry land at any time, no matter how complicated its trajectory is; if the trajectory converts the whole of the body's kinetic energy into potential energy, it will only reach the shore.

Moreover, the body cannot[5] "jump" over dry land, as that would require going through areas of potential higher than the total energy. It is confined to the "lake" in which it started.

The plots below show various regions allowed by the total energy in the previously shown potential, together with example trajectories at these energies. Note that the trajectories are computed assuming the potential is constant (which is not true in the case of Pluto and Charon, since these bodies revolve around each other). We'll look at a more realistic situation in a later post.

3 Generalised coordinates

We will now look at another strength of the Hamiltonian formulation of classical mechanics: it allows for the use of coordinate systems more appropriate to the problem at hand.

[5] In quantum mechanics this happens: this is quantum tunnelling.

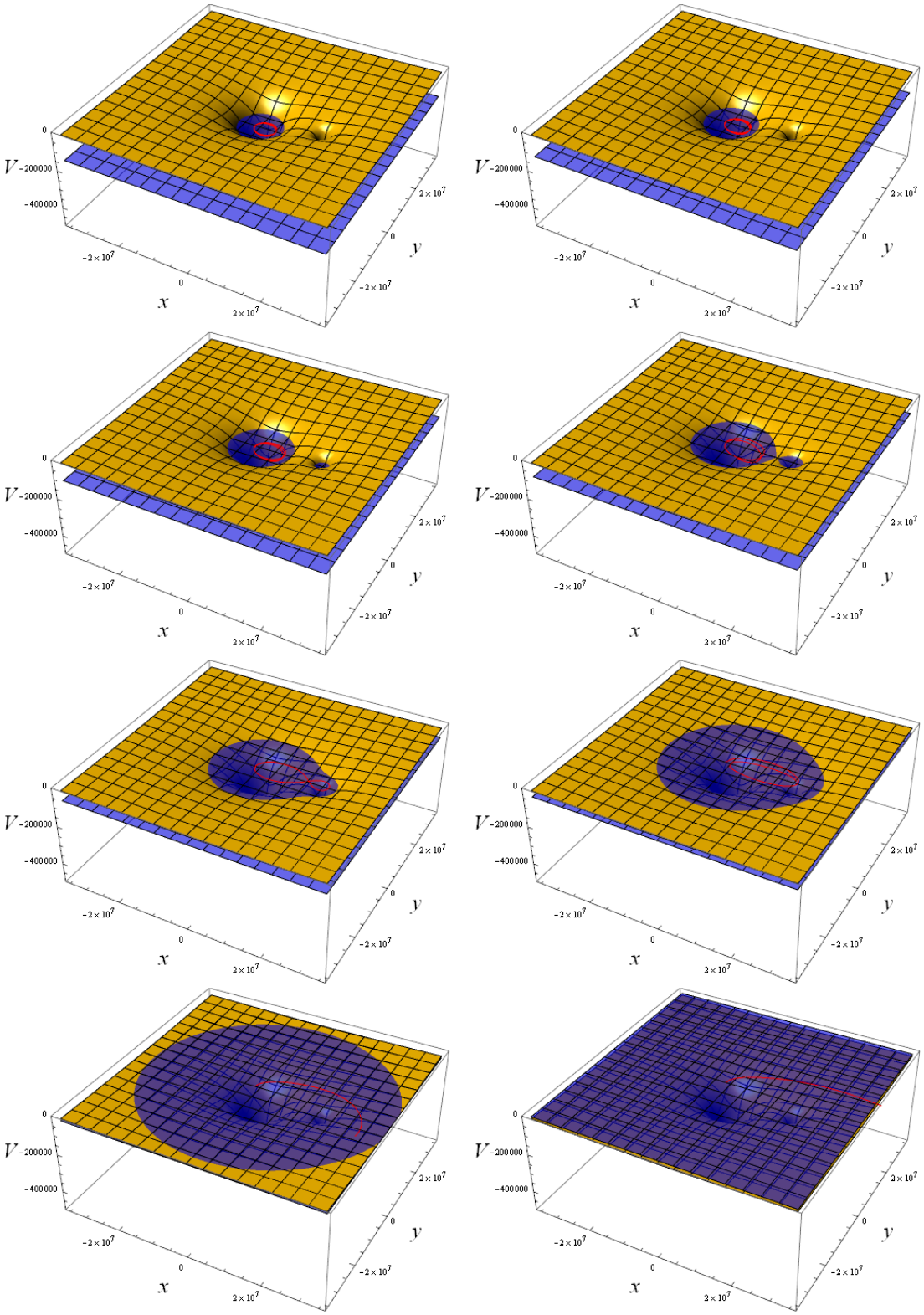

Figure 2. Forbidden regions (due to potential higher than the initial energy) for various initial energies, with example trajectories. The energy of the body is the blue plane, the potential is the yellow surface.

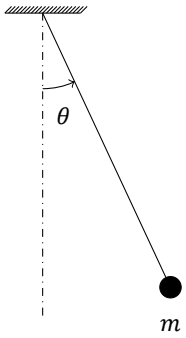

Figure 3. A mathematical pendulum.

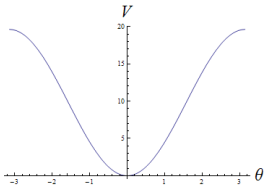

Figure 4. The potential of the pendulum, with $m = 1$ kg and $r = 1$ m. V in Joules, θ in radians.

Consider a pendulum made of a point mass m suspended in a vacuum with a massless rod of length r from a frictionless hinge[6], under the influence of uniform standard gravity g_0.

At first glance, this may seem like a 2-dimensional problem since the pendulum does not move in a straight line. However, since the pendulum is restricted by the rod to a circle around the pivot, we can describe its position uniquely by the oriented angle θ between the rod and the vertical: we shall use this as our *generalised position*.

Lagrangian mechanics, which is beyond the scope of this overview, is needed to derive the corresponding generalised momentum. We shall take for granted that this is the angular momentum $L = mr^2\omega$, where $\omega = \frac{\mathrm{d}\,\theta}{\mathrm{d}\,t}$ is the angular velocity.

Our state (θ, L) thus lies in a 2-dimensonial phase space. We can now compute the Hamiltonian. The kinetic energy of our mass is

$$T = \frac{1}{2}mv^2 = \frac{1}{2}m(r\omega)^2 = \frac{L^2}{2mr^2}.$$

The potential energy is mg_0h, where h is the height of the mass, so we can express it as

$$V = mg_0h = -mg_0(\cos\theta - 1).$$

We can then apply the equations of motions to that problem, and solve it as a 1-dimensional problem, using these more convenient coordinates. We will come back to this problem in the next post to study another fundamental conservation law related to Hamiltonian systems.

4 Conclusion

We see that the nature of the possible trajectories changes fundamentally when the energy changes, from strongly-bound orbits to transfers to outright escapes. It would therefore be useful to be able to guarantee that energy does not drift too much even over long periods of time when numerically computing these trajectories. Surprisingly, while guaranteeing that the actual position does not drift away from the truth is impossible, it *is* possible to ensure that the *energy* does not drift, thus ensuring that the essential nature of the trajectory remains unchanged.

Integrators which enforce conservation of energy are called *symplectic* integrators. They rely on another property of Hamiltonian systems, symplecticity, which will be the focus of the next post.

[6] We will not be needing the spherical cows today.