Why not just integrate Newtons second law numerically? †

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†This contribution is dedicated to the memory of Prof. Dr. Roman Gaida

1. Introduction

The provocative question in the title is a natural one when encountering a book on classical mechanics. Why is there all that fuss about Lagrangian dynamics, conservation laws, Hamiltonian canonical equations of motion and so on? Why don't we stop right after presenting Newtons equations of motion (NEOM) and give the numerical results for some cases of interest?

In this report I shall present modern aspects of classical mechanics[1]. Even in recent books or courses on theoretical mechanics they are hardly mentioned. I will argue that it is more worthwhile than ever to look for general aspects and properties of the NEOM and not just integrate them on a computer (admittedly no reasonable physicist would do so).

For only a few (N) pointlike particles it is rather easy to numerically integrate **Newtons equations of motion**

$$m_i \ddot{\mathbf{r}}_i = \mathbf{F}_i \left(\{ \mathbf{r}_j \} \right) , \quad i = 1, \ldots, N , \tag{NEOM}$$

where m_i and $\mathbf{r}_i(t)$ are the masses and positions respectively of the particles (In the following we consider only **conservative systems**, i.e. $\mathbf{F}_i \left(\{ \mathbf{r}_j \} \right) = -\boldsymbol{\nabla}_i V \left(\{ \mathbf{r}_j \} \right)$, where V is the potential; also we use in the following the notation $\dot{a} = \frac{da}{dt}$, so that $m_i \ddot{\mathbf{r}}_i = m_i \frac{d^2 \mathbf{r}_i}{dt^2}$). But nobody would be content with a simple printout of the resulting sequence of coordinates:

5.197753757238388E-002	-.1036242246627808
.1033616736531258	-.1011988669633865
.1535586565732956	-9.733060747385025E-002
.2019750475883484	-9.227080643177032E-002
.2480203658342361	-8.635251969099045E-002
.2911123335361481	-7.99727737903595E-002
.3306850492954254	-7.357125729322433E-002
.3661999404430389	-6.760651618242264E-002
.397159218788147	-6.253085285425186E-002
.4231205582618713	-5.876516923308372E-002
.4437121450901031	-5.667513236403465E-002
.4586465954780579	-5.654985830187798E-002
.4677322208881378	-5.858432129025459E-002
.4708806276321411	-6.286641210317612E-002
.468109667301178	-6.936939060688019E-002
.4595413208007812	-7.795010507106781E-002
.4453944265842438	-8.835316449403763E-002
.4259730875492096	-.1002207696437836
.4016517102718353	-.1131077483296394
.372857928276062	-.1265010088682175
.3400549590587616	-.1398424804210663
.....	.....

[1]For more details and references see my book "Klassichna mechanika", Lviv national university, Lviv 1999 (in german: "Klassische Mechanik", Trauner-Verlag, Linz 1996).

At least she/he would try to plot the result. So let us plot the **orbits** of the particles $(\mathbf{r}_1(t), \mathbf{r}_2(t), \ldots)$: If one is lucky the result may look like figure 2.10. The orbit looks like a rotating ellipse, e.g. like the orbit of Mercury. The angular velocity $\dot{\phi}$ of the orbit (as seen from m_2) has always the same sign, e.g. $\dot{\phi} > 0$. But starting from different initial conditions the result may be the one shown in figure 2.12. The important point to recognize here is that $\dot{\phi}$ changes sign, i.e. $\dot{\phi} \geq 0$ as well as $\dot{\phi} \leq 0$ occurs. For several particles the probability that the orbits may intersect and intertwine increases. So it is hard to follow the particles. In conclusion: The graphical representation of the orbit(s) is also of rather limited value.

There is a possibility for a unique representation of the dynamics. Consider the 2 sets of independent **dynamical variables** $\{\mathbf{r}_i\}$ and $\{\mathbf{p}_i = m_i\dot{\mathbf{r}}_i\}$ (they are independent because the NEOM are differential equations of second order). For each particle they are coordinates in the 6-dimensional **phase space**. The NEOM in these variables are now coupled 1^{st} order differential equations

$$\begin{aligned} \mathbf{p}_i &= m_i\dot{\mathbf{r}}_i \\ \dot{\mathbf{p}}_i &= \mathbf{F}_i(\{\mathbf{r}_j\}), \quad i = 1, \ldots, N \ . \end{aligned}$$

Under rather general assumptions their solutions, the **trajectories** $(\mathbf{r}_i(t), \mathbf{p}_i(t))$, do not intersect. But now a new problem arises: How to plot a 6 dimensional space? How can one reduce the number of dimensions necessary for a graphical representation?

That is now the point where we should look for useful general properties (i.e. some that do not rely on the calculational power of a computer) of the NEOM and their solutions[2].

The dynamics of the system is represented in phase space by the trajectories of many different initial values - the **flow in phase space**. An important question is then the **stability of the system**: Do trajectories which are close to each other at some time stay close? The reason to search for an answer to that question is apparent: Then one does not need to know the initial conditions exactly to predict the future state of a system; in fact one allways knows the initially given values of the coordinates in phase space only within a certain precision.

