介绍

求解一般一阶方程组的简单方法

考虑系统

$$\begin{cases} \dot{y} = f(t, y) \\ y(t_0) = y_0 \end{cases}$$

显 $Euler$ 法

显 $Euler$ 法迭代公式:

$$y_1 = y_0 + h \cdot f(t, y_0)$$

自治系统的显 $Euler$ 程序

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
import warnings
warnings.filterwarnings("ignore")
```

In [2]:
```
def explicit_euler(model):
    y_cur = model.y0
    for i in range(model.epoch):
        y_cur = y_cur + model.h * model.f(y_cur)
        model.add_res(y_cur)
    return model.get_res()
```

隐 $Euler$ 法

隐 $Euler$ 法迭代公式:

$$y_1 = y_0 + h \cdot f(t, y_1)$$

自治系统的隐 $Euler$ 程序

In [3]:
```
from scipy.optimize import fsolve
```

In [4]:
```
def implicit_euler(model):
    y_cur = model.y0
    for i in range(model.epoch):
        fc = lambda x: y_cur + model.h * model.f(x) - x
        y_cur = fsolve(fc, y_cur)
        model.add_res(y_cur)
    return model.get_res()
```

隐中点法

隐中点法 迭代公式:

$$y_1 = y_0 + h \cdot f(t, \frac{y_0 + y_1}{2})$$

自治系统的隐中点法程序

In [5]:
```
def implicit_midpoint(model):
    y_cur = model.y0
    for i in range(model.epoch):
        fc = lambda x: y_cur + model.h * model.f( (y_cur + x) / 2 ) - x
        y_cur = fsolve(fc, y_cur)
        model.add_res(y_cur)
    return model.get_res()
```

求解分离系统的简单方法

考虑系统:

$$\begin{cases} \dot{u} = a(u, v) \\ \dot{v} = b(u, v) \end{cases}$$

辛 $Euler$ 法

辛 $Euler$ 法迭代公式:

- $$\begin{cases} u_{n+1} = u_n + ha(u_n, v_{n+1}) \\ v_{n+1} = v_n + hb(u_n, v_{n+1}) \end{cases}$$
- $$\begin{cases} u_{n+1} = u_n + ha(u_{n+1}, v_n) \\ v_{n+1} = v_n + hb(u_{n+1}, v_n) \end{cases}$$

自治系统的辛 $Euler$ 法程序

In [6]:
```
def symplectic_euler(model):
    tt_l = len(model.y0)
    u_cur, v_cur = model.y0[0: tt_l // 2], model.y0[tt_l // 2:]
    a = lambda u, v: model.f(np.hstack((u, v)))[0: tt_l // 2]
    b = lambda u, v: model.f(np.hstack((u, v)))[tt_l // 2 :]
    for i in range(model.epoch):
        fc = lambda x: np.array([
            x[0: tt_l // 2]  - u_cur - model.h * a(u_cur, x[tt_l // 2 :]),
            x[tt_l // 2:] - v_cur - model.h * b(u_cur, x[tt_l // 2 :])
        ]).flatten()
        uv = fsolve(fc, np.hstack((u_cur, v_cur)))
        model.add_res(uv)
        u_cur, v_cur = uv[0: tt_l // 2], uv[tt_l // 2:]
    return model.get_res()
```

求解二阶系统的简单方法

考虑系统

$$\ddot{q} = f(q)$$

变量替换

容易知道,可以使用变量替换 $p = \dot{q}$, 从而将上述二阶系统改写为一阶系统:

$$\begin{cases} \dot{p} = f(q) \\ \dot{q} = p \end{cases}$$

利用上述求解一阶系统的方法对上述方程进行求解

$Störmer-Verlet$ 方法

$Störmer-Verlet$ 单步法迭代公式:

$$\begin{cases} p_{n+1/2} = p_n + \frac{h}{2}f(q_n) \\ q_{n+1} = q_n + hp_{n+1/2} \\ p_{n+1} = p_{n+1/2} + \frac{h}{2}f(q_{n+1}) \end{cases}$$

$Störmer-Verket$ 法程序

In [7]:
```
def stormer_verlet(model):
    tt_l = len(model.y0)
    p_cur, q_cur = model.y0[0: tt_l // 2], model.y0[tt_l // 2:]
    for i in range(model.epoch):
        p_mid = p_cur + (model.h / 2) * model.f_stormer(q_cur)
        q_cur = q_cur + model.h * p_mid
        p_cur = p_mid + (model.h / 2) * model.f_stormer(q_cur)
        model.add_res(np.hstack((p_cur, q_cur)))
    return model.get_res()
```

简单模型问题

$Lotka-Volterra$ 模型

$$\begin{cases} \dot{u} = u(v-2) \\ \dot{v} = v(1-u) \end{cases}$$

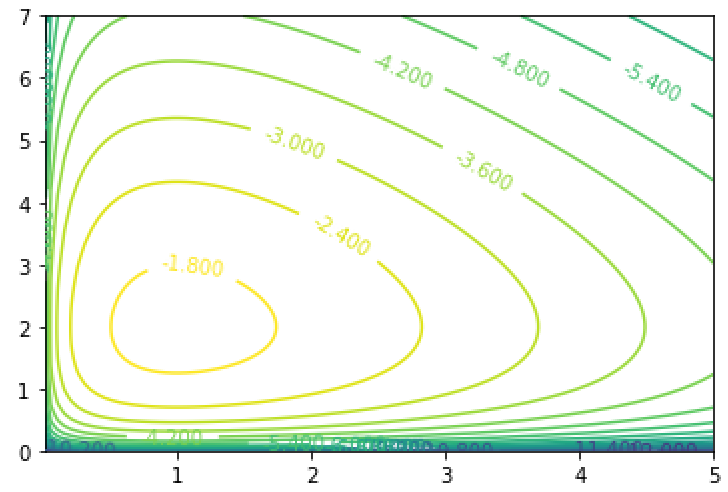
$Lotal-Vikterra$ 模型有如下首次积分:

$$lnu - u + 2lnv - v = C$$

等值线如下:

In [8]:
```
# 方便起见定义等势线绘制函数
def my_draw_contour(func, var1_devid, var2_devid, curve_number = 10, is_ilustrate = True):
    x = np.linspace(var1_devid[0],  var1_devid[1],  var1_devid[2])
    y = np.linspace(var2_devid[0], var2_devid[1],  var2_devid[2])
    X, Y = np.meshgrid(x, y); Z = func(X, Y)
    ctor = plt.contour(X, Y, Z, curve_number)
    if is_ilustrate:
        plt.clabel(ctor)

# 为了数值模拟定义绘制解曲线的函数
def draw_numeric(res_record, color = "red", marker = None):
    x_plt = []; y_plt = []
    for point in res_record:
        x_plt.append(point[0]); y_plt.append(point[1])
    plt.plot(x_plt, y_plt, color = color, marker = marker)
```

In [9]:
```
f_lotka = lambda u,v: np.log(u) - u + 2 * np.log(v) - v
my_draw_contour(f_lotka, (0.01, 5, 100), (0.01, 7, 100), curve_number = 20)
plt.show()
```



数值模拟

分别利用 显 $Euler$ 法; 隐 $Euler$ 法; 辛 $Euler$ 法求解上述系统,规定各个方法的初始条件以及迭代次数如下:

- 显 $Euler$ 法: $h = 0.12 \quad (u_0, v_0) = (2, 2) \quad epoch = 100$
- 隐 $Euler$ 法: $h = 0.12 \quad (u_0, v_0) = (4, 8) \quad epoch = 100$
- 辛 $Euler$ 法: $h = 0.12 \quad (u_0, v_0) = (6, 2) \quad epoch = 100$

并在相空间中绘制出数值解曲线

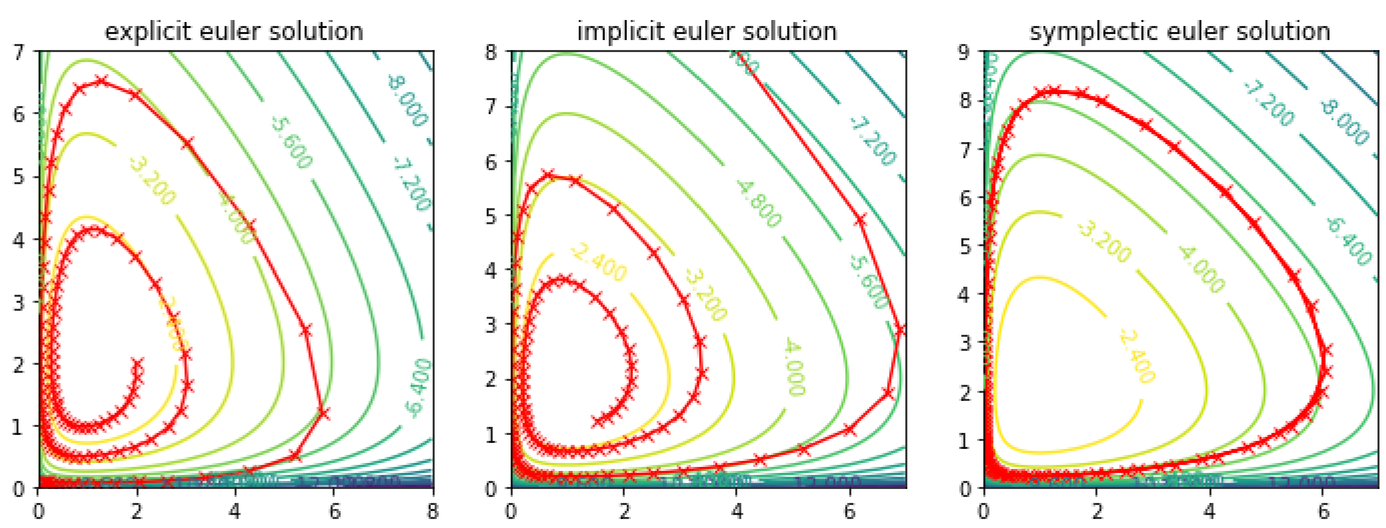
设置模型参数

In [10]:
```python
class Lotka:
    def __init__(self, t0, y0, h, epoch):
        self.t0 = t0
        self.y0 = y0
        self.h = h
        self.epoch = epoch
        self.res = [self.y0]

    def t_mesh(self):
        end = self.t0 + self.epoch * self.h
        t = np.linspace(self.t0, end + self.h, self.epoch + 1)
        return t

    def f(self, y):
        return np.array([y[0] * (y[1] - 2), y[1] * (1 - y[0])])

    def add_res(self, y):
        self.res.append(y)

    def get_res(self):
        return self.res
```

测试程序

In [11]:
```python
def lotka_test():
    # 初始化
    t0 = [0, 0, 0]
    y0 = [np.array([2, 2]), np.array([4, 8]), np.array([6, 2])]
    h = [0.12, 0.12, 0.12]
    epoch = [100, 100, 100]

    lotka_exp_euler = Lotka(t0[0], y0[0], h[0], epoch[0])
    lotka_imp_euler = Lotka(t0[1], y0[1], h[1], epoch[1])
    lotka_symp_euler = Lotka(t0[2], y0[2], h[2], epoch[2])

    # 求解
    exp_euler_res = explicit_euler(lotka_exp_euler)
    imp_euler_res = implicit_euler(lotka_imp_euler)
    symp_euler_res = symplectic_euler(lotka_symp_euler)

