Physics 115/242

Comparison of methods for integrating the simple harmonic oscillator.

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I. THE SIMPLE HARMONIC OSCILLATOR

The energy (sometimes called the "Hamiltonian") of the simple harmonic oscillator is

$$E = \frac{p^2}{2m} + \frac{1}{2}kx^2 \tag{1}$$

where m is the mass, k is the spring constant, and $p = m\dot{x}$ is the momentum. In the numerical examples we will set $m = k = 1$ so the angular frequency, ω and period, T, are given by

$$\omega = \sqrt{\frac{k}{m}} = 1, \qquad T = \frac{2\pi}{\omega} = 2\pi. \tag{2}$$

We also have

$$2E = p^2 + x^2 \qquad \text{(a const.)} \tag{3}$$

Hence a "phase space" plot, i.e. the trajectory in the x-p plane, should be a circle of radius $\sqrt{2E}$.

Following standard practice when solving ODE's numerically, Newton's equation of motion,

$$\ddot{x} = -x\,, \tag{4}$$

will be written as two first order differential equations

$$\dot{x} = p, \tag{5}$$

$$\dot{p} = -x. \tag{6}$$

We will numerically integrate these equations for three methods that have been described in class:

- Euler method,
- second order Runge Kutta (RK2),
- fourth order Runge Kutta (RK4),

with initial conditions, $x = 1, p = 0$. Hence $2E = 1$ and the radius of the circle in the phase space plots is unity. We will use a time step $h = 0.02T$ so it takes 50 time steps to go perform one cycle of the oscillator.

The formulae for stepping forward in time the differential equations (5) and (6) are:

- Euler method

$$x_{n+1} = x_n + hp_n, \qquad p_{n+1} = p_n - hx_n. \tag{7}$$

- second order Runge Kutta (RK2)

$$k_1^x = p_n, \qquad k_1^p = -x_n, \tag{8a}$$

$$k_2^x = p_n + hk_1^p, \qquad k_2^p = -(x_n + hk_1^x), \tag{8b}$$

$$x_{n+1} = x_n + \frac{h}{2}(k_1^x + k_2^x), \qquad p_{n+1} = p_n + \frac{h}{2}(k_1^p + k_2^p). \tag{8c}$$

- fourth order Runge Kutta (RK4)

$$k_1^x = p_n, \qquad k_1^p = -x_n, \tag{9a}$$

$$k_2^x = p_n + \frac{h}{2}k_1^p, \qquad k_2^p = -(x_n + \frac{h}{2}k_1^x), \tag{9b}$$

$$k_3^x = p_n + \frac{h}{2}k_2^p, \qquad k_3^p = -(x_n + \frac{h}{2}k_2^x), \tag{9c}$$

$$k_4^x = p_n + hk_3^p, \qquad k_4^p = -(x_n + hk_3^x), \tag{9d}$$

$$x_{n+1} = x_n + \frac{h}{6}(k_1^x + 2k_2^x + 2k_3^x + k_4^x), \qquad p_{n+1} = p_n + \frac{h}{6}(k_1^p + 2k_2^p + 2k_3^p + k_4^p). \tag{9e}$$

Below we give numerical results obtained by iterating these equations. However, the solutions can also be obtained analytically as shown in Appendix A.

II. EULER METHOD

Figure 1 show that the energy very quickly deviates from its correct value and grows without bound. The phase space plot is badly in error even after one cycle. This illustrates that the Euler method is terrible and so **I don't recommend its use.**

III. SECOND ORDER RUNGE-KUTTA (RK2)

The first figure in Fig. 2 shows that the energy deviates from its exact value much more slowly than with the Euler method and the phase space plot shows that one cycle is tracked pretty