Morover one would like to know which **part of phase space is occupied by the flow**? Does it remain in that part forever? In many cases it is possible to take advantage of general properties of the flow in phase space. An important role is played here by the socalled first integrals; these are functions of the dynamical

[2]Why are we (the physicists) looking for general features at all? Because we believe that they reflect symmetry, beauty, economy (E. Mach) of nature.

variables $\hat{I}_k\left(\{\mathbf{r}_i(t)\},\{\mathbf{p}_i(t)\},t\right)$ with

$$\frac{d}{dt}\hat{I}_k\left(\{\mathbf{r}_i(t)\},\{\mathbf{p}_i(t)\},t\right)=0.$$

If $\hat{I}_k$ is time independent, it is a called a **conserved quantity**; examples are energy or angular momentum. Such a conserved quantity law reduces the size and the "complexity" of that part in phase space that is covered by the trajectories. Under some physically not too restrictive assumptions there exist - in an abstract, mathematical sense - $3N$ first integrals from which one can obtain (by eliminating t with one of these integrals) $3N-1$ conserved quantities

$$I_k\left(\{\mathbf{r}_i(t)\},\{\mathbf{p}_i(t)\}\right) \qquad \text{with} \qquad dI_k/dt=0.$$

But it turns out that, though such quantities exist in principle, very often they cannot be given explicitly enough: such first integrals are useless or, more technically speaking, they are **not separating**. If one knows a **sufficient number of separating independent first integrals** one knows the solution of the problem: this is the socalled **integrable case**. There are very few such cases (these usually we learn about in lectures and they are given in textbooks). The overwhelming majority of problems is not integrable, and even shows **chaotic behaviour**. That means, there is an extremely sensitive dependence of the future state of such a system on only minute changes in the initial conditions.

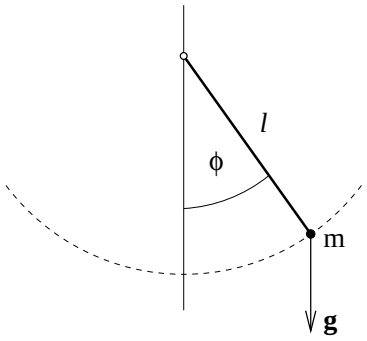
But for many of these nonintegrable systems there exists an integrable limiting case when some parameter is turned down. One may ask now: How does **integrability turn into nonintegrability**? An partial answer is given by the **KAM-theorem**. Loosely speaking it states: A small disturbance of an integrable system only destroys "weak" trajectories, the "strong" ones are kept. In this way phase space is divided into regions with some regularity and such ones, which were formerly occupied by the weak trajectories and which are now chaotic. The application of the theorem to the question of stability of the solar system yields a not too convincing result.

2. Examples

2.1 1-d systems: the pendulum

The EOM for conservative 1-d-systems is always integrable i.e reducible to an integral (see also below). In particular this is also true when the force is a nonlinear function of the (generalized) coordinate as in our example: the **mathematical pendulum,** a pointlike mass m suspended on a rigid stick of length l with no weight, whose motion is restricted to a plane. It experiences only the gravitational force, which here is considered to be constant

$$|\mathbf{F}| = mg.$$



Its Newtonian equation of motion is

$$\ddot{\phi} + \omega^2 \sin\phi = 0,$$

where

$$\omega^2 = g/l$$

By multiplying the equation with $\dot{\phi}$ one readily finds that the energy

$$E = \frac{\dot{\phi}^2}{2} - \omega^2 \cos\phi$$

is conserved

$$E = \text{ constant}$$

(from the conservation one easily gets $\dot{\phi} = f(\phi)$ and then $t = \int d\phi / f(\phi)$). Its conservation is due to the independence of the system of the choice of the starting point in time. Saying it a different way: The overall features of the pendulum are the same for alltimes (due to the time independence of m, l, and g).

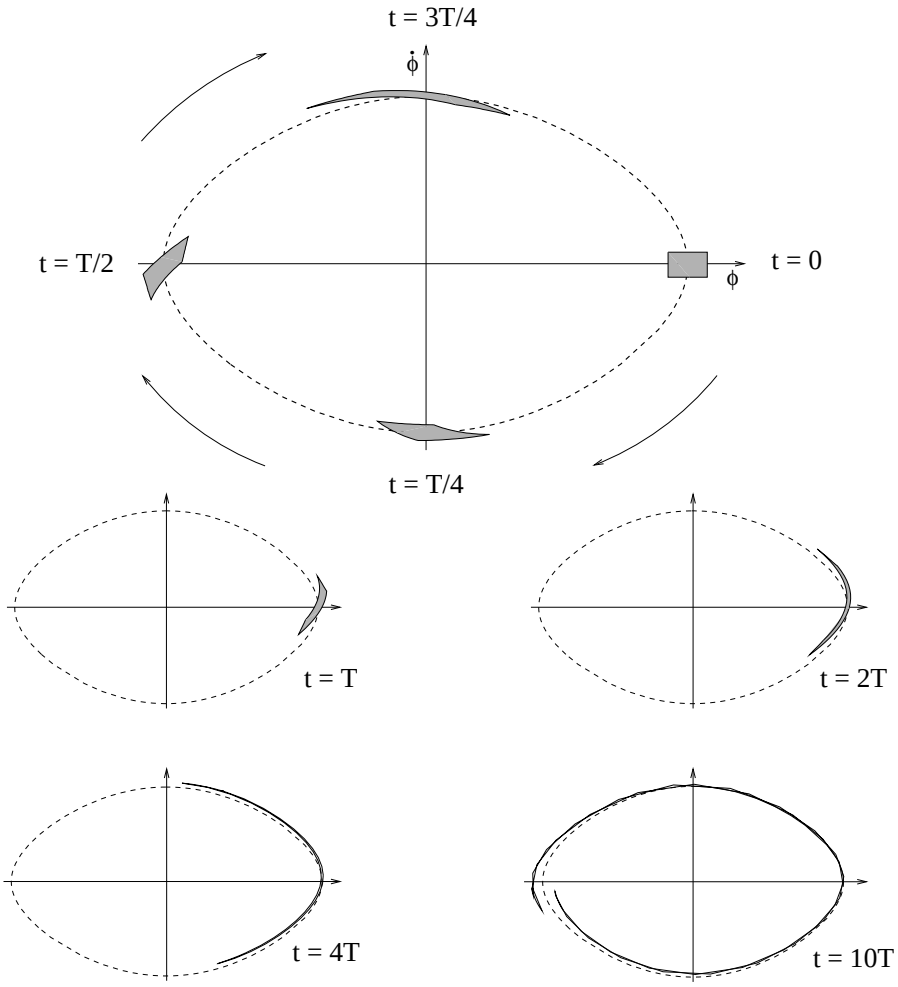


Figure 2.1: The change in shape of an initially rectangular region of starting points for different realisations of the swinging pendulum.