    # 可视化
    plt.figure(figsize = (12, 4))
    plt.subplot(131)
    my_draw_contour(f_lotka, (0.01, 8, 100), (0.01, 7, 100), curve_number = 20)
    draw_numeric(exp_euler_res, marker = 'x')
    plt.title('explicit euler solution')

    plt.subplot(132)
    my_draw_contour(f_lotka, (0.01, 7, 100), (0.01, 8, 100), curve_number = 20)
    draw_numeric(imp_euler_res, marker = 'x')
    plt.title('implicit euler solution')

    plt.subplot(133)
    my_draw_contour(f_lotka, (0.01, 7, 100), (0.01, 9, 100), curve_number = 20)
    draw_numeric(symp_euler_res, marker = 'x')
    plt.title('symplectic euler solution')
    plt.show()
```

In [12]:
```python
lotka_test()
```



单摆模型

单摆模型由如下系统给出

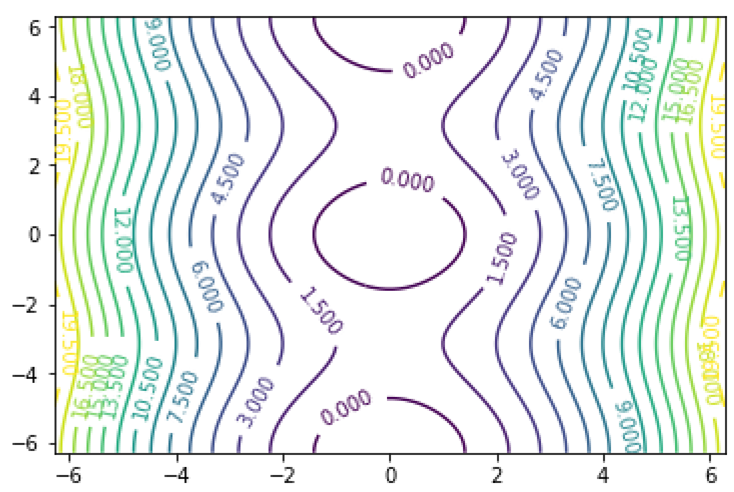
$$\begin{cases} \dot{p} = -sinq \\ \dot{q} = p \end{cases}$$

单摆模型作为哈密顿系统有如下守恒量

$$H(p,q) = \frac{1}{2}p^2 - cosq$$

等值线如下:

In [13]:
```python
f_pendulum = lambda p, q: 0.5 * p**2 - np.cos(q)
my_draw_contour(f_pendulum, (-2 * np.pi, 2 * np.pi, 100), (-2 * np.pi, 2 * np.pi, 100), curve_number = 20)
plt.show()
```



数值模拟

在上述单摆模型中 取初始迭代点 $(0, \frac{\pi}{2})$, 时间步长0.15, 迭代次数100次, 分别利用 显 $Euler$, 隐中点, 辛 $Euler$方法对上述

系统进行求解, 在相空间中绘制出积分曲线.

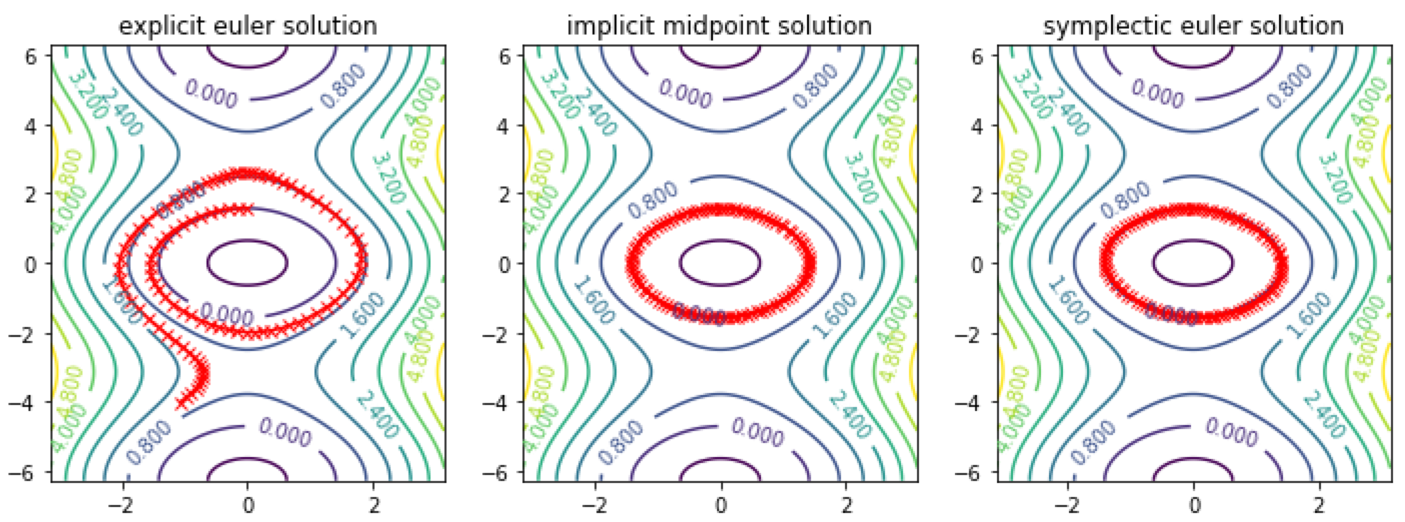
设置模型参数

In [14]:
```python
class Pendulum:
    def __init__(self, t0, y0, h, epoch):
        self.t0 = t0
        self.y0 = y0
        self.h = h
        self.epoch = epoch
        self.res = [self.y0]

    def t_mesh(self):
        end = self.t0 + self.epoch * self.h
        t = np.linspace(self.t0, end + self.h, self.epoch + 1)
        return t

    def f(self, y):
        return np.array([-np.sin(y[1]), y[0]])

    def add_res(self, y):
        self.res.append(y)

    def get_res(self):
        return self.res
```

测试程序

In [15]:
```python
def pendulum_test():
    # 初始化
    t0 = [0, 0, 0]
    y0 = [np.array([0, np.pi / 2]), np.array([0, np.pi / 2]), np.array([0, np.pi / 2])]
    h = [0.15, 0.15, 0.15]
    epoch = [100, 100, 100]

    pendulum_exp_euler = Pendulum(t0[0], y0[0], h[0], epoch[0])
    pendulum_imp_mid = Pendulum(t0[1], y0[1], h[1], epoch[1])
    pendulum_symp_euler = Pendulum(t0[2], y0[2], h[2], epoch[2])

    # 求解
    exp_euler_res = explicit_euler(pendulum_exp_euler)
    imp_mid_res = implicit_midpoint(pendulum_imp_mid)
    symp_euler_res = symplectic_euler(pendulum_symp_euler)

    #
    plt.figure(figsize = (12, 4))
    plt.subplot(131)
    my_draw_contour(f_pendulum, (- np.pi , np.pi , 100), (-2 * np.pi, 2 * np.pi, 100), curve_number = 10)
    draw_numeric(exp_euler_res, marker = 'x')
    plt.title('explicit euler solution')

    plt.subplot(132)
    my_draw_contour(f_pendulum, (-  np.pi , np.pi , 100), (-2 * np.pi, 2 * np.pi, 100), curve_number = 10)
    draw_numeric(imp_mid_res, marker = 'x')
    plt.title('implicit midpoint solution')

    plt.subplot(133)
    my_draw_contour(f_pendulum, (- np.pi , np.pi , 100), (-2 * np.pi, 2 * np.pi, 100), curve_number = 10)
    draw_numeric(symp_euler_res, marker = 'x')
    plt.title('symplectic euler solution')
    plt.show()
```

In [16]:
```python
pendulum_test()
```



Kepler 模型

$Kepler$问题 对应的微分方程组:

$$\ddot{q}_1 = -\frac{q_1}{(q_1^2+q_2^2)^{3/2}} \quad , \quad \ddot{q}_2 = -\frac{q_2}{(q_1^2+q_2^2)^{3/2}}$$

作变量替换之后, 可得如下一阶系统:

$$\begin{cases} \dot{p}_1 = -\dfrac{q_1}{(q_1^2+q_2^2)^{3/2}} \\ \dot{p}_2 = -\dfrac{q_2}{(q_1^2+q_2^2)^{3/2}} \\ \dot{q}_1 = p_1 \\ \dot{q}_2 = p_2 \end{cases}$$

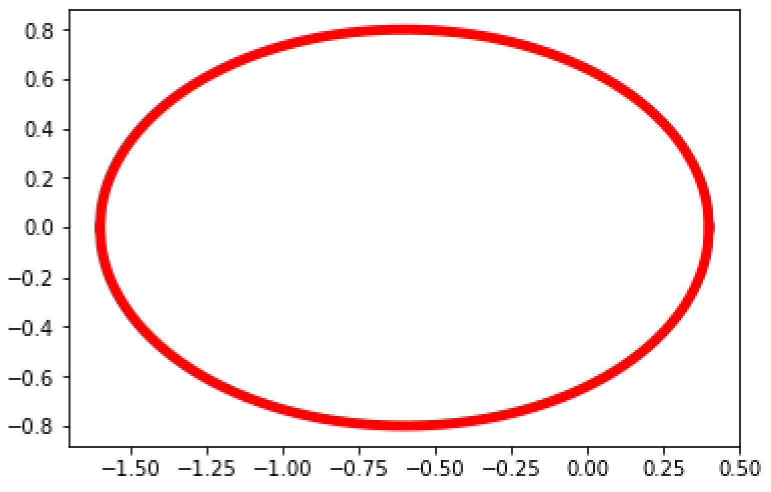
$d = 1 - e^2, e = 0.6$时该方程组直角坐标系下相空间中的积分曲线由下式出

$$x^2 + y^2 - (0.64 - 0.6x)^2 = 0$$

绘制真解图像

In [17]:
```python
def show_solution():
    number_of_points = 500
    q1_plt = np.linspace(-1.6, 0.4, number_of_points)
    q2_plt_pos = np.sqrt( (0.64 - 0.6 * q1_plt )**2 - q1_plt**2)
    q2_plt_neg = -q2_plt_pos
    plt.plot(q1_plt, q2_plt_pos, "r",  linewidth = 5, label = "exact flow")
    plt.plot(q1_plt, q2_plt_neg, "r", linewidth=5)
```

In [18]:
```
show_solution()
```



数值模拟

分别利用 显 $Euler$ 法; 辛 $Euler$ 法; 隐中点法; $Störmer-Verlet$ 求解上述系统,规定各个方法的初始条件以及迭代次数如下:

- 显 $Euler$ 法: $h=0.0005 \quad (p_1,p_2,q_1,q_2)=(0,2,0.4,0) \quad epoch=400000$
- 辛 $Euler$ 法: $h=0.05 \quad (p_1,p_2,q_1,q_2)=(0,2,0.4,0) \quad epoch=4000$
- 隐中点法: $h=0.05 \quad (p_1,p_2,q_1,q_2)=(0,2,0.4,0) \quad epoch=4000$
- $Störmer-Verlet: h=0.05 \quad (p_1,p_2,q_1,q_2)=(0,2,0.4,0) \quad epoch=4000$

并在相空间中绘制出数值解曲线

绘制 显 $Euler$ 法; 辛 $Euler$ 法;在求解过程中的能量变化曲线
绘制 显 $Euler$ 法; 辛 $Euler$ 法;在求解过程中与真解的误差曲线

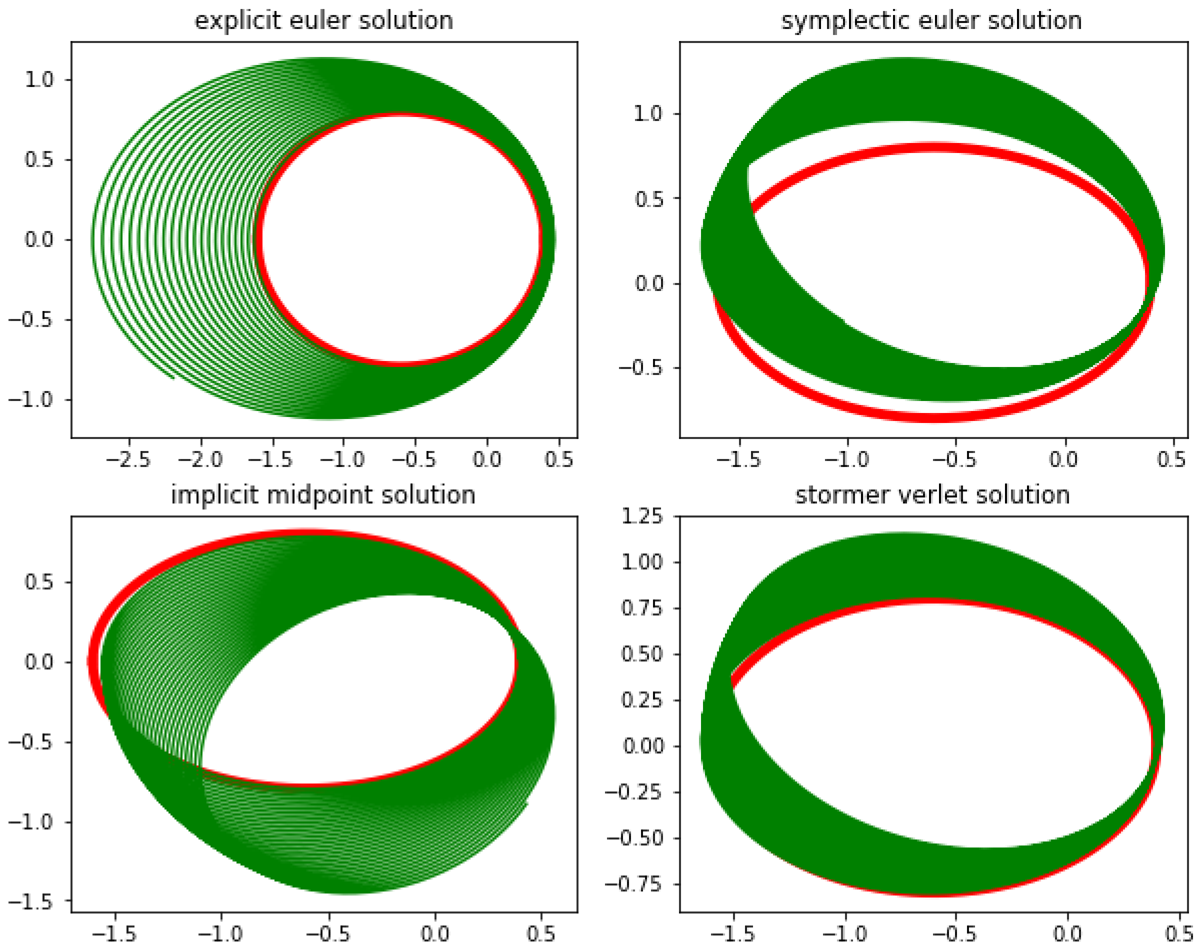
积分曲线的模拟

In [19]:
```
class Kepler1:
    def __init__(self, t0, y0, h, epoch):
        self.t0 = t0
        self.y0 = y0
        self.h = h
        self.epoch = epoch
        self.res = [self.y0[2:4]]