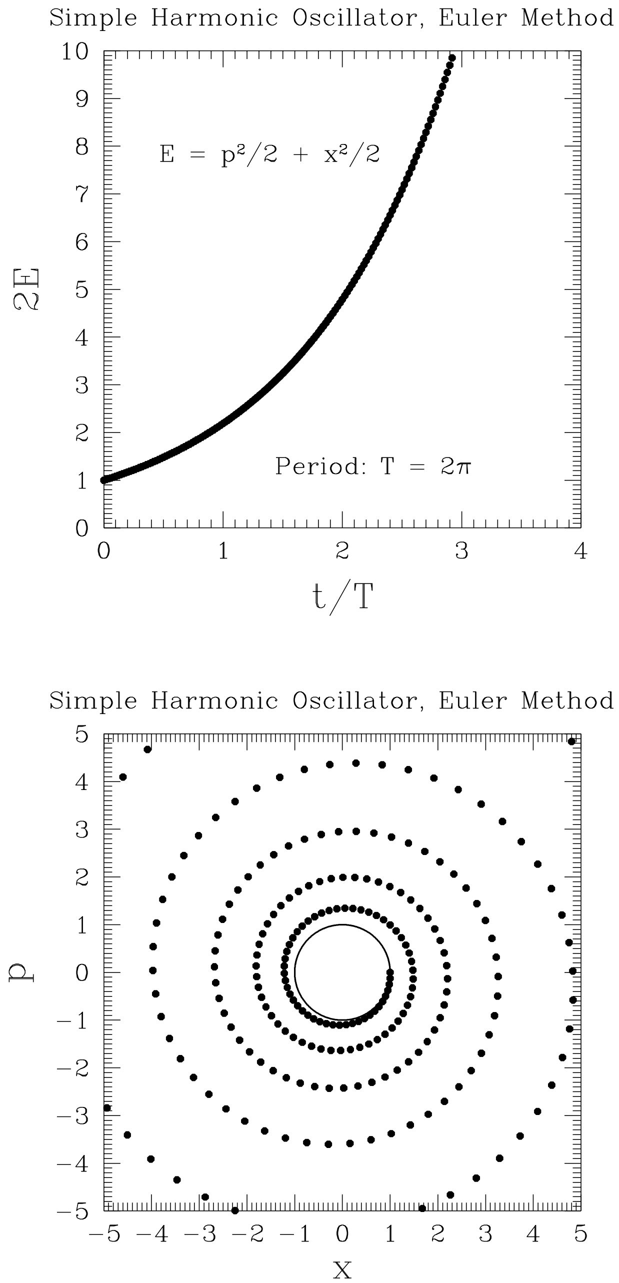
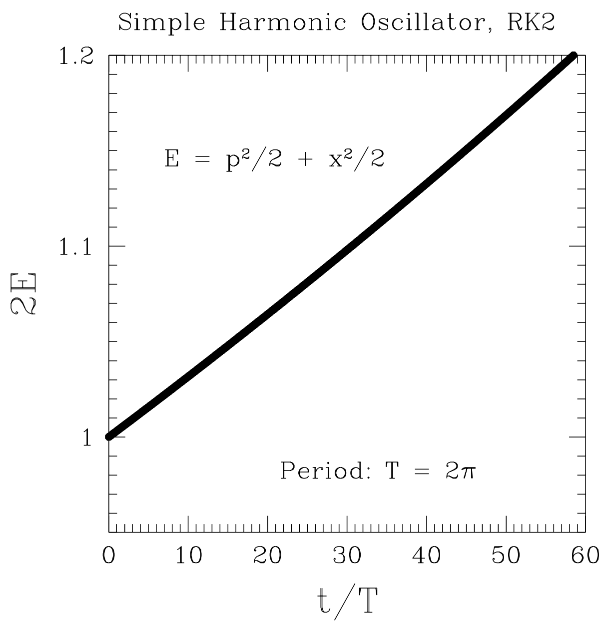


FIG. 1: Numerical results for the Euler method

accurately, within the thickness of the lines. (Remember the exact phase space plot is a circle of radius unity.) Hence, if you want a simple scheme, **use RK2 but not Euler**.