For not too large initial velocities $\dot{\phi}_0$ and not too large values of ϕ_0 the orbits $\phi(t)$ stay within $(-\pi, \pi)$. The corresponding trajectories $\left(\phi(t), p_\phi(t) = \dot{\phi}\right)$ are calculated from

$$\begin{aligned} p_\phi &= \dot{\phi} \\ \dot{p}_\phi &= -\omega^2 \sin\phi \end{aligned}$$

and look similar to ellipses (see dashed lines in figure 2.1).

Let us consider the swinging of the pendulum in many experiments. We arrange that the initial conditions for the positions ϕ and the velocities $\dot{\phi}$ such that they form, by choice, the rectangle shown at $t = 0$ in figure 2.1. Now we consider all the runs together in the phase space $\left(\phi, \dot{\phi}\right)$. As time goes on, there is an distortion

of the rectangle as shown in the figure. So already for $t = 10T$ the different realisations spread along the dotted trajectory, which denotes the behaviour of the center of the rectangle: Initially nearby points do not stay close. Nevertheless all points within the rectangle stay close to the dotted trajectory: Close trajectories stay close. The system is not completely stable: If there is an uncertainty about the intial values (and there always is only a limited precision in the intial values) the future position in phase space cannot be predicted with the same uncertainty. It can be only said that the trajectories will stay close.

2.2 2-d systems: linear and nonlinear oscillators

2.2.1 The harmonic oscillator

Let us now first review a linear 2-dimensional model system, the **harmonic oscillator**

$$\begin{aligned} \ddot{x} + \omega_1^2 x &= 0 \\ \ddot{y} + \omega_2^2 y &= 0. \end{aligned}$$

These equations of motion may again result from a mathematical pendulum, whose motion is now not restricted to a plane, but only small deviations from the rest position ($x = 0, y = 0$) are allowed.

For general values of the ratio $\omega := \omega_1/\omega_2$ there are 2 conserved quantities: the x-mode energy $E_x = \frac{1}{2}\left(\dot{x}^2 + \omega_1^2 x^2\right)$ and the y-mode energy $E_y = \frac{1}{2}\left(\dot{y}^2 + \omega_2^2 y^2\right)$ (it is easy to verify that their time derivatives vanish). Of course the total energy $E = E_x + E_y$ is also conserved.

Before we carry on, we consider the **isotropic case**:

$$\omega_1 = \omega_2 .$$

There are now 3 conserved quantities: the x-mode energy E_x, the y-mode energy E_y, and the angular momentum $L = x\dot{y} - y\dot{x}$. The additional conservation of L is due to the rotational symmetry of the system. The trajectories are in a 4-d phase space, which is hard to visualize. But we may use the constancy of E_x to express $\dot{x}$ as a function of x and thus reduce the number of dimensions to represent the trajectories graphically. We consider this restricted phase space $(x, y, \dot{y})$ and look for a trajectory $\left(x\left(t\right), y\left(t\right), p_y\left(t\right) = \dot{y}\right)$. It still has to fulfill the conservation laws for E_y and L. Both correspond to surfaces in the restricted phase space. This is shown in figure 2.2: The elliptic cylinder is the surface $E_y = const$ and the hyperbolic cylinder is obtained from $L = const$. Since the trajectory has to stay on both surfaces it is just the line where both surfaces intersect or touch (as in the figure) each other. It can be seen from the figure that the trajectory crosses

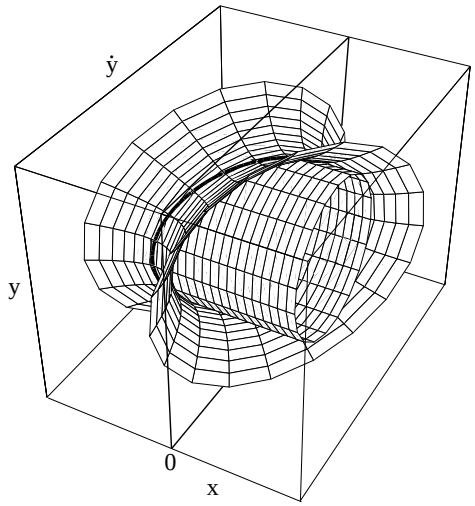


Figure 2.2: The trajectory in restricted phase space $(x, y, \dot{y})$ for an isotropic oscillator is the line where the two surfaces touch. The surfaces represent 2 conserved quantities: the energy E_y and the angular momentum L (compare text).

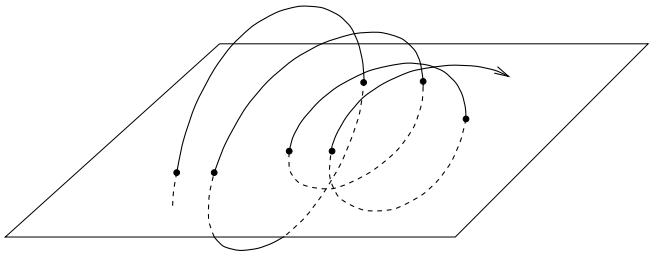


Figure 2.3: A trajectory and the Poincaré surface of section

the $(x = 0)$-plane in two points only. The orbit, an ellipse, is just the projection of the trajectory onto the (x, y)-plane.