    def t_mesh(self):
        end = self.t0 + self.epoch * self.h
        t = np.linspace(self.t0, end + self.h, self.epoch + 1)
        return t

    # 一般的一阶数系统的右端函数
    def f(self, y):
        p1 = y[0]; p2 = y[1] ; q1 = y[2]; q2 = y[3]
        return np.array([-q1 / (q1**2 + q2**2)**1.5, -q2 / (q1**2 + q2**2)**1.5, p1, p2])

    # 用于 stormer-verlert 迭代构造的函数
    def f_stormer(self, y):
        return np.array([-y[0] / (y[0] ** 2 + y[1] ** 2)**1.5, -y[1] / (y[0] ** 2 + y[1] ** 2)**1.5])

    def solution(self, t):
        phi = [0]
        solution = []
        for i in range(len(t)):
            f = lambda phi: 4 * np.arctan(np.tan(phi / 2) / 2) \
            - 4.8 * (np.tan( phi / 2) / ( np.tan(phi / 2) ** 2 + 4)) - t[i]
            phi2 = fsolve(f, phi[i])
            phi.append(phi2)
            solution.append(np.array([0.64 * np.cos(phi2) / (1 + 0.6 * np.cos(phi2)),
                                      0.64 * np.sin(phi2) / (1 + 0.6 * np.cos(phi2))]).flatten())
        return solution

    def add_res(self, y):
        self.res.append(y[2:4])

    def get_res(self):
        return self.res
```

测试程序1

In [20]:
```
# 可视化
def kepler_test1():
    # 初始化
    t0 = [0, 0, 0, 0]
    y0 = [np.array([0, 2, 0.4, 0]), np.array([0, 2, 0.4, 0]), np.array([0, 2, 0.4, 0]), np.array([0, 2, 0.4, 0])]
    h = [0.0005, 0.05, 0.05, 0.05]
    epoch = [400000, 4000, 4000, 4000]

    kepler_exp_euler = Kepler1(t0[0], y0[0], h[0], epoch[0])
    kepler_symp_euler = Kepler1(t0[1], y0[1], h[1], epoch[1])
    kepler_imp_mid = Kepler1(t0[2], y0[2], h[2], epoch[2])
    kepler_stormer = Kepler1(t0[3], y0[3], h[3], epoch[3])

    # 求解
    exp_euler_res = explicit_euler(kepler_exp_euler)
    symp_euler_res = symplectic_euler(kepler_symp_euler)
    imp_mid_res = implicit_midpoint(kepler_imp_mid)
    stormer_res = stormer_verlet(kepler_stormer)

    #
    plt.figure(figsize = (10, 8))
    plt.subplot(221)
    show_solution()
    draw_numeric(exp_euler_res, color = 'g')
    plt.title('explicit euler solution')

    plt.subplot(222)
    show_solution()
    draw_numeric(symp_euler_res, color = 'g')
    plt.title('symplectic euler solution')

    plt.subplot(223)
    show_solution()
    draw_numeric(imp_mid_res, color = 'g')
    plt.title('implicit midpoint solution')

    plt.subplot(224)
    show_solution()
    draw_numeric(stormer_res, color = 'g')
    plt.title('stormer verlet solution')

    plt.show()
```

In [21]:
```
kepler_test1()
```



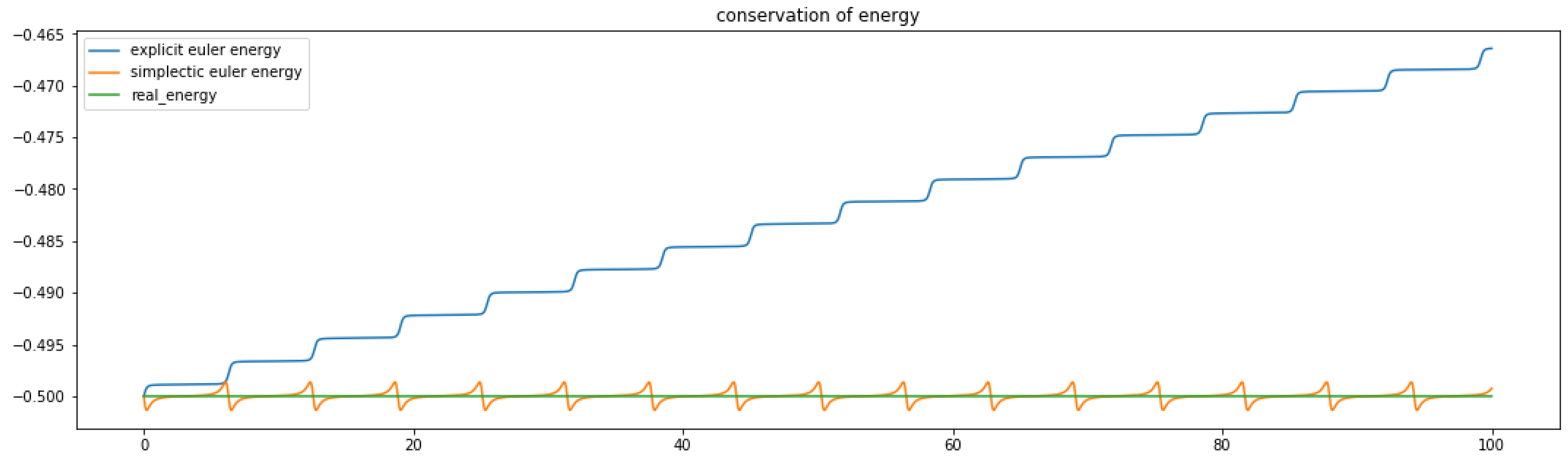
绘制显 $Euler$ 法和辛 $Euler$ 法的误差和能量曲线

In [22]:
```
# 重新定义模型参数如下
class Kepler2:
    def __init__(self, t0, y0, h, epoch):
        self.t0 = t0
        self.y0 = y0
        self.h = h
        self.epoch = epoch
        self.res = [self.y0]

    def t_mesh(self):
        end = self.t0 + self.epoch * self.h
        t = np.linspace(self.t0, end + self.h, self.epoch + 1)
        return t

    def f(self, y):
        p1 = y[0]; p2 = y[1] ; q1 = y[2]; q2 = y[3]
        return np.array([-q1 / (q1**2 + q2**2)**1.5, -q2 / (q1**2 + q2**2)**1.5, p1, p2])

    # Hamiltonian 能量函数定义
    def H(self, y):
        return 0.5 * (y[0] ** 2 + y[1] ** 2) - 1 / np.sqrt(y[2] ** 2 + y[3] ** 2)

    def add_res(self, y):
        self.res.append(y)

    def get_res(self):
        return self.res
```

测试程序2

In [23]:
```
def kepler_test2():
    # 初始化
    t0 = [0, 0]
    y0 = [np.array([0, 2, 0.4, 0]), np.array([0, 2, 0.4, 0])]
    h = [0.0001, 0.001]
    epoch = [1000000, 100000]

    kepler_exp_euler = Kepler2(t0[0], y0[0], h[0], epoch[0])
    kepler_symp_euler = Kepler2(t0[1], y0[1], h[1], epoch[1])

    # 获取时间网格, 数值解能量, 真实能量
    t_exp_euler = kepler_exp_euler.t_mesh()
    t_symp_euler = kepler_symp_euler.t_mesh()

    exp_euler_res = explicit_euler(kepler_exp_euler)
    symp_euler_res = symplectic_euler(kepler_symp_euler)

    H0 = kepler_symp_euler.H(y0[0])
    H_real = np.full_like(t_exp_euler ,H0)
    H_exp_euler = np.zeros_like(t_exp_euler)
    H_symp_euler = np.zeros_like(t_symp_euler)

    for i in range(len(H_exp_euler)):
        H_exp_euler[i] = kepler_exp_euler.H(exp_euler_res[i])

    for j in range(len(H_symp_euler)):
        H_symp_euler[j] = kepler_symp_euler.H(symp_euler_res[j])