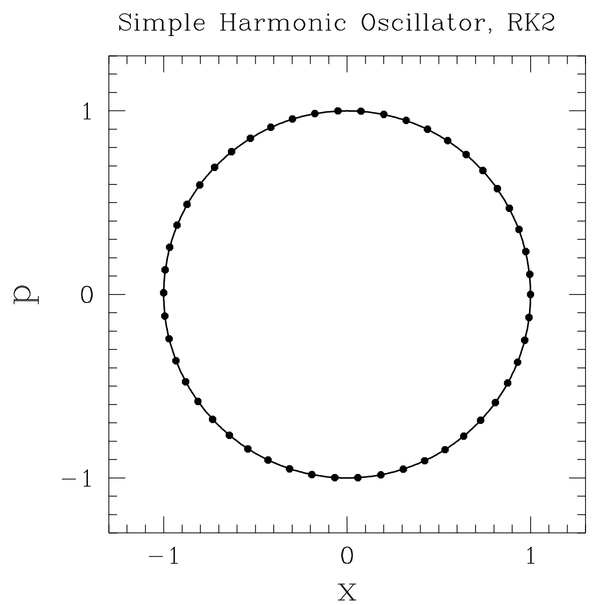


FIG. 2: Numerical results for second order Runge-Kutta.

IV. FOURTH ORDER RUNGE-KUTTA (RK4)

Figure 3, which has a highly blown up scale on the vertical axis, shows that RK4 keeps the energy constant to very high precision. All in all, **RK4 is very accurate** but quite simple and so is the method of choice for many people. Combined with "adaptive stepsize control" (not necessary

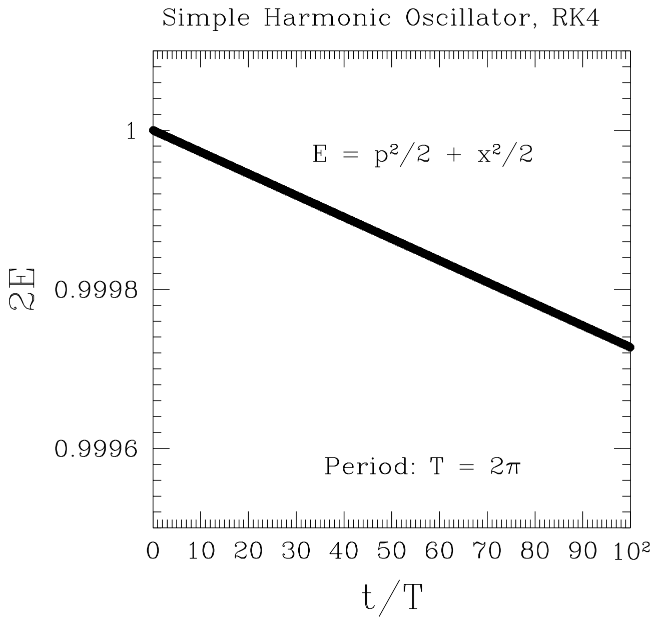


FIG. 3: Numerical results for fourth order Runge-Kutta.

for the simple harmonic oscillator, and not covered in this course) it is very powerful. A phase space plot (not shown) looks essentially perfect.

V. ANHARMONIC OSCILLATOR

We conclude by showing in Fig. 4 some results for an anharmonic oscillator using the RK2 method. We take the potential energy to be

$$V(x) = \frac{x^6}{6}\,, \tag{10}$$

which is close to zero for $|x| < 1$ and then has very steep (almost vertical) walls at $x = \pm 1$. Hence the particle will travel with almost constant velocity for $|x| < 1$, and will rebound suddenly when it gets to $x = \pm 1$. The figures below show that this expected behavior is well reproduced by RK2.