Now we return to the **anisotropic case:** ω_1/ω_2 arbitrary but $\neq 1$. The complexity of the orbits $(x(t), y(t))$ depends on the ratio ω_1/ω_2. They form the well knom **Lissajous figures**. Some examples are the left hand parts of figs. 2.4 and 2.5.

The trajectories $(x(t), y(t), p_x(t) = \dot{x}, p_y(t) = \dot{y})$ are curves in a 4-dimensional space. With the help of the conservation of the total energy we can again reduce the number of coordinates in phase space necessary for a graphical representation. Now we shall introduce a method due to Poincaré to represent the dynamics of such a system in two dimensions.

If a surface in this 3d space is coveniently chosen such that the sequence of points of intersection (crossings) of the trajectories is a complete representation of the

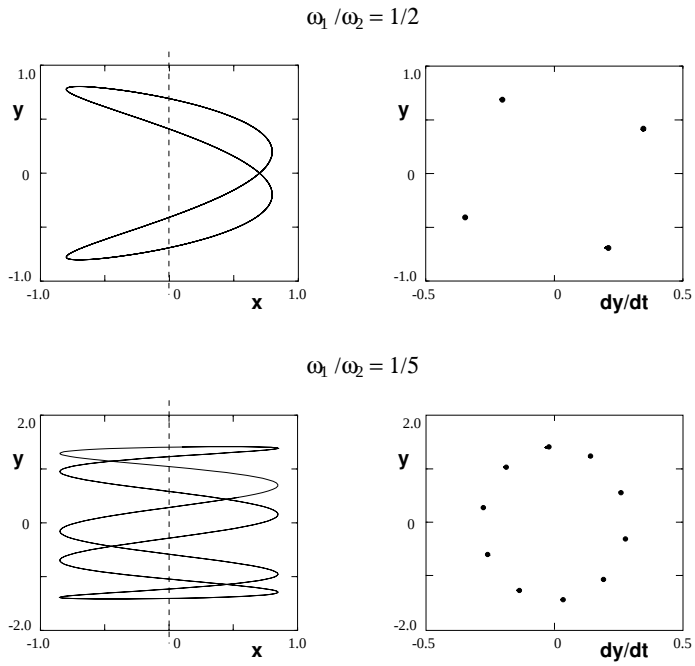


Figure 2.4: Orbits and PSS points of an 2-dimensional harmonic oscillator for rational frequency ratio

dynamics (cf. the sketch of figure 2.3; see the examples below) such a surface is called a **Poincaré surface of section** (PSS) (Usually one adds the condition that only the intersections of trajectories coming from a chosen side of the plane are recorded; so in fig. 2.3 one would omit e.g. the points where the trajectory comes from below the surface).

We now apply this concept to the harmonic oscillator. We reduce the dimensionality of phase space with the help of energy conservation $E = E_x + E_y = const$

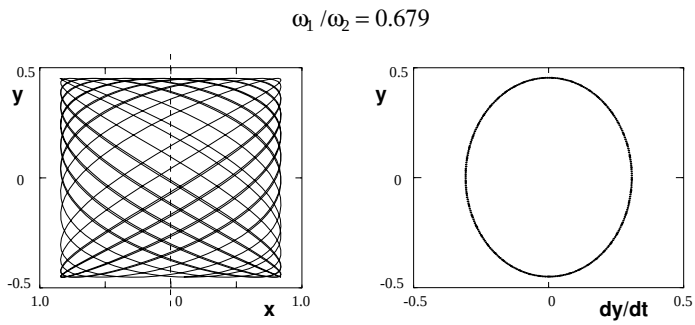


Figure 2.5: Orbits and PSS points of an 2-dimensional harmonic oscillator for irrational frequency ratio

giving $\dot{x}$ as a function of the remaining variables: $\dot{x} = f(x, y, \dot{y})$. Then we introduce the plane $x = 0$ as PSS (and possibly accept only points with e.g. $\dot{y} > 0$).

Consider first two examples for rational frequency ratio $\omega = \omega_1/\omega_2$ (figure 2.4). As can be seen on the left hand side the orbits are closed. They form the well known Lissajous figures, whose appearance depends on the ratio ω. On the right hand side the corresponding points in the PSS are shown: there is only a finite number of them depending also on ω (in the figures all penetration points are shown).

Now we turn to an irrational value of ω. The orbits are not closed anymore (see figure 2.5); with time an orbit would cover all the area allowed by energy conservation. Such orbits are called **almost periodic**. Further there now is an infinite number of PSS points lying on a curve, which is just the cutting line of the surface $E_y = const$ with the PSS. So the reason for the PSS points to lie on a curve is the existence of a conserved quantitiy, which here is a simple function of the coordinates y and dy/dt. Such an integral is called separating.

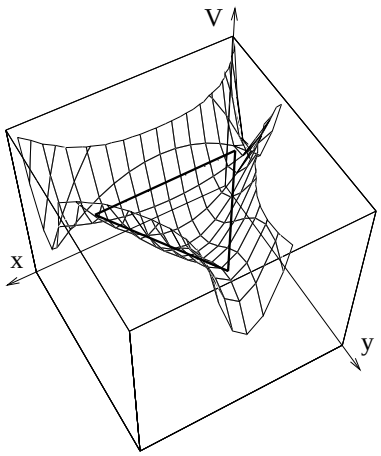


Figure 2.6: The potential of the Hénon-Heiles system

2.2.2 The Hénon-Heiles system

The equations of motion

$$\begin{aligned} \ddot{x} &= -x - 2xy \\ \ddot{y} &= -y + y^2 - x^2 \end{aligned}$$