    #
    plt.figure(figsize = (40, 5))
    ax1 = plt.subplot(121)
    ax1.plot(t_exp_euler, H_exp_euler, label = 'explicit euler energy')
    ax1.plot(t_symp_euler, H_symp_euler, label = 'simplectic euler energy')
    ax1.plot(t_exp_euler, H_real, label = 'real_energy')
    plt.legend()
    plt.title('conservation of energy')

    plt.show()
```

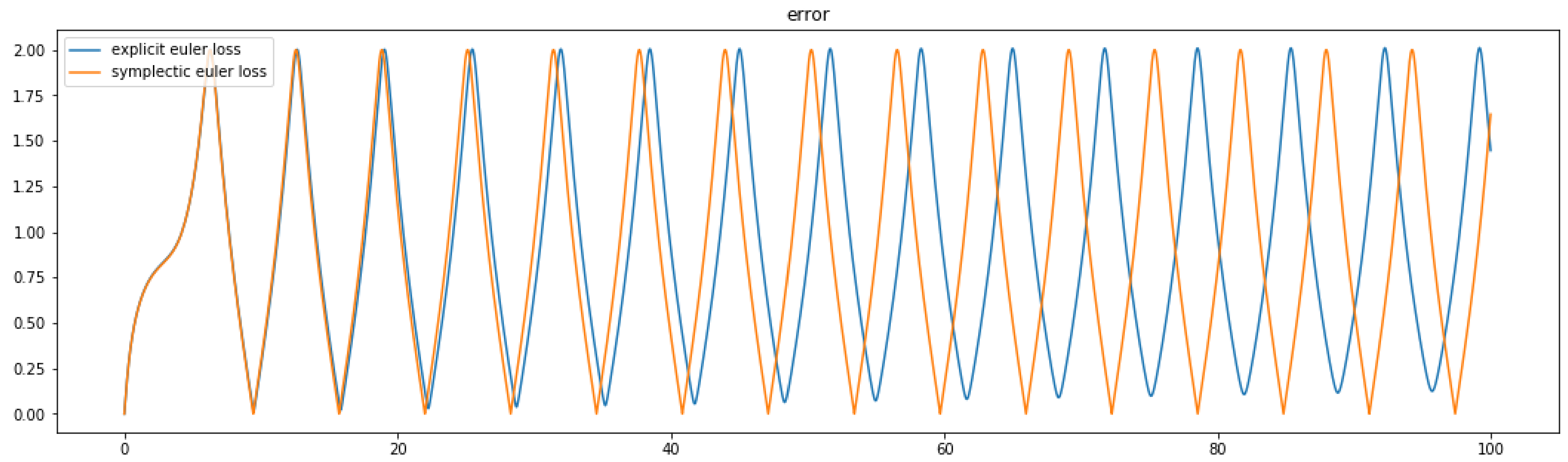
In [24]:
```
kepler_test2()
```



测试程序3

In [25]:
```
# 定义误差函数
def loss_comp(solution, y):
    loss = np.zeros(len(solution), dtype = np.float64)
    for i in range(len(solution)):
        loss[i] = np.linalg.norm(solution[i] - y[i])
    return loss


def kepler_test3():
    # 初始化
    t0 = [0, 0]
    y0 = [np.array([0, 2, 0.4, 0]), np.array([0, 2, 0.4, 0])]
    h = [0.0001, 0.001]
    epoch = [1000000, 100000]

    kepler_exp_euler = Kepler1(t0[0], y0[0], h[0], epoch[0])
    kepler_symp_euler = Kepler1(t0[1], y0[1], h[1], epoch[1])

    # 获取时间网格， 数值解, 真实解
    t_exp_euler = kepler_exp_euler.t_mesh()
    t_symp_euler = kepler_symp_euler.t_mesh()

    exp_euler_res = explicit_euler(kepler_exp_euler)
    symp_euler_res = symplectic_euler(kepler_symp_euler)


    solution_exp = kepler_exp_euler.solution(t_exp_euler)
    solution_symp = kepler_symp_euler.solution(t_symp_euler)

    loss_exp_euler = loss_comp(solution_exp, exp_euler_res)
    loss_symp_euler = loss_comp(solution_symp, symp_euler_res)


    #
    plt.figure(figsize = (40, 5))
    ax1 = plt.subplot(121)
    ax1.plot(t_exp_euler, loss_exp_euler, label = 'explicit euler loss')
    ax1.plot(t_symp_euler, loss_symp_euler, label = 'symplectic euler loss')

    plt.legend()
    plt.title('error')

    plt.show()
```

In [26]:
```
kepler_test3()
```



??????????这个那本书上怎么画的。。。。画不出来难受啊

外太阳系系统

考虑对 描述 5 个和太阳相关的外行星的运动的系统使用数值方法,该系统的哈密顿函数如下:

$$H(p,q)=\frac{1}{2}\sum_{i=0}^{5}\frac{1}{m_i}p_i^T p_i-G\sum_{i=1}^{5}\sum_{j=0}^{i-1}\frac{m_i\,m_j}{\|q_i-q_j\|}$$

其中

$$\begin{cases} p=(p_0,p_1,p_2,p_3,p_4,p_5) & p_i\in R^3 \\ q=(p_0,q_1,q_2,q_3,q_4,q_5) & q_i\in R^3 \end{cases}$$

m_i表示行星和太阳的相对质量

取太阳的相对质量: $m_0=1.00000597682$

取万有引力常数: $G=2.95912208286\times 10^{-4}$

取太阳的初始位置和速度: $q_0(0)=(0,0,0)\quad \dot{q_0}(0)=(0,0,0)$

其余五个行星和太阳的相对质量以及初始条件如下:

- $Jupiter\quad m_1=0.000954786104043\quad q_1(0)=(-3.5023653,-3.8169847,-1.5507963)$
  $\dot{q_1}(0)=(0.00565429,-0.00412490,-0.00190589)$
- $Saturn\quad m_2=0.000285583733151\quad q_2(0)=(9.0755314,-3.0458353,-1.6483708)\quad \dot{q_2}(0)=(0.00168318,0.00483525,0.00192462)$
- $Uranus\quad m_3=0.0000437273164546\quad q_3(0)=(8.3101420,-16.2901086,-7.2521278)$
  $\dot{q_3}(0)=(0.00354178,0.00137102,0.00055029)$
- $Neptune\quad m_4=0.0000517759138449\quad q_4(0)=(11.4707666,-25.7294829,-10.8169456)$
  $\dot{q_4}(0)=(0.00288930,0.00114527,0.00039677)$
- $Pluto\quad m_5=1/(1.3\cdot 10^8)\quad q_5(0)=(-15.5387357,-25.2225594,-3.1902382)\quad \dot{q_5}(0)=(0.00276725,-0.00170702,-0.00136504)$

外太阳系数值模拟

分别用显 $Euler$ 法; 隐 $Euler$ 法; 辛 $Euler$ 法; $Stórmer-Verlet$ 方法求解上述系统, 在一个时间周期

(200000 天) 求解上述系统, 时间步长分别如下取值:

- 显 $Euler$ 法 : h = 10
- 隐 $Euler$ 法 : h = 10
- 辛 $Euler$ 法 : h = 100
- $Stórmer-Verlet$ 方法 : h = 200

设置模型参数

写出原方程对应的一阶系统如下:

$$\begin{cases} \dot{p_k}=-G\sum\limits_{\substack{i=0\\ i\neq k}}^{5}\frac{m_i\,m_k}{\|q_k-q_i\|^3}(q_k-q_i) \\ \dot{q_k}=p_k/m_k \end{cases}$$

$\dot{p}$ 的数组化定义方式:

定义如下数组:

$$-G\begin{pmatrix} 0 & \frac{m_0m_1}{\|q_1-q_0\|^3}(q_1-q_0) & \cdots & \frac{m_0m_5}{\|q_5-q_0\|^3}(q_5-q_0) \\ \frac{m_1m_0}{\|q_0-q_1\|^3}(q_0-q_1) & 0 & \cdots & \frac{m_1m_5}{\|q_5-q_1\|^3}(q_5-q_1) \\ \frac{m_2m_0}{\|q_0-q_2\|^3}(q_0-q_2) & \frac{m_2m_1}{\|q_1-q_2\|^3}(q_1-q_2) & \cdots & \frac{m_2m_5}{\|q_5-q_2\|^3}(q_5-q_2) \\ & \cdots & \cdots & \\ \frac{m_5m_0}{\|q_0-q_5\|^3}(q_0-q_5) & \frac{m_5m_1}{\|q_1-q_5\|^3}(q_1-q_5) & \cdots & 0 \end{pmatrix}$$

其中

$$A[i,3j:3j+3]=\begin{cases} 0 & i=j \\ \frac{m_im_j}{\|q[3j:3j+3]-q[3i:3i+3]\|}(q[3j:3j+3]-q[3i:3i+3]) & i\neq j \end{cases}$$

利用 sum 函数沿着行的方向求和即可

对于利用 $Stórmer-Verlet$ 方法进行迭代时,把方程改如下:

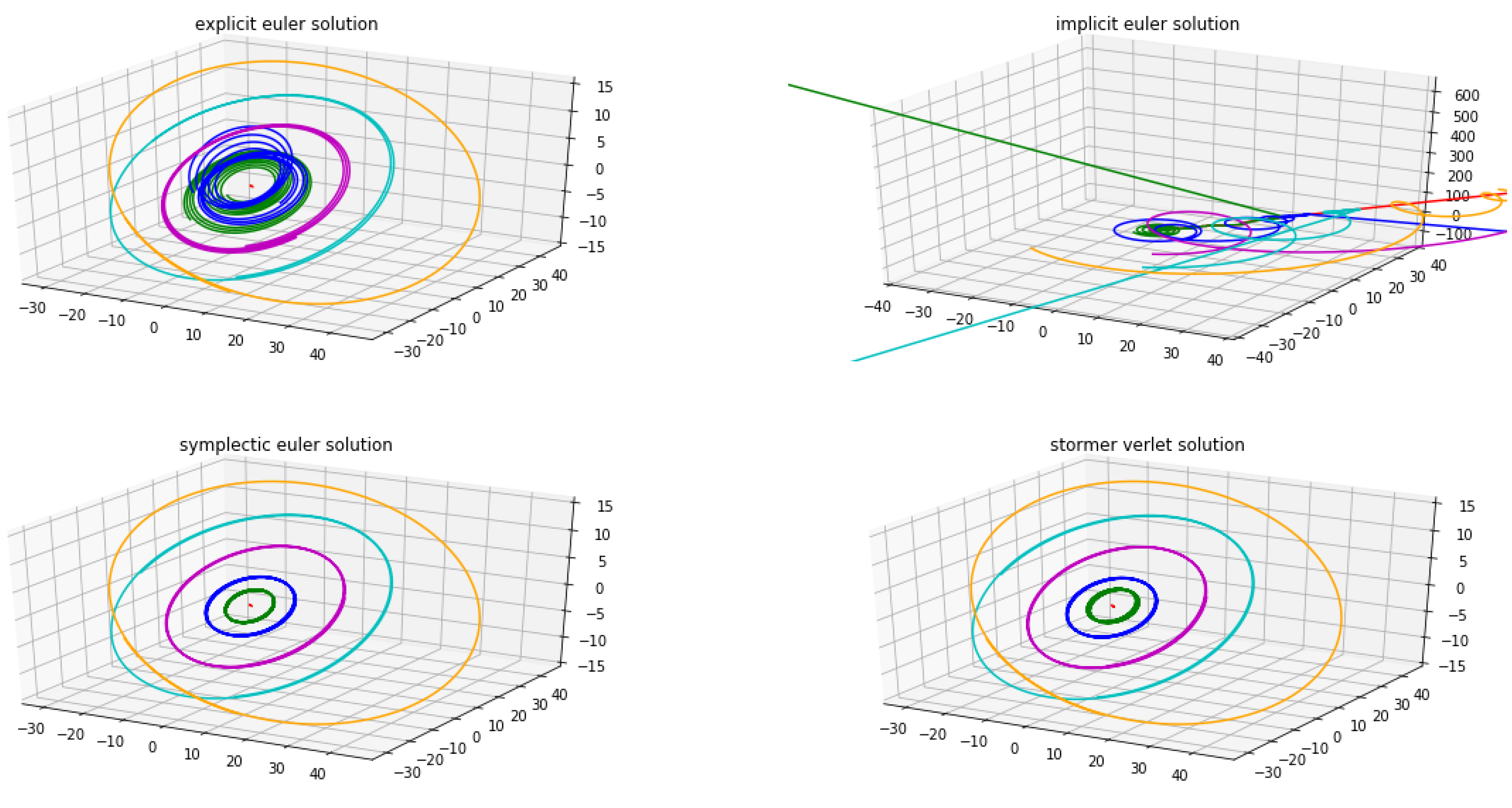
$$\begin{cases} \dot{v_k}=-G\sum\limits_{\substack{i=0\\ i\neq k}}^{5}\frac{m_i}{\|q_k-q_i\|^3}(q_k-q_i) \\ \dot{q_k}=v_k \end{cases}$$

In [27]:
```python
from scipy.linalg import block_diag
class Outer_Solar:
    def __init__(self, t0, y0, h, m, epoch):
        self.t0 = t0
        self.y0 = y0
        self.h = h
        self.epoch = epoch
        self.res = [self.y0[18:]]
        self.G = 2.95912208286 * 1e-4
        self.m = m

    def t_mesh(self):
        end = self.t0 + self.epoch * self.h
        t = np.linspace(self.t0, end + self.h, self.epoch + 1)
        return t