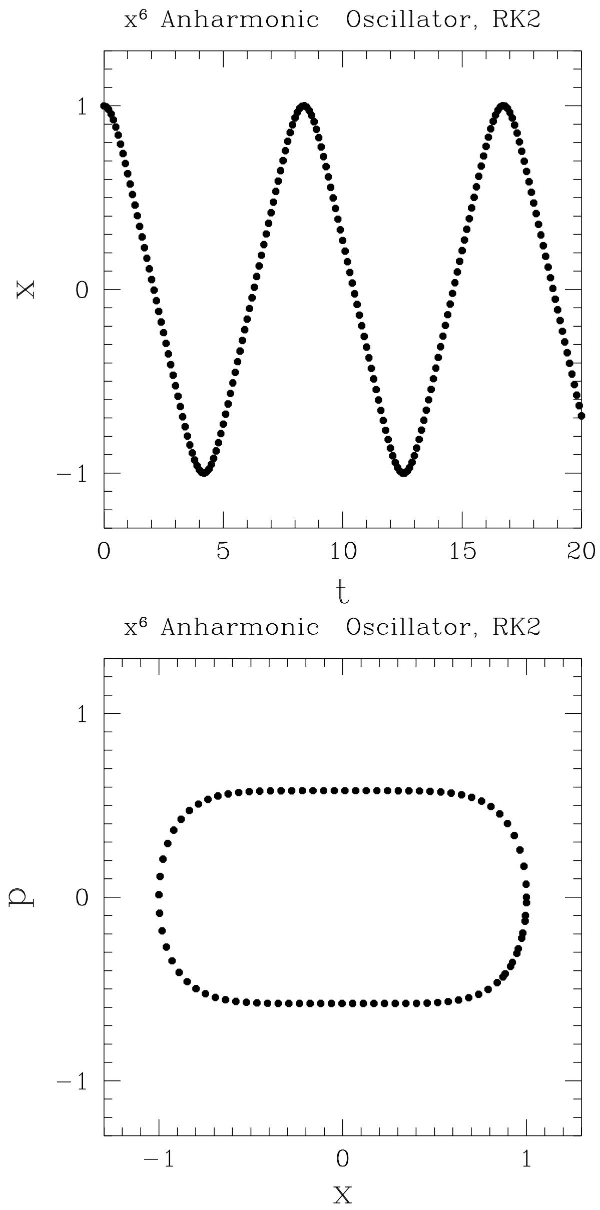


FIG. 4: Numerical results for the anharmonic ($x^6/6$) potential using RK2.

Appendix A: Analytical results for the simple harmonic oscillator

The results for the simple harmonic oscillator found above numerically can also be obtained analytically, as we show in this appendix.

One can write the formulae used in the this handout to step forward by one time step in matrix notation as

$$\begin{pmatrix} x_{n+1} \\ p_{n+1} \end{pmatrix} = A \begin{pmatrix} x_n \\ p_n \end{pmatrix} , \tag{A1}$$

where A is a 2×2 matrix. For the simple harmonic oscillator the matrix A is constant, i.e. independent of x and p, and, for the numerical methods described here, has the form

$$A = \begin{pmatrix} c & d \\ -d & c \end{pmatrix} , \tag{A2}$$

where c are d are constants which are different for the different numerical schemes. For $h \to 0$ we will see below that that $c \to 1$ and $d \to h$. The eigenvalues of A are $\lambda_{\frac{1}{2}} = c \pm id$, which can be written in polar form as

$$\lambda_{\frac{1}{2}} = re^{\pm i\theta} , \tag{A3}$$

where

$$r = \sqrt{c^2 + d^2}, \qquad \theta = \tan^{-1}(d/c) , \tag{A4}$$

so, for $h \to 0, r \to 1$ and $\theta \to h$. The eigenvectors actually don't depend on c and d are are given by

$$\vec{e}_{(1)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} , \qquad \vec{e}_{(2)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} . \tag{A5}$$

Although A is not Hermitian, so its eigenvalues are complex, it is "normal" which means that it commutes with its Hermitian conjugate (as is easily checked)[1]. This means that it can be diagonalized by a unitary transformation, and so the eigenvectors are orthogonal, as can easily be verified in Eq. (A5).

Because the elements of A are constants, we can step forward n time steps just by taking the n-th power of A, i.e.

$$\begin{pmatrix} x_n \\ p_n \end{pmatrix} = A^n \begin{pmatrix} x_0 \\ p_0 \end{pmatrix} , \tag{A6}$$