have their origin in modelling a galactic system. They are due to M. Hénon and C. Heiles (Astron. J. **69**,73(1964)). They can also be considered as the equations of motion for an anharmonic oscillator. The only known explicit first integral is

the energy

$$E = \frac{1}{2}\left(\dot{x}^2 + \dot{y}^2\right) + V\left(x, y\right)$$

where the potential

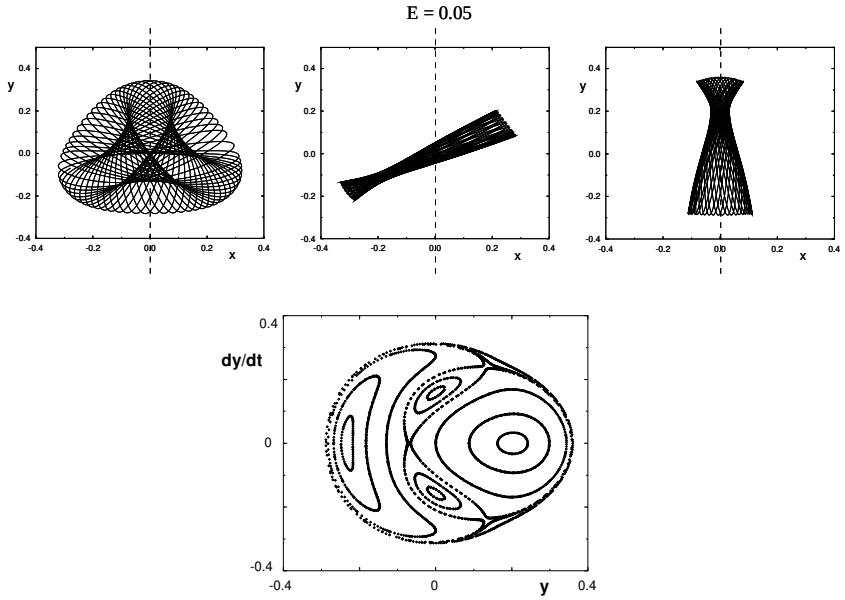
$$V\left(x, y\right) = \frac{1}{2}\left(x^2 + y^2\right) + x^2 y - \frac{1}{3}y^3$$

is shown in figure 2.6. Bounded motion can occur only for energies in the range

$$0 \leq E \leq 1/6 = 0.1666;$$

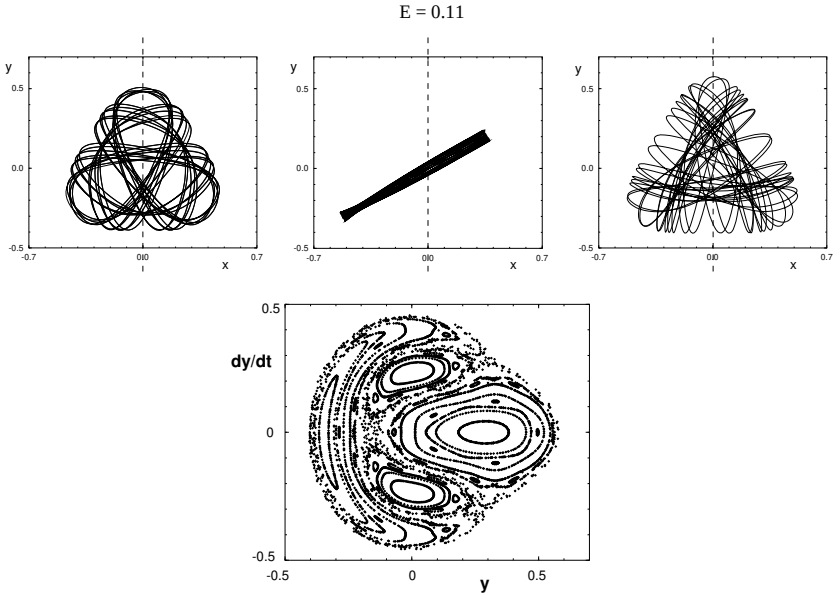
the motion then stays within the triangular region.

In the following figures, orbits (top row) and PSSs (bottom) for increasing energy $E = 0.05,\ 0.11,\ 0.13,\ 0.1666$ are presented. For a small energy, $E = 0.05$, the orbits look like more complicated Lissajous figures. The PSS points all lie on appearently smooth curves. Each curve results from a trajectory starting from a particular set of initial values.

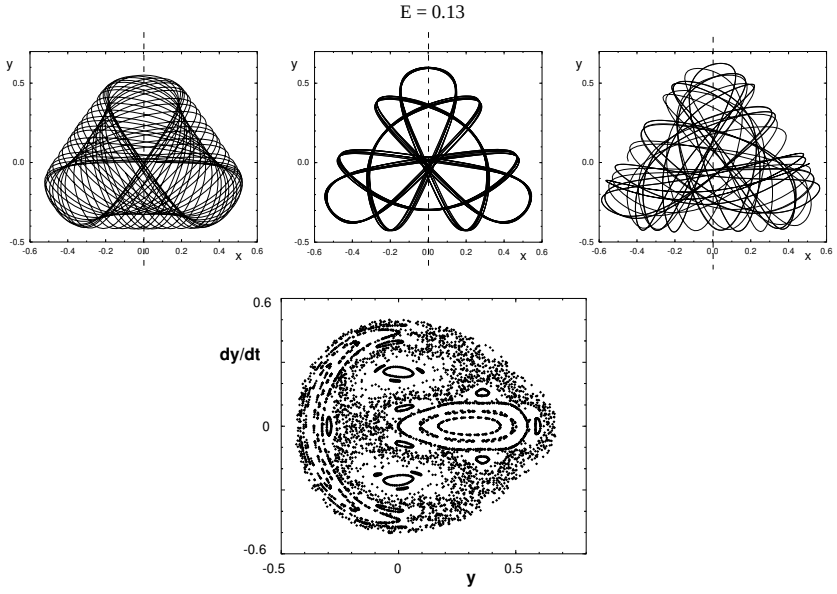


This seems to indicate the existence of a further conserved quantity I_2 (as is the case for the harmonic oscillator discussed above): The different curves in the PSS would then correspond to different values of I_2 $(= const)$.