    # 一般的一阶数系统的右端函数
    def f(self, y):     # y : 长度为36的数组
        ttl = len(y)
        lq = ttl // 2
        p = y[0 : ttl // 2]
        q = y[ttl // 2 :]

        a = np.ones(3)
        support = block_diag(a, a, a, a, a, a)

        # 创建二维数组 A
        A = np.zeros((6, 18))
        for i in range(6):
            for j in range(6):
                if i != j:
                    qi = q[3 * i : 3 * i + 3]
                    qj = q[3 * j : 3 * j + 3]
                    A[i,3 * j : 3 * j + 3] = ( (self.m[i] * self.m[j])/ (np.linalg.norm(qj - qi)) ** 3) * (qj - qi)
        # 创建右端项矩阵
        dp = -self.G * np.sum(A, axis = 0)
        dq = p / np.dot(self.m.reshape(1, -1), support).flatten()
        return np.hstack((dp, dq))

    # 用于 stormer-verlert 迭代构造的函数
    def f_stormer(self, s):
        A = np.zeros((6, 18))
        for i in range(6):
            for j in range(6):
                if i != j:
                    si = s[3 * i : 3 * i + 3]
                    sj = s[3 * j : 3 * j + 3]
                    A[i,3 * j : 3 * j + 3] = ( (self.m[i] )/ (np.linalg.norm(sj - si)) ** 3 ) * (sj - si)
        ds = -self.G * np.sum( A, axis = 0 )
        return ds


    def add_res(self, y):
        self.res.append(y[18:])

    def get_res(self):
        return self.res
```

测试程序

In [28]:
```python
from mpl_toolkits.mplot3d import Axes3D

def draw_numeric_outer(ax, res_record, color = ['r', 'g', 'b', 'm', 'c', 'orange']):
    for i in range(6):
        x_rec = []
        y_rec = []
        z_rec = []
        for j in range(len(res_record)):
            x_rec.append(res_record[j][i * 3])
            y_rec.append(res_record[j][i * 3 + 1])
            z_rec.append(res_record[j][i * 3 + 2])
        ax.plot(x_rec, y_rec, z_rec, color = color[i])

def outer_solar_test():
    # 初始化
    m = np.array([1.00000597682, 0.000954786104043,0.000285583733151,\
                  0.0000437273164546, 0.0000517759138449, 1 / (1.3 * 1e8)])
    t0 = [0, 0, 0, 0]
    v0 = np.array([
        0, 0, 0,
        0.00565429, -0.00412490, -0.00190589,
        0.00168318, 0.00483525, 0.00192462,
        0.00354178, 0.00137102, 0.00055029,
        0.00288930, 0.00114527, 0.00039677,
        0.00276725, -0.00170702, -0.00136504
    ])

    # 将速度初值转换为动量初值
    a = np.ones(3)
    support = block_diag(a, a, a, a, a, a)
    p0 = v0 * np.dot(m.reshape(1, -1), support).flatten()

    q0 = np.array([
        0, 0, 0,
        -3.5023653, -3.8169847, -1.5507963,
        9.0755314, -3.0458353, -1.6483708,
        8.3101420, -16.2901086, -7.2521278,
        11.4707666, -25.7294829, -10.8169456,
        -15.5387357, -25.2225594, -3.1902382
    ])
    y0 = np.hstack((p0, q0))
    h = [10, 10, 100, 200]
    epoch = [10000, 5000, 1000, 500]

    #
    outer_exp_euler = Outer_Solar(t0[0], y0, h[0], m, epoch[0])
    outer_imp_euler = Outer_Solar(t0[1], y0, h[1], m, epoch[1])
    outer_symp_euler = Outer_Solar(t0[2], y0, h[2], m, epoch[2])

    # stormer-verlet 法初值需要代速度
    outer_stormer = Outer_Solar(t0[3], np.hstack((v0, q0)), h[3], m, epoch[3])

    # 求解
    exp_euler_res = explicit_euler(outer_exp_euler)
    imp_euler_res = implicit_euler(outer_imp_euler)
    symp_euler_res = symplectic_euler(outer_symp_euler)
    stormer_res = stormer_verlet(outer_stormer)


    # 绘制积分曲线
    plt.figure(figsize = (20, 10))

    ax1 = plt.subplot(221, projection = '3d')
    draw_numeric_outer(ax1, exp_euler_res)
    plt.title('explicit euler solution')

    ax2 = plt.subplot(222, projection = '3d')
    draw_numeric_outer(ax2, imp_euler_res)
    plt.xlim(-40, 40)
    plt.ylim(-40, 40)
    plt.title('implicit euler solution')

    ax3 = plt.subplot(223, projection = '3d')
    draw_numeric_outer(ax3, symp_euler_res)
    plt.title('symplectic euler solution')

    ax4 = plt.subplot(224, projection = '3d')
    draw_numeric_outer(ax4, stormer_res)
    plt.title('stormer verlet solution')

    plt.show()
```

In [29]:
```python
outer_solar_test()
```



$Henon - Heiles$ 模型

$Henon - Heiles$ 模型用于描述恒星运动

在降维之后, 带有两个自由度的哈密顿系统的哈密顿函数如下:

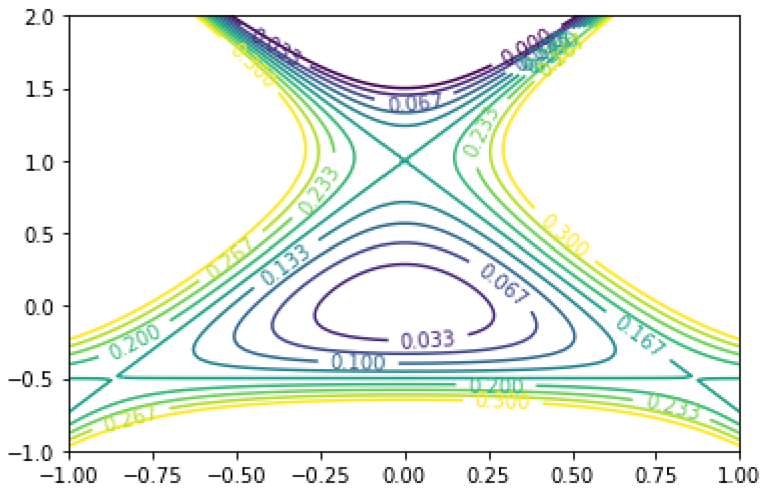
$$H(p,q) = \frac{1}{2}(p_1^2 + p_2^2) + U(q)$$

其中, $U(q)$ 如下选取:

$$U(q) = \frac{1}{2}(q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3}q_2^3$$

势能的等值线如下:

In [30]:
```
def my_draw_contourhh(func, var1_devid, var2_devid, is_ilustrate = True):
    x = np.linspace(var1_devid[0],  var1_devid[1],  var1_devid[2])
    y = np.linspace(var2_devid[0], var2_devid[1],  var2_devid[2])
    X, Y = np.meshgrid(x, y); Z = func(X, Y)
    ctor = plt.contour(X, Y, Z, np.linspace(0, 0.3, 10))
    if is_ilustrate:
        plt.clabel(ctor)
pot_hh = lambda x,y: 0.5 * (x ** 2 + y ** 2) + x**2 * y - (1 / 3) * y ** 3
my_draw_contourhh(pot_hh, (-1, 1, 100), (-1, 2, 100))
plt.show()
```



由图,当势能 $U = \frac{1}{6}$时, U的等值线趋向于等边三角形, 其顶点为 U的鞍点, 势能 U 取为上式时,相应的系统如下:

$$\begin{cases} \ddot{q_1} = -q_1 - 2q_1 q_2 \\ \ddot{q_2} = -q_2 - q_1^2 + q_2^2 \end{cases}$$

或者将上述系统改写为一阶系统如下:

$$\begin{cases} \dot{p_1} = -q_1 - 2q_1 q_2 \\ \dot{p_2} = -q_2 - q_1^2 + q_2^2 \\ \dot{q_1} = p_1 \\ \dot{q_2} = p_2 \end{cases}$$

上述系统的解具有非平凡的性质, 对于给定的初值如果使得 $H(p(0), q(0)) < \frac{1}{6}$ 并且 $q(0)$ 在三角形 $U \leq \frac{1}{6}$

$Poncare$ 截面数值模拟:

固定初始能量 H_0 令: $q_{10} = 0$, 任取 $P_0 = (q_{20}\ , p_{20}\ )$, 则可以从哈密顿函数中解出,并取 $p_{10} = \sqrt{2H_0 - 2U_0 - p_{20}^2}$ 沿着数值解走, 直到解再次在正向 $p_1 > 0$ 出现在面 $q_1 = 0$ 上, 此时获取第二个点$P_1 = (q_{21}, p_{21}\ )$, 同理计算得到: $P_2 = (q_{22}\ , p_{22}\ )\cdots$

模拟数据:

取 $H_0 = \frac{1}{12}, h = 10^{-5}, q_{10} = 0,\ q_{20} = 0.25,\ p_{20} = -0.15$

$p_{10} = \sqrt{2H_0 - 2U_0 - p_{20}^2}$

利用显$Euler$ 迭代求解上述系统, 在 $t \in [0, 300000]$ 上求解绘制(迭代 $3 * 10^{11}$ 次)

跑不动 跑不动。。。。。

分子动力学

分子动力学需要哈密顿系统的解, 哈密顿函数如下给出:

$$H(p,q) = \frac{1}{2}\sum_{i=1}^{N}\frac{1}{m_i}p_i^T p_i + \sum_{i=2}^{N}\sum_{j=1}^{i-1}V_{ij}(\|q_i - q_j\|)$$

其中:$V_{ij}(r)$ 是给定的势能函数, q_i 表示位置, p_i 表示原子动量, m_i 表示第 i 个原子的质量

在外太阳系系统中, 势能函数由$Vij(r) = -G\frac{m_i m_j}{r}$ 给出,在分子动力学中,通常考虑 $Lennard - Jones$ 势能:

$$V_{ij}(r) = 4\epsilon_{ij}[(\frac{\sigma_{ij}}{r})^{12} - (\frac{\sigma_{ij}}{r})^{6}]$$

其中 ϵ_{ij} 以及 σ_{ij} 是由原子所决定的合适常数

上述势能函数在当 $r = \sigma ij\sqrt[6]{2}$时取得全局极小值, 这个值的含义是: 当 两个原子之间的距离小于这个值时, 由上述势能产

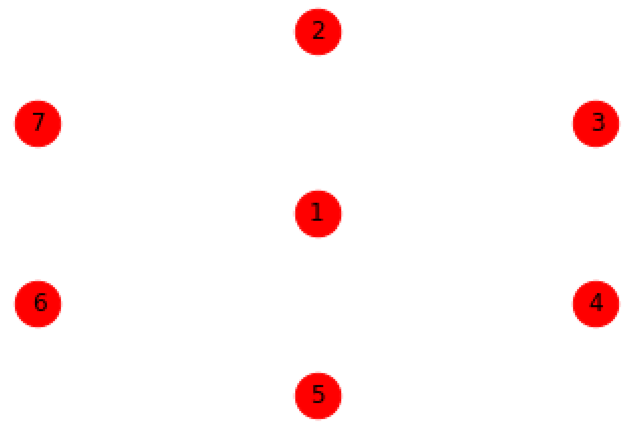
生的力将会排斥两个原子, 当两个原子之间的距离超过这个值时, 由上述势能产生的力将会吸引两个原子.

冻结氩晶体的数值模拟

如下图所示在平面上考虑如下排列 7个氩原子之间的相互作用:

其中一个位于中心, 剩余的留个对称地排列在四周

In [31]:
```python
import networkx as nx
G = nx.Graph()
num = 7
nodes = [i for i in range(1, 8)]
G.add_nodes_from(nodes)