The n-th power of a matrix is conveniently found by diagonalizing A. We have

$$U^\dagger A U = D , \tag{A7}$$

where

$$D = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \tag{A8}$$

is a diagonal matrix with the eigenvalues λ_1 and λ_2 on the diagonal, and U is the (unitary) matrix

$$U = \left(\vec{e}_{(1)},\ \vec{e}_{(2)}\right) = \begin{pmatrix} e^x_{(1)} & e^x_{(2)} \\ e^p_{(1)} & e^p_{(2)} \end{pmatrix} \tag{A9}$$

formed by stacking the normalized (column) eigenvectors $\vec{e}_{(1)}$ and $\vec{e}_{(2)}$ side by side. Hence

$$A = U\,D\,U^\dagger, \tag{A10}$$

and so

$$A^n = U \begin{pmatrix} \lambda_1^n & 0 \\ 0 & \lambda_2^n \end{pmatrix} U^\dagger, \tag{A11}$$

where we used that $U^\dagger U = I$, the identity matrix. Substituting Eq. (A11) into Eq. (A6), and using the initial condition that $x_0 = 1, p_0 = 0$, we have

$$\begin{aligned}
\begin{pmatrix} x_n \\ p_n \end{pmatrix} &= U \begin{pmatrix} \lambda_1^n & 0 \\ 0 & \lambda_2^n \end{pmatrix} U^\dagger \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\
&= \begin{pmatrix} e^x_{(1)} & e^x_{(2)} \\ e^p_{(1)} & e^p_{(2)} \end{pmatrix} \begin{pmatrix} \lambda_1^n & 0 \\ 0 & \lambda_2^n \end{pmatrix} \begin{pmatrix} e^{x*}_{(1)} \\ e^{x*}_{(2)} \end{pmatrix} \\
&= \begin{pmatrix} e^x_{(1)} & e^x_{(2)} \\ e^p_{(1)} & e^p_{(2)} \end{pmatrix} \begin{pmatrix} \lambda_1^n\, e^{x*}_{(1)} \\ \lambda_2^n\, e^{x*}_{(2)} \end{pmatrix} \\
&= \begin{pmatrix} \displaystyle\sum_{\alpha=1,2} \lambda_\alpha^n \left| e^x_{(\alpha)} \right|^2 \\ \displaystyle\sum_{\alpha=1,2} \lambda_\alpha^n\, e^p_{(\alpha)}\, e^{x*}_{(\alpha)} \end{pmatrix}.
\end{aligned} \tag{A12}$$

Time is given by $t = nh$. Hence, using Eqs. (A3), (A5) and (A12), the numerical solution is given by

$$\boxed{\begin{pmatrix} x(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} e^{(\ln(r)/h)\,t}\ \cos\left[(\theta/h)\,t\right] \\ -e^{(\ln(r)/h)\,t}\ \sin\left[(\theta/h)\,t\right] \end{pmatrix},} \tag{A13}$$

and

$$\boxed{2E = r^{2n} = e^{(2\ln(r)/h)\,t},} \tag{A14}$$

where r and θ are given by Eq. (A4). For $h \to 0$ these results go over to the exact solution, $x(t) = \cos t$, $p(t) = -\sin t$, $2E = 1$, since $\theta \to h$ and, as we shall see, in this limit, $r \to 1 + O(h^k)$ where $k > 1$.

We now give results for the different numerical schemes used in this handout. Some of the detailed calculations are done in a Mathematica notebook, which is also on the class web site (in a pdf version) at http://young.physics.ucsc.edu/115/ode_solve.nb.pdf.

1. Euler

From the formulae for the Euler method in Eq. (7) we find

$$A = \begin{pmatrix} 1 & h \\ -h & 1 \end{pmatrix} , \tag{A15}$$

so $\lambda_{\frac{1}{2}} = 1 \pm ih$ and hence, from Eq. (A3), we have

$$r = \sqrt{1 + h^2} = 1 + \frac{h^2}{2} + \cdots , \qquad \theta = \tan^{-1}(h) = h - \frac{h^3}{3} + \cdots . \tag{A16}$$

If follows from Eq. (A14) that

$$2E = \exp\left[\frac{\ln(1 + h^2)}{h}\, t\right]] \simeq \boxed{\exp\left[h\, t\right] ,} \tag{A17}$$

which agrees precisely with the data for $2E$ in Fig. 1.