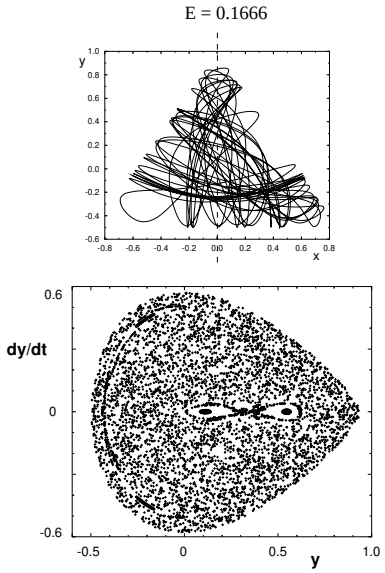
Allready for $E = 0.11$ some orbits become irregular. For some initial values the PSS points do definitely not lie on smooth curves; they are scattered in some small areas.



Increasing the energy further to $E = 0.13$ the number of irregular orbits also increases. But more interesting is the increase of the area in the PSS covered by scattered points. All those points belong to only 2 different trajectories.



Coming finally to the maximum energy for bounded motion ($E = 0.1666$), the orbits are completely irregular (We have shown only one typical example) and would fill after sufficiently long time ($t \to \infty$) all the triangular area also shown in figure 2.6. In the PSS <u>all</u> the scattered points belong to just <u>one</u> trajectory.



It has been attempted by Gustavson to calculate a further first integral for the Hénon-Heiles system by perturbation theory. The result (figure 2.7) up to $E = 1/12$ shows a very good agreement with the numerical calculations. But then there is a clear discrepancy. Gustavsons result can not show chaotic behaviour, due to the basic assumption of any perturbation theory: smooth dependence of the results on the perturbation parameter. So it is important not to start directly integrating the equations of motion, but it is equally important to check the solutions numerically.

2.3 Chaotic behaviour

When is the behaviour of a system called chaotic?

A qualitative answer to this question is: When there is an **extremely sensitive dependence** of the future state **on the initial values**. Allready a minute difference in the initial state leads to completely different values in the future.

The important resulting feature of a chaotic system is the **unpredictability** of the future state, since allways initial (starting) values are known only up to some precision.

A more mathematical formulation: Chaotic behaviour can occur in a system of more than two autonomous, nonlinear differential equations

$$\dot{x}_i = g_i\left(x_1, \ldots, x_f\right), \quad i = 1, \ldots, f, \quad f \geq 3,$$

where g is a nonlinear function of $\{x_i\}$. Let us consider the formal solution

$$x_i = x_i\left(\left\{x_j^0\right\}, t\right) \quad \text{where} \quad x_j^0 = x_j\left(\left\{x_k^0\right\}, t = 0\right),$$

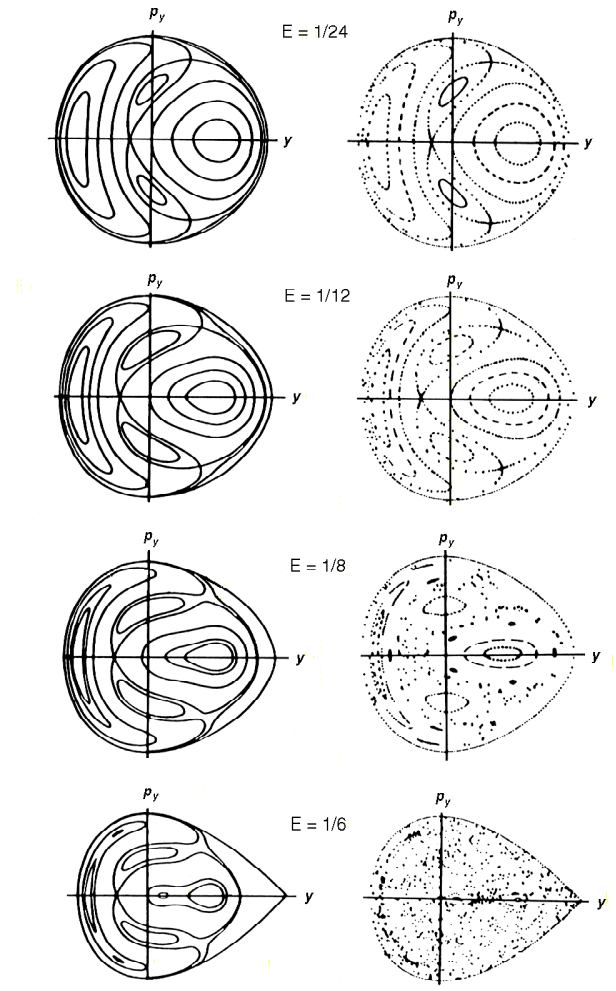


Figure 2.7: The result of Gustavson obtained in perturbation theory compared to the numerical calculation.

for two adjacent initial values $\left\{x_j^0\right\}$ and $\left\{x_j^0 + \delta x_j^0\right\}$. In the chaotic case the values of $x_i = x_i\left(\left\{x_j^0\right\}, t\right)$ and $\bar{x}_i = x_i\left(\left\{x_j^0 + \delta x_j^0\right\}, t\right)$ can become arbitrarily distant (in some measure) with time t. The distance $\|\bar{x}_i - x_i\|$ has to depend on time exponentially:

$$\lim_{t\to\infty} \|\bar{x}_i - x_i\| = const \times e^{\lambda t},$$

where the **Ljapunov exponent** λ has to be positive.