coordinates = [[0, 0], [0, 1.5], [0.5, 0.75], [0.5, -0.75], [0, -1.5], [-0.5, -0.75], [-0.5, 0.75]]
vnode= np.array(coordinates)
npos = dict(zip(nodes, vnode))
nlabels = dict(zip(nodes, nodes))
nx.draw_networkx_nodes(G, npos, node_size=500, node_color="red")
nx.draw_networkx_labels(G, npos, nlabels)
x_max,y_max = vnode.max(axis=0)
x_min, y_min = vnode.min(axis=0)
x_num = (x_max - x_min) / 10
y_num = (y_max - y_min) / 10
# print(x_max, y_max, x_min, y_min)
plt.xlim(x_min - x_num, x_max + x_num)
plt.ylim(y_min - y_num, y_max + y_num)
plt.axis('off')
plt.show()
```



取哈密顿量即为上述的哈密顿量, $N=7$, $m_i=m=66.34\cdot 10^{-27}[kg]$

$$\epsilon_{ij}=\epsilon=119.8k_B[J],\quad \sigma_{ij}=\sigma=0.341[nm]$$

其中 $k_B=1.380658\cdot 10^{-23}\ [J/K]$为波尔兹曼常数, 质量单位取 $[kg]$, 长度单位取纳米$1[nm]=10^{-9}\ [m]$, 时间单位取纳秒 $1[nsec]=10^{-9}\ [sec]$, 各个原子的初始位置 $[nm]$, 初始速度 $[nm]/[nsec]$ 在下面给出, 距离的选取按照适当的规则,并且下述距离选取使得系统总动量为0, 因此最中心原子将不会发生移动, 初始位置时刻的能量大约为 $-1260.2k_B[J]$

- 1号: 初始位置: (0.00, 0.00) , 初始速度:(-30, -20)
- 2号: 初始位置: (0.02, 0.39) , 初始速度:(50, -90)
- 3号: 初始位置: (0.34, 0.17) , 初始速度:(-70, -60)
- 4号: 初始位置: (0.36, -0.21) , 初始速度:(90, 40)
- 5号: 初始位置: (-0.02, -0.40) , 初始速度:(80, 90)
- 6号: 初始位置: (-0.35, -0.16) , 初始速度:(-40, 100)
- 7号: 初始位置: (-0.31, 0.21) , 初始速度:(-80, -60)

在对分子动力学系统的计算中, 一般不关心原子的轨迹, 一般对一些宏观量比较感兴趣(如: 温度, 压力, 内能等), 在此处, 考虑哈密顿能量以及温度, 温度的计算公式如下:

$$T=\frac{1}{2Nk_B}\sum_{i=1}^{N}m_i\|\dot{q}_i\|^2$$

模拟要求如下:

- 分别利用显$Euler$法 以及 辛$Euler$法对上述系统进行求解; 取时间步长分别为 $0.5[fec], 10[fec]$ $(1[fec]=10^{-6}\ [nec])$ 在时间区间 $[0,0.1]$ (即, 分别迭代 200000次, 10000次)上绘制出总能量变化曲线(用 $H(p_n,q_n)-H(p_0,q_0)/k_B$)
- 分别利用显$Euler$法 以及 辛$Euler$法对上述系统进行求解; 取时间步长分别为 $10[fec], 10[fec]$ $(1[fec]=10^{-6}\ [nec])$ 在时间区间 $[0,0.1]$ (即, 分别迭代 10000次, 10000次)上利用上述温度公式,绘制出温度变化曲线
- 利用SV方法进行两次求解, 取时间步长分别为 $40[fec], 80[fec]$ $(1[fec]=10^{-6}\ [nec])$ 在时间区间 $[0,0.1]$ (即, 分别迭代 2500次, 1250次)上绘制出总能量变化曲线(用 $H(p_n,q_n)-H(p_0,q_0)/k_B$)
- 利用SV方法进行两次求解, 取时间步长分别为 $10[fec], 20[fec]$ $(1[fec]=10^{-6}\ [nec])$ 在时间区间 $[0,0.1]$ (即, 分别迭代 10000次, 5000次)上绘制出温度变化曲线

将原系统改写如下:

$$\begin{cases}\dot{p_k}=-24\epsilon\sigma^6\sum\limits_{\substack{i=1\\i\neq k}}^{7}\dfrac{1}{\|q_k-q_i\|^8}(1-\dfrac{2\sigma^6}{\|q_k-q_i\|^6})(q_k-q_i)\\ \dot{q_k}=p_k/m\end{cases}$$

对于 SV 方法, 需要将系统改写如下:

$$\begin{cases}\dot{v_k}=-24\dfrac{\epsilon\sigma^6}{m}\sum\limits_{\substack{i=1\\i\neq k}}^{7}\dfrac{1}{\|q_k-q_i\|^8}(1-\dfrac{2\sigma^6}{\|q_k-q_i\|^6})(q_k-q_i)\\ \dot{q_k}=v_k\end{cases}$$

模型参数

```python
In [32]: class Md_Model:
    def __init__(self, t0, y0, h, epoch):
        self.t0 = t0
        self.y0 = y0
        self.h = h
        self.epoch = epoch
        self.res = [self.y0]
        self.kB = 1.380658 * 1e-23
        self.epsilon = 119.8 * self.kB
        self.sigma = 0.341
        self.m = 66.34 * 1e-27
        self.H0 = -1260.2 * self.kB
        self.T0 = 22.72

    def t_mesh(self):
        end = self.t0 + self.epoch * self.h
        t = np.linspace(self.t0, end, self.epoch + 1)
        return t

    # 一般的一阶数系统的右端函数
    def f(self, y):     # y : 长度为 28 的数组
        ttl = len(y)
        lq = ttl // 2
        p = y[0 : ttl // 2]
        q = y[ttl // 2 :]
        # 创建二维数组 A
        A = np.zeros((7, 14))
        for i in range(7):
            for j in range(7):
                if i != j:
                    qi = q[2 * i : 2 * i + 2]
                    qj = q[2 * j : 2 * j + 2]
                    A[i, 2 * j : 2 * j + 2] \
                    = (1 / np.linalg.norm(qj - qi) ** 8) * \
                    (1 - 2 * (self.sigma / np.linalg.norm(qj - qi)) ** 6) * (qj - qi)
        # 创建右端项矩阵
        dp = -24 * self.epsilon * (self.sigma ** 6) * np.sum(A, axis = 0)
        dq = p / self.m
        return np.hstack((dp, dq))

    # 用于 stormer-verlert 迭代构造的函数
    def f_stormer(self, q):
        A = np.zeros((7, 14))
        for i in range(7):
            for j in range(7):
                if i != j:
                    qi = q[2 * i : 2 * i + 2]
                    qj = q[2 * j : 2 * j + 2]
                    A[i, 2 * j : 2 * j + 2] = \
                    (1 / np.linalg.norm(qj - qi) ** 8) \
                    * (1 - 2 * (self.sigma  / np.linalg.norm(qj - qi)) ** 6) * (qj - qi)
        # 创建右端项矩阵
        res = -24 * self.epsilon * (self.sigma ** 6) * np.sum(A, axis = 0) / self.m
        return res

    # y: 28 维数组
    # y: 0 - 14 分别表示 1-7号 原子的 动量或者速度, 注意搞清迭代获得的是速度分量还是动量
    # y: 14 - 27 分别表示 1-7号原子的 位置坐标

    # 下面程序中:
    # switch = 0 时,表示代入的前14个是动量分量
    # switch = 1 时 表示代入的前14个是速度分量

    # 势能函数
    def V(self, r):
        return 4 * self.epsilon * \
    ( (self.sigma / np.linalg.norm(r)) ** 12 - (self.sigma / np.linalg.norm(r)) ** 6 )

    # Hamiltonian 能量函数
    def H(self, y, switch = 0):
        if switch == 1:  # 将速度分量转换为动量分量
            p = self.m * y[0:14]
        else:
            p = y[0: 14]
        q = y[14:]

        # 计算总动能 ttm
        rcm = np.zeros(7)
        for i in range(7):
            rcm[i] = np.linalg.norm(p[2 * i : 2 * i + 2]) ** 2
        ttm = np.sum(rcm) / (2 * self.m)

        # 计算总势能 ttp
        rcp = np.zeros((6, 6))
        for i in range(6):
            for j in range(6):
                if i >= j:
                    rcp[i, j] = self.V(q[2 * (i+1) : 2 * (i+1) + 2]  -  q[2 * j : 2 * j + 2 ])
        ttp = np.sum(rcp)
        return ttm + ttp

    # 系统温度函数
    def temprature(self, p, switch = 0):
        if switch == 0: # 传入的是动量时, 将动量转换为速度
            v = (p / self.m)[0:14]
        else:
            v = p[0: 14]
        recv = np.zeros(7)
        for i in range(7):
            recv[i] = np.linalg.norm(v[2 * i : 2 * i + 2]) ** 2
        temprature = np.sum(recv) * (self.m / (2 * 7 * self.kB))
        return temprature

    def add_res(self, y):
        self.res.append(y)

    def get_res(self):
        return self.res
```

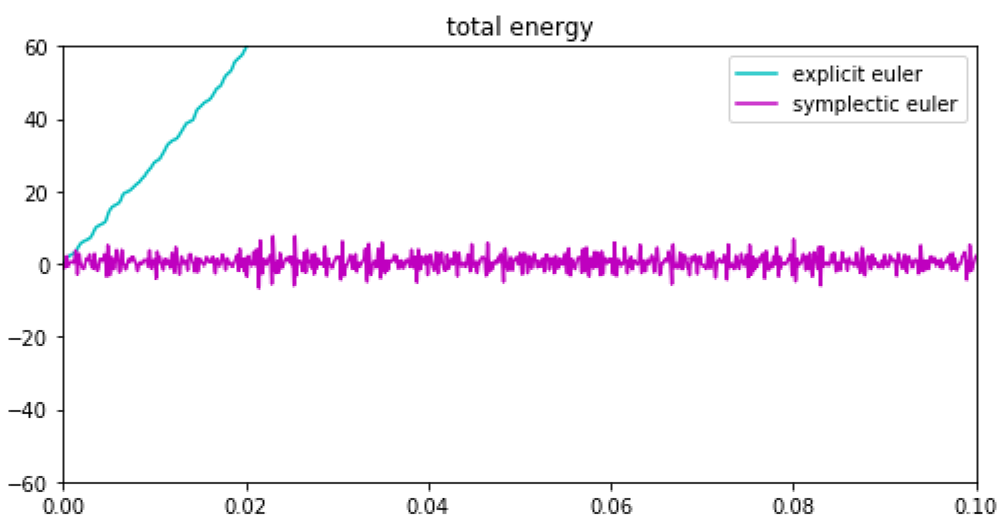
误差函数

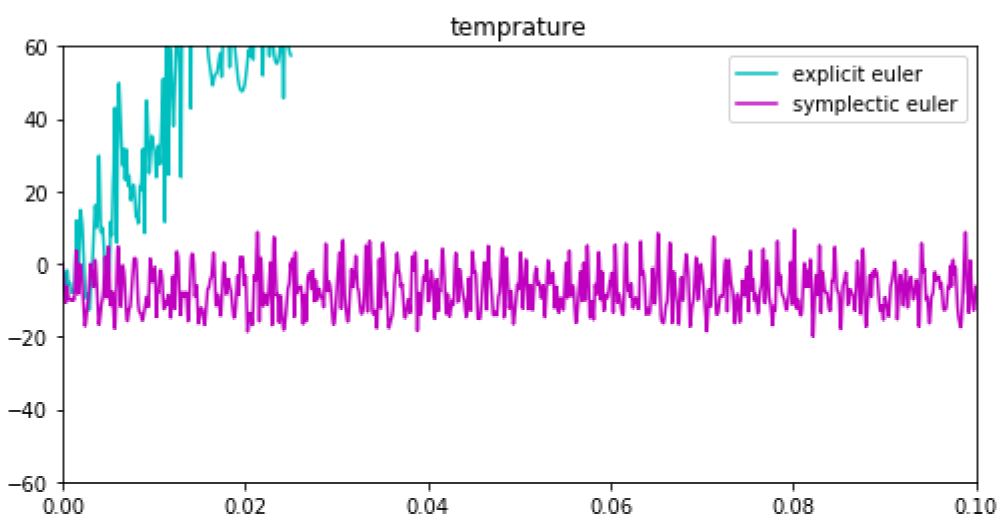
In [33]:
```python
def loss_hamiltonian(model, res, switch = 0):
    lth = len(res)
    plt_arr = np.zeros(lth)
    for i in range(lth):
        plt_arr[i] = (model.H(res[i], switch) - model.H0) / model.kB
    return plt_arr