2. RK2

From the formulae for RK2 in Eq. (8) I find

$$A = \begin{pmatrix} 1 - \frac{h^2}{2} & h \\ -h & 1 - \frac{h^2}{2} \end{pmatrix} , \tag{A18}$$

so $\lambda_{\frac{1}{2}} = 1 - h^2/2 \pm ih$ and hence, from Eq. (A3), we have

$$r = \sqrt{1 + h^4/4} = 1 + \frac{h^4}{8} + \cdots , \qquad \theta = \tan^{-1}(h/(1 - h^2/2)) = h + \frac{h^3}{6} + \cdots . \tag{A19}$$

If follows from Eq. (A14) that

$$2E = \exp\left[\frac{\ln(1 + h^4/4)}{h}\, t\right] \simeq \boxed{\exp\left[\frac{h^3}{4}\, t\right] .} \tag{A20}$$

which agrees precisely with the data for $2E$ in Fig. 2.

3. RK4

With some help from Mathematica I find that the formulae for RK4 in Eq. (9) give

$$A = \begin{pmatrix} 1 - \frac{h^2}{2} + h^4/24 & h - h^3/6 \\ -h + h^3/6 & 1 - \frac{h^2}{2} + h^4/24 \end{pmatrix}, \tag{A21}$$

so $\lambda_{\frac{1}{2}} = 1 - h^2/2 + h^4/24 \pm i(h - h^3/6)$ and hence, from Eq. (A3), we have

$$r = \sqrt{1 - h^6/72 + h^8/576} = 1 - \frac{h^6}{144} + \cdots, \tag{A22}$$

$$\theta = \tan^{-1}((h - h^3/6)/(1 - h^2/2 + h^4/24)) = h - \frac{h^5}{120} + \cdots. \tag{A23}$$

If follows from Eq. (A14) that

$$2E = \exp\left[\frac{\ln(1 - h^6/72 + h^8/576)}{h}\, t\right] \simeq \boxed{\exp\left[-\frac{h^5}{72}\, t\right]}, \tag{A24}$$

which agrees precisely with the data for $2E$ in Fig. 3.

4. Comments

Note that the correction to the energy for the Euler method, given in Eq. (A17) is of order h, as expected since this is a first order method.

However, for RK2 and RK4, the correction to the energy given in Eqs. (A20) and (A24) respectively is one higher order than expected, $O(h^3)$ for RK2 whereas $O(h^2)$ is expected since RK2 is a second order method, and $O(h^5)$ for RK4 whereas $O(h^4)$ is expected since RK4 is a fourth order method. This leads to better than expected long time stability for these methods. Is this is special feature of the simple harmonic oscillator or true more generally? I don't have a definitive answer but I have experimented numerically with RK2 and RK4 for an *anharmonic* oscillator and found that the energy change, at fixed time, varies with h in the same way as for the simple harmonic oscillator, namely $O(h^3)$ for RK2 and $O(h^5)$ for RK4. Enhanced long-term stability for Runge-Kutta methods for oscillator problems therefore seems to be an unexpected, and as far as I can see an unpublicized, bonus of these methods. Note, however, that the error in $x(t)$ and $p(t)$ *is* that expected for RK2 and RK4, since θ/h, which is unity in the exact solution according to Eq. (A13), is $1 + O(h^2)$ for RK2 from Eq. (A19), and $1 + O(h^4)$ for RK4 from Eq. (A23). Thus the error in the *phase* of the oscillation is of the order expected for RK2 and RK4, but the error in the *amplitude* is of one higher order. Curious.

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[1] The matrix A is only normal because its off-diagonal elements are equal in magnitude which, in turn, comes from our setting $m = k = 1$, where m is the mass and k the force constant. If we put back *general* values of m and k then A is not normal, and the eigenvectors are not orthogonal so the matrix of eigenvectors U is not unitary. We therefore have to use U^{-1} instead of $U^\dagger$ in Eqs. (A7), (A10), (A11), and (A12). The end result is almost the same as what we find here in which we set $m = k = 1$. The differences are that the time step h has to be multiplied everywhere by $\sqrt{k/m}$ (which has the dimensions of $(\text{time})^{-1}$; note that t appears in the combination t/h in the solution given in Eq. (A13) so t is multiplied by $\sqrt{m/k}$, the natural unit of time), the expression for the momentum has to be multiplied by $\sqrt{mk}$, and the expression for the energy has to be multiplied by k.