The EOMs in phase space for a conservative system with time independent potential are in general an autonomous, nonlinear system of differential equations of first order. Therefore allready for one particle in 2 dimensions ($N = 1$ and $d = 2$) chaotic behaviour can occur as in the Hénon-Heiles system discussed above. In chaotic mechanical systems, too many of the first integrals - which in principle

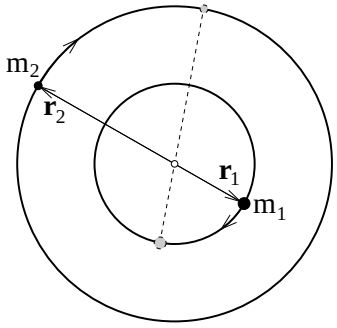
exist! - are useless, nonseparating ones. To get an idea of such an integral imagine a curve in phase space, which looks like a Lissajous figure for a frequency ratio close to an irrational value: the curve consists of very many, very short pieces (branches), where it is unique (and therfore useful).

2.4 3 body systems

We consider 3 particles which interact only pairwise via gravitational forces

$$\mathbf{F}_{ij}\left(\mathbf{r}_i, \mathbf{r}_j\right) = -\frac{G m_i m_j}{\left|\mathbf{r}_i - \mathbf{r}_j\right|^3}\left(\mathbf{r}_i - \mathbf{r}_j\right), \qquad i, j = 1, 2, 3,\ i \neq j.$$

In general the motion of 3 masses is already very complicated, but there exists a special situation which can be treated more easily: the socalled **restricted 3-bodies problem.**



2 heavy bodies m_1, m_2 move under their mutual gravitational forces on circular Kepler orbits with constant circular velocity ω in a plane. Further there is a light mass m ($\ll m_1, m_2$, i.e. m does not influence the motion of m_1 and m_2) moving only in that given plane.

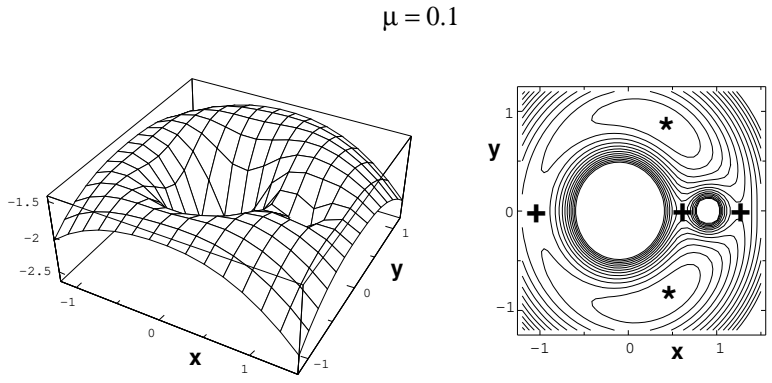


Figure 2.8: The potential of the restricted 3-body system as seen in the corotating frame

It is convenient to consider the motion of m in the rotating frame of reference, where m_1 and m_2 at rest. The only known first integral of the resulting equations of motion is the energy E, which in scaled and reduced units ($m = \omega = 1$) and $\mu = m_1/(m_1 + m_2)$ is

$$E = \frac{1}{2}\left(\dot{x}^2 + \dot{y}^2\right) + V(x, y).$$

The potential

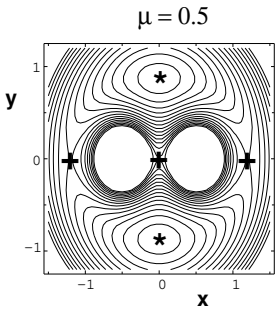


Figure 2.9: The potential in the rotating system for $\mu = 0.5$

$$V = -\frac{1}{2}\left(x^2 + y^2\right) - \frac{\mu}{r_1} - \frac{1-\mu}{r_2},$$

(r_1 and r_2 being the respective scaled distances to the masses m_1 and m_2) acting on m in the rotating system is shown in figure 2.8 for $\mu = 0.1$. There are socalled 5 Lagrangean points: 2 maxima of V (indicated by ★ in the figure) and 3 saddle points of V (indicated by $+$).

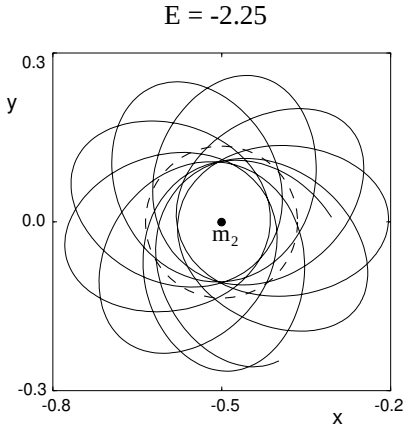


Figure 2.10: Seemingly regular orbit around one of the heavy masses

In the following we show the orbits for $\mu = 0.5$ (i.e. $m_1 = m_2$). If

$$E \leq -2$$

then the energy is smaller than the value of the potential V at the saddle point between the two masses, $V(0,0) = -2$, and the orbits stay in the vicinity of one of the masses. Figure 2.10 shows a seemingly regular orbit for $E = -2.25$ but coming closer to $E = -2$, figure 2.11 shows an indication of something going on for the light particle at energies $E \lesssim -2$.