def loss_temprature(model, res, switch = 0):
    lth = len(res)
    plt_arr = np.zeros(lth)
    for i in range(lth):
        plt_arr[i] = model.temprature(res[i], switch) - model.T0
    return plt_arr
```

测试程序1

In [34]:
```python
# 显 Euler 和 辛 Euler 的能量， 温度曲线
def md_test1():
    # 初始化 时间， 速度， 动量， 位置， 时间步长， 迭代次数
    t0 = [0, 0, 0]
    v0 = np.array([
        -30, -20,
        50, -90,
        -70, -60,
        90, 40,
        80, 90,
        -40, 100,
        -80, -60
    ], dtype = np.float64)
    p0 = (66.34 * 1e-27) * v0
    q0 = np.array([
        0.00, 0.00,
        0.02, 0.39,
        0.34, 0.17,
        0.36, -0.21,
        -0.02, -0.40,
        -0.35, -0.16,
        -0.31, 0.21
    ])
    y0 = np.hstack((p0, q0))
    h = [0.5 * 1e-6, 10 * 1e-6, 10 * 1e-6]
    epoch = [50000, 10000, 2500]

    # 显 Euler 能量计算
    md_exp_euler1 = Md_Model(t0[0], y0, h[0], epoch[0])
    t_exp_euler1 = md_exp_euler1.t_mesh()
    md_exp_res1 = explicit_euler(md_exp_euler1)
    loss_exp1 = loss_hamiltonian(md_exp_euler1, md_exp_res1)

    # 显 Euler 温度计算
    md_exp_euler2 = Md_Model(t0[2], y0, h[2], epoch[2])
    t_exp_euler2 = md_exp_euler2.t_mesh()
    md_exp_res2 = explicit_euler(md_exp_euler2)
    loss_exp2 = loss_temprature(md_exp_euler2, md_exp_res2)

    # 辛 Euler 能量， 温度计算
    md_sym_euler1 = Md_Model(t0[1], y0, h[1], epoch[1])
    t_sym_euler1 = md_sym_euler1.t_mesh()
    md_sym_res1 = symplectic_euler(md_sym_euler1)
    loss_sym1 = loss_hamiltonian(md_sym_euler1, md_sym_res1)
    loss_sym2 = loss_temprature(md_sym_euler1, md_sym_res1)

    plt.figure(figsize = (18, 4))
    ax1 = plt.subplot(121)
    ax1.plot(t_exp_euler1, loss_exp1, color = 'c', label = 'explicit euler')
    ax1.plot(t_sym_euler1, loss_sym1, color = 'm', label = 'symplectic euler')
    ax1.set_ylim(-60, 60)
    ax1.set_xlim(0, 0.1)
    ax1.legend()
    ax1.set_title('total energy')

    ax2 = plt.subplot(122)
    ax2.plot(t_exp_euler2, loss_exp2, color = 'c', label = 'explicit euler')
    ax2.plot(t_sym_euler1, loss_sym2, color = 'm', label = 'symplectic euler')
    ax2.set_ylim(-60, 60)
    ax2.set_xlim(0, 0.1)
    ax2.legend()
    ax2.set_title('temprature')

    plt.legend()
    plt.show()
```

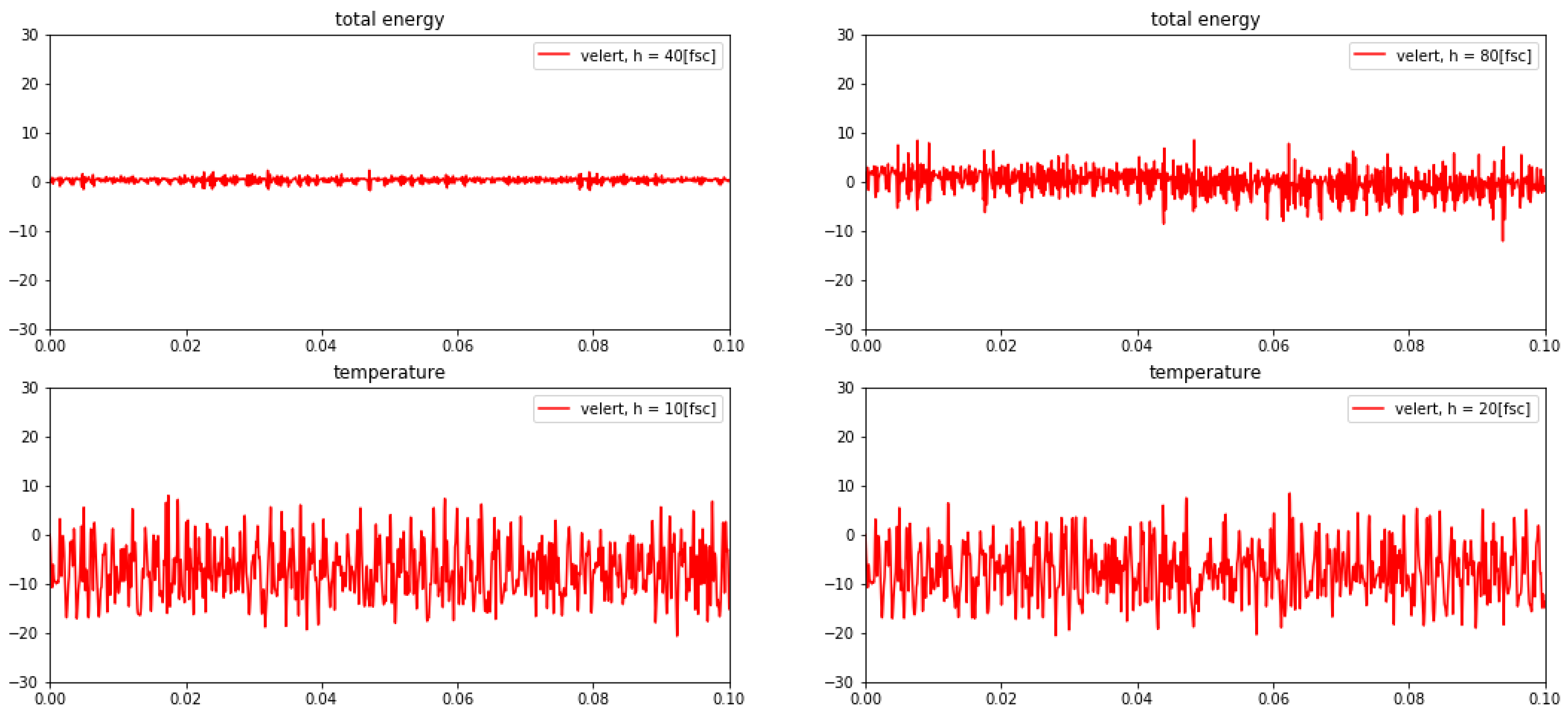
In [35]:
```python
md_test1()
```





In [36]:
```python
# sv 能量, 温度
def md_test2():

    # 初始化 时间, 速度, 位置, 时间步长, 迭代次数
    t0 = [0, 0, 0, 0]
    v0 = np.array([
        -30, -20,
        50, -90,
        -70, -60,
        90, 40,
        80, 90,
        -40, 100,
        -80, -60
    ], dtype = np.float64)
    q0 = np.array([
        0.00, 0.00,
        0.02, 0.39,
        0.34, 0.17,
        0.36, -0.21,
        -0.02, -0.40,
        -0.35, -0.16,
        -0.31, 0.21
    ])
    y0 = np.hstack((v0, q0))
    h = [40 * 1e-6, 80 * 1e-6, 10 * 1e-6, 20 * 1e-6]
    epoch = [2500, 1250, 10000, 5000]

    # sv 能量计算
    md_sv1 = Md_Model(t0[0], y0, h[0], epoch[0])
    t_sv1 = md_sv1.t_mesh()
    md_sv_res1 = stormer_verlet(md_sv1)
    loss_sv1 = loss_hamiltonian(md_sv1, md_sv_res1, 1)

    md_sv2 = Md_Model(t0[1], y0, h[1], epoch[1])
    t_sv2 = md_sv2.t_mesh()
    md_sv_res2 = stormer_verlet(md_sv2)
    loss_sv2 = loss_hamiltonian(md_sv2, md_sv_res2, 1)

    # sv 温度计算
    md_sv3 = Md_Model(t0[2], y0, h[2], epoch[2])
    t_sv3 = md_sv3.t_mesh()
    md_sv_res3 = stormer_verlet(md_sv3)
    loss_sv3 = loss_temprature(md_sv3, md_sv_res3, 1)

    md_sv4 = Md_Model(t0[3], y0, h[3], epoch[3])
    t_sv4 = md_sv4.t_mesh()
    md_sv_res4 = stormer_verlet(md_sv4)
    loss_sv4 = loss_temprature(md_sv4, md_sv_res4, 1)

    plt.figure(figsize = (18, 8))
    ax1 = plt.subplot(221)
    ax1.plot(t_sv1, loss_sv1, label = 'velert, h = 40[fsc]', color = 'r')
    ax1.legend()
    ax1.set_ylim(-30, 30)
    ax1.set_xlim(0, 0.1)
    ax1.set_title('total energy')

    ax2 = plt.subplot(222)
    ax2.plot(t_sv2, loss_sv2, label = 'velert, h = 80[fsc]',color = 'r')
    ax2.legend()
    ax2.set_ylim(-30, 30)
    ax2.set_xlim(0, 0.1)
    ax2.set_title('total energy')

    ax3 = plt.subplot(223)
    ax3.plot(t_sv3, loss_sv3, label = 'velert, h = 10[fsc]', color = 'r')
    ax3.legend()
    ax3.set_ylim(-30, 30)
    ax3.set_xlim(0, 0.1)
    ax3.set_title('temperature')

    ax4 = plt.subplot(224)
    ax4.plot(t_sv4, loss_sv4, label = 'velert, h = 20[fsc]', color = 'r')
    ax4.legend()
    ax4.set_ylim(-30, 30)
    ax4.set_xlim(0, 0.1)
    ax4.set_title('temperature')

