An Introduction Hamiltonian Mechanics

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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 Newtonian viewpoint

Recall the formulation by forces of the gravitational N-body problem: each body i, located at position $\boldsymbol{Q}_i$ exerts a force $\boldsymbol{F}_{ij}$ on every other body j, located at $\boldsymbol{Q}_j$ whose magnitude is

$$F_{ij} = \frac{G m_i m_j}{|\boldsymbol{Q}_i - \boldsymbol{Q}_j|^2}.$$

The force on j is directed toward i, so

$$\boldsymbol{F}_{ij} = F_{ij} \frac{\boldsymbol{Q}_i - \boldsymbol{Q}_j}{|\boldsymbol{Q}_i - \boldsymbol{Q}_j|} = \frac{G m_i m_j}{|\boldsymbol{Q}_i - \boldsymbol{Q}_j|^2} \frac{\boldsymbol{Q}_i - \boldsymbol{Q}_j}{|\boldsymbol{Q}_i - \boldsymbol{Q}_j|} = \frac{G m_i m_j}{|\boldsymbol{Q}_i - \boldsymbol{Q}_j|^3} (\boldsymbol{Q}_i - \boldsymbol{Q}_j).$$

Adding up all the forces exerted on j by the bodies $1, \ldots, j-1, j+1, \ldots, N$, we get the total force $\boldsymbol{F}_j$ on j,

$$\begin{aligned} \boldsymbol{F}_j &= \boldsymbol{F}_{1j} + \boldsymbol{F}_{2j} + \cdots + \boldsymbol{F}_{j-1\,j} + \boldsymbol{F}_{j+1\,j} + \boldsymbol{F}_{N\,j} \\ &= \sum_{\substack{i=1 \\ i \neq j}}^{N} \boldsymbol{F}_{ij} \end{aligned}$$

This force then changes the velocity of j according to Newton's second law,

$$\frac{\mathrm{d}\,\boldsymbol{v}_j}{\mathrm{d}\,t} = \frac{\boldsymbol{F}_j}{m_j}.$$

What is the energy of that N-body system? Part of it is the energy due to the motion of the bodies, the so-called *kinetic*[1] energy T,

$$T = \sum_{j=1}^{N} \frac{1}{2} m_j v_j^2.$$

[1]From ancient Greek *κινεῖν*, to move.

The other form in which energy is present is gravitational potential energy,

$$V = \sum_{i=1}^{N} \sum_{\substack{i=1 \\ i \neq j}}^{N} \frac{G m_i m_j}{|\boldsymbol{Q}_i - \boldsymbol{Q}_j|}$$

From the Newtonian viewpoint, it happens that gravity is a conservative force (it doesn't waste energy in heat or something else), so that $T + V$, the total energy, is conserved, and we can prove this from the expression of $\boldsymbol{F}$.

In the Hamiltonian approach, we start instead with the energy, and *derive* the effect of the gravitational interaction from it, ensuring that it conserves energy: The energy defines the evolution of the system, and we no longer care about individual forces.

3 Gravitation from a Hamiltonian viewpoint

We consider a system of N bodies 1 through N, with masses m_1 through m_j. 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*[2] *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 given for each component $i \in \{1, \dots, 3N\}$, by

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

This is can beReaders 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 $\frac{\mathrm{d}}{\mathrm{d}\,t}\begin{pmatrix}\boldsymbol{q} \\ \boldsymbol{p}\end{pmatrix} = \begin{pmatrix}\boldsymbol{0} & \mathbb{1} \\ -\mathbb{1} & \boldsymbol{0}\end{pmatrix} \boldsymbol{\nabla}\mathcal{H}$. written as

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

In this way, we have *defined* the change in position and momentum as a function of time, and thus completely desccribed how the system will evolve from an initial state $(\boldsymbol{q}_0, vp_0)$.

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