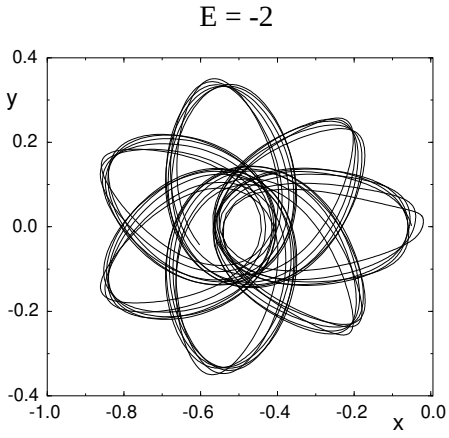


Figure 2.11: A not so regular orbit around on of the heavy masses

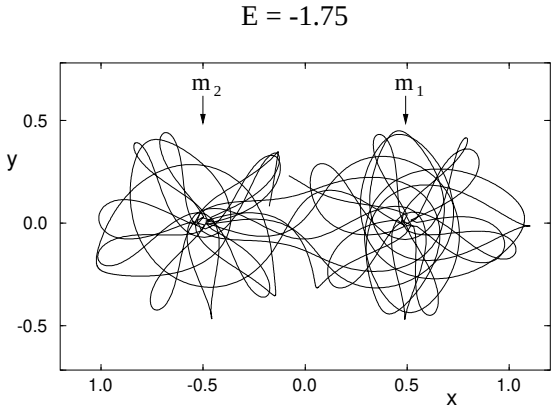


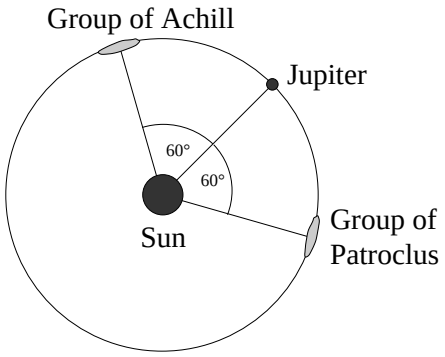
Figure 2.12: An apparently chaotic orbit around both masses

If

$$-2 \leq E \leq 1.743,$$

where 1.743 is the value of the potential V at the two other saddle points at $\left(\pm\sqrt{5}/2, 0\right)$, the orbits are still bounded and around both masses (see figure 2.12). The orbit shown is clearly irregular and even chaotic. This can be inferred from the PSS (not given here, they can be found in the original papers).

Linear stability analysis shows that for values $\mu < 0.038$ also the two Lagrangian points ★ are stable, stationary solutions of the equations of motion: There is a small region of stable, bounded motion close to these maxima of V. The motion is stabilized by the Coriolis force. A system to which this considerations are applicable are the **Trojans**, 2 groups of asteroids in a configuration shown below; the heavy masses are Sun and Jupiter.



2.5 Is the solar system stable?

Consider only Sun, Jupiter and Earth. The ratio of their masses is

$$m_S : m_J : m_E = 330000 : 318 : 1.$$

Is this system stable? To get an answer using analytic methods one would start from an "unperturbed system", which consists of the Sun and Jupiter only. Neglecting the orbit of the Sun around the common center of mass, Jupiter performs an Kepler-ellipse around the Sun, with period T_J of approximately 12 years: $T_J \simeq 12$yrs; the corresponding frequency is $\omega = 1/T_J$. To calculate the orbit of the Earth analytically one would use canonical perturbation theory with an expansion parameter $\varepsilon \sim m_E/(m_S + m_J)$. This is now the point where Hamilton-Jacobi theory enters, which in turn is based on the analytical mechanics of Lagrange and Hamiltons principle. For a systematic perturbation theory Hamilton-Jacobi theory is indispensible, but this is not our topic now. We only mention that the result of the perturbative calculation will be non chaotic due to the method (like Gustavsons result shown in fig. 2.7 for the Hénon-Heiles system). But we know from the preceeding discussion that there are chaotic solutions. These we can find only numerically. Whether a solution will be chaotic or regular cannot be said without an analytic and numerical investigation. Concerning the analytic approach there is the

K(olmogorov)**A**(rnol'd)**M**(oser)**-Theorem**:

> For certain frequencies ω of the unperturbed trajectories a small perturbation of strength ε will only change the trajectory a little (and not destroy it).

A more pictorial consequence of the KAM - Theorem is the mass distribution in the rings of Saturn (see picture 2.13). Here the rings are due to small masses attracted by Saturn. One of the inner moons (Mimas) serves as the perturbation. The orbits occupied correspond to stable trajectories of the unperturbed system Saturn - dust surviving the influence of Mimas.

Returning to the system Sun-Jupiter-Earth: From the astronomical evidence we may deduce that $\omega = 1/T_J$ is one of these "stable" frequencies (or at least it is very close). Proceeding to the solar system by adding further planets one must mention that with increasing number of particles the chaotic region inreases tremendously so that eventually the system is totally chaotic. The conclusion one may draw about the solar system:

It is not impossible that the solar system is stable

but very unlikely; only the very long (as compared to the lifetime of the Sun) characteristic times for chaotic behaviour may save us from chaos.

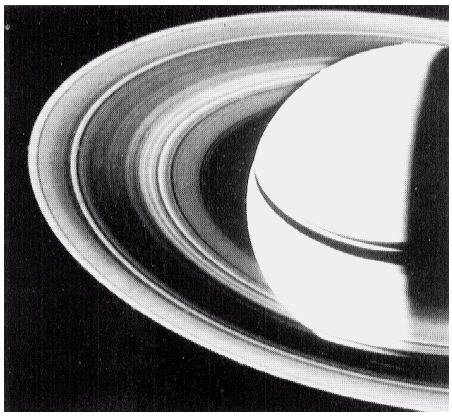


Figure 2.13: The rings of Saturn

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