    plt.show()
```

In [37]:
```python
md_test2()
```



高震荡问题

$Fermi - Pasta - Ulam$ **问题介绍**

考虑将 $2m$ 个质点由非线性轻弹簧以及线性硬弹簧混合连接构成的系统, 并且将端点处固定 ($q_0 = q_{2m+1} = 0$) 并且记 $p_i = \dot{q}_i$ 表示质

点的速度,则 该系统为具有如下总能量的哈密顿系统:

$$H(p,q) = \frac{1}{2}\sum_{i=1}^{m}(p_{2i-1}^2 + p_{2i}^2) + \frac{\omega^2}{4}\sum_{i=1}^{m}(q_{2i} - q_{2i-1})^2 + \sum_{i=0}^{m}(q_{2i+1} - q_{2i})^4$$

其中,需要假设 ω 较大, 自然地, 可以作变量替换如下:

$$\begin{aligned} x_{0,i} &= (q_{2i} + q_{2i-1})/\sqrt{2} \qquad & x_{1,i} &= (q_{2i} - q_{2i-1})/\sqrt{2} \\ y_{0,i} &= (p_{2i} + p_{2i-1})/\sqrt{2} \qquad & y_{1,i} &= (p_{2i} - p_{2i-1})/\sqrt{2} \end{aligned}$$

其中, $x_{0,i}$ 表示第 i 个刚性弹簧的标度位移, $x_{1,i}$ 表示第i个刚性弹簧的伸长量, $y_{0,i}$ 以及 $y_{1,i}$ 表示速度(或动量)

在上述坐标变换后的新坐标下, 运动被描述为以下哈密顿系统:

$$H(y,x) = \frac{1}{2}\sum_{i=1}^{m}(y_{0,i}^2 + y_{1,i}^2) + \frac{\omega^2}{2}\sum_{i=1}^{m} x_{1,i}^2 + \frac{1}{4}[(x_{0,1} - x_{1,1})^4 + \sum_{i=1}^{m-1}(x_{0,i+1} - x_{1,i+1} - x_{0,i} - x_{1,i})^4 + (x_{0,m} + x_{1,m})^4]$$

上述运动方程除了哈密顿能量是守恒的以外, 一般还具有一个有趣的特性:

$$I_j\ (x_{1,j}\ ,\ y_{1,j}\ ) = \frac{1}{2}(y_{1,j}^2 + \omega^2 x_{1,j}{}^2\ )$$

上式描述了第 j个刚性弹簧的能量, 上式表明, 在刚性弹簧之间具有能量的交换, 但是总能量 $I = I_1 + \cdots + I_m$ 一直保持在一个常数

实际上, 有 $I(x(t),y(t)) = I(x(0),y(0))$

经典数值积分方法的应用

当将步长h 和 高频率 ω 作乘积时, 前面所述的方法否还能正确地定性模拟系统?

线性稳定性分析:

为了得到最大容许步长, 忽略 哈密顿函数中的四次项, 则原微分方程将变为两个二维问题:

$$\begin{aligned} \dot{y}_{0,i} &= 0 \qquad & \dot{x}_{0,i} &= y_{0,i} \\ \dot{y}_{1,i} &= -\omega^2 x_{1,i} \qquad & \dot{x}_{1,i} &= y_{1,i} \end{aligned}$$

忽略下标之后, 上述微分方程的解为:

$$\begin{pmatrix} y(t) \\ \omega x(t) \end{pmatrix} = \begin{pmatrix} \cos\omega t & -\sin\omega t \\ \sin\omega t & \cos\omega t \end{pmatrix} \begin{pmatrix} y(0) \\ \omega x(0) \end{pmatrix}$$

对上述系统使用单步法获得的为:

$$\begin{pmatrix} y_{n+1} \\ \omega x_{n+1} \end{pmatrix} = M(h\omega) \begin{pmatrix} y_n \\ \omega x_n \end{pmatrix}$$

并且矩阵 $M(h\omega)$ 的特征值 λ_i 决定了数值解的长时间的行为.

数值解的稳定性需要特征值的模长不超过1

对显 $Euler$ 能量$I_n = (y_n^2 + \omega^2 x_n^2\ )\ /\ 2$ 以 $(1 + h^2\omega^2)^{n/2}$ 增长

对隐 $Euler$ 能量 以 $(1 + h^2\omega^2)^{-n/2}$ 衰减

对于隐中点法, 由于矩阵 $M(h\omega)$ 正交, 因此, 能够将 I_n 在任意时刻精确保持.

对于辛$Euler$方法以及 SV 方法, 有:

$$M(h\omega) = \begin{pmatrix} 1 & -h\omega \\ h\omega & 1 - h^2\omega^2 \end{pmatrix} \qquad M(h\omega) = \begin{pmatrix} 1 - \dfrac{h^2\omega^2}{2} & -\dfrac{h\omega}{2}(1 - \dfrac{h^2\omega^2}{4}) \\ \dfrac{h\omega}{2} & 1 - \dfrac{h^2\omega^2}{2} \end{pmatrix}$$

上述两个方程组的特征多项式均为 $\lambda^2 - (2 - h^2\omega^2)\lambda + 1$,因此特征值的模长小于等于1当且仅当$|h\omega| \leq 2$

$Fermi - Pasta - Ulam$ 问题数值实验

分别利用 隐中点,辛$Euler$法, SV 方法 求解上述系统两次, 两次步长分别取为 $h = 0.001, h = 0.03$ 在 $t \in [0,200]$上进行求解

(即分别迭代200000 , 6667次), 其余参数如下设置:

$\omega = 50$

$x_{0,1}(0) = 1, \qquad y_{0,1}(0) = 1, \qquad x_{1,1}(0) = \omega^{-1} = 0.02, \qquad y_{1,1}(0) = 1$

其余均设置为 0

改写原系统如下:

$$\begin{cases} \dot{y} = -RHS \\ \dot{x} = y \end{cases}$$

模型参数

In [38]:
```python
class Fpu_Model:
    def __init__(self, t0, y0, h, omega, epoch, N = 3):     # N: 硬弹簧个数
        self.t0 = t0
        self.y0 = y0
        self.h = h
        self.omega = omega
        self.epoch = epoch
        self.res = [self.y0]
        self. N = N

    def t_mesh(self):
        end = self.t0 + self.epoch * self.h
        t = np.linspace(self.t0, end, self.epoch + 1)
        return t

    # 一般的一阶数系统的右端函数
    def f(self, z):     # z : 长度为 12 的数组
        y = z[0 : 6]
        x = z[6 : ]
        vec = np.array([
            [0, x[1], 0, x[3], 0, x[5]],
            [1, -1, 0, 0, 0, 0],
            [0, 0, 0, 0, 1, 1],
            [1, 1, -1, 1, 0, 0],
            [0, 0, 1, 1, -1, 1]
        ], dtype = np.float64)
        # 编写 y 导数的右端项
        dy = self.omega**2 * vec[0] + (x[0] - x[1])**3 * vec[1] + (x[4] + x[5])**3 * vec[2] \
        + (x[0] + x[1] + x[3] - x[2])**3 * vec[3] + (x[2] + x[3] + x[5] - x[4])**3 * vec[4]
        dx = y
        return np.hstack((-dy, dx))

    # 用于 stormer-verlert 迭代构造的函数
    def f_stormer(self, x):
        vec = np.array([
            [0, x[1], 0, x[3], 0, x[5]],
            [1, -1, 0, 0, 0, 0],
            [0, 0, 0, 0, 1, 1],
            [1, 1, -1, 1, 0, 0],
            [0, 0, 1, 1, -1, 1]
        ], dtype = np.float64)
        # 编写 y 导数的右端项
        dy = self.omega**2 * vec[0] + (x[0] - x[1])**3 * vec[1] + (x[4] + x[5])**3 * vec[2] \
        + (x[0] + x[1] + x[3] - x[2])**3 * vec[3] + (x[2] + x[3] + x[5] - x[4])**3 * vec[4]
        return -dy

    # z : 12 维数组, z前6个位置表示y分量, z后六个位置表示z分量
    # I
    # pos : 0 - 2
    def I_part(self, z, pos):
        y = z[0 : 6]
        x = z[6 : ]
        return 0.5 * (y[2 * pos + 1]**2 + self.omega**2 * x[2 * pos + 1]**2)

    def add_res(self, y):
        self.res.append(y)

    def get_res(self):
        return self.res
```

测试程序:

In [39]:

```python
def draw_fpu(ax, model, numeric, t_mesh):
    len_numeric  = len(numeric)
    I = np.zeros((3, len_numeric))

    color_markers = ['m', 'g', 'c']
    for i in range(len_numeric):
        for j in range(3):
            I[j, i] = model.I_part(numeric[i], j)
    I_tt = np.sum(I, axis = 0)

    for i in range(3):
        ax.plot(t_mesh, I[i, :], color = color_markers[i])
    ax.plot(t_mesh, I_tt, color = 'orange')


def fpu_test():
    # 初始化
    omega = 50
    t0 = 0
    x0 = np.array([1, omega ** (-1), 0, 0, 0, 0])
    y0 = np.array([1, 1, 0, 0, 0, 0])
    z0 = np.hstack((y0, x0))
    h = [0.001, 0.03]
    epoch = [200000, 6667]

    fpu_impmidp1 = Fpu_Model(t0, z0, h[0], omega, epoch[0])
    t_mesh1 = fpu_impmidp1.t_mesh()
    fpu_impmidp_res1 = implicit_midpoint(fpu_impmidp1)

    fpu_symp1 = Fpu_Model(t0, z0, h[0], omega, epoch[0])
    fpu_symp_res1 = symplectic_euler(fpu_symp1)

    fpu_sv1 = Fpu_Model(t0, z0, h[0], omega, epoch[0])
    fpu_sv_res1 = stormer_verlet(fpu_sv1)

    fpu_impmidp2 = Fpu_Model(t0, z0, h[1], omega, epoch[1])
    t_mesh2 = fpu_impmidp2.t_mesh()
    fpu_impmidp_res2 = implicit_midpoint(fpu_impmidp2)

    fpu_symp2 = Fpu_Model(t0, z0, h[1], omega, epoch[1])
    fpu_symp_res2 = symplectic_euler(fpu_symp2)

    fpu_sv2 = Fpu_Model(t0, z0, h[1], omega, epoch[1])
    fpu_sv_res2 = stormer_verlet(fpu_sv2)

    plt.figure(figsize = (18, 8))
    ax1 = plt.subplot(231)
    draw_fpu(ax1, fpu_impmidp1, fpu_impmidp_res1, t_mesh1)
    ax1.set_xlim(0, 200)
    ax1.set_title('implict mid-point h = 0.001')

    ax2 = plt.subplot(232)
    draw_fpu(ax2, fpu_symp1, fpu_symp_res1, t_mesh1)
    ax2.set_xlim(0, 200)
    ax2.set_title('symplectic euler h = 0.001')

    ax3 = plt.subplot(233)
    draw_fpu(ax3, fpu_sv1, fpu_sv_res1, t_mesh1)
    ax3.set_xlim(0, 200)
    ax3.set_title('stormer-verlet h = 0.001')

    ax4 = plt.subplot(234)
    draw_fpu(ax4, fpu_impmidp2, fpu_impmidp_res2, t_mesh2)
    ax4.set_xlim(0, 200)
    ax4.set_title('implict mid-point h = 0.3')

    ax5 = plt.subplot(235)
    draw_fpu(ax5, fpu_symp2, fpu_symp_res2, t_mesh2)
    ax5.set_xlim(0, 200)
    ax5.set_title('symplectic euler h = 0.3')

    ax6 = plt.subplot(236)
    draw_fpu(ax6, fpu_sv2, fpu_sv_res2, t_mesh2)
    ax6.set_xlim(0, 200)
    ax6.set_title('stormer-verlet h = 0.3')
```

In [40]:

```python
fpu_test()
```