24-623/12-623 HW#2 Solutions

1. (10 points) (a) (i)

$$\begin{aligned}
\frac{\partial|\mathbf{p}_i|^2}{\partial\mathbf{p}_i} &= \frac{\partial}{\partial\mathbf{p}_i}(p_{i,x}^2+p_{i,y}^2+p_{i,z}^2)\\
&= \frac{\partial}{\partial p_{i,x}}(p_{i,x}^2+p_{i,y}^2+p_{i,z}^2)\mathbf{i}+\frac{\partial}{\partial p_{i,y}}(p_{i,x}^2+p_{i,y}^2+p_{i,z}^2)\mathbf{j}+\frac{\partial}{\partial p_{i,z}}(p_{i,x}^2+p_{i,y}^2+p_{i,z}^2)\mathbf{k}\\
&= 2p_{i,x}\mathbf{i}+2p_{i,y}\mathbf{j}+2p_{i,z}\mathbf{k}\\
&= 2\mathbf{p}_i.
\end{aligned}$$

So that

$$\frac{1}{2m_i}\frac{\partial|\mathbf{p}_i|^2}{\partial\mathbf{p}_i}=\left(\frac{1}{2m_i}\right)(2\mathbf{p}_i)=\frac{\mathbf{p}_i}{m_i}.$$

(ii)

$$\begin{aligned}
\frac{\partial r_{ij}}{\partial\mathbf{r}_i} &= \frac{\partial}{\partial\mathbf{r}_i}[(r_{i,x}-r_{j,x})^2+(r_{i,y}-r_{j,y})^2+(r_{i,z}-r_{j,z})^2]^{1/2}\\
&= \frac{\partial}{\partial r_{i,x}}[(r_{i,x}-r_{j,x})^2+(r_{i,y}-r_{j,y})^2+(r_{i,z}-r_{j,z})^2]^{1/2}\mathbf{i}\\
&+ \frac{\partial}{\partial r_{i,y}}[(r_{i,x}-r_{j,x})^2+(r_{i,y}-r_{j,y})^2+(r_{i,z}-r_{j,z})^2]^{1/2}\mathbf{j}\\
&+ \frac{\partial}{\partial r_{i,z}}[(r_{i,x}-r_{j,x})^2+(r_{i,y}-r_{j,y})^2+(r_{i,z}-r_{j,z})^2]^{1/2}\mathbf{k}\\
&= \frac{1}{2[\cdot]}2(r_{i,x}-r_{j,x})\mathbf{i}+\frac{1}{2[\cdot]}2(r_{i,y}-r_{j,y})\mathbf{j}+\frac{1}{2[\cdot]}2(r_{i,z}-r_{j,z})\mathbf{k}\\
&= \frac{1}{r_{ij}}(r_{ij,x}\mathbf{i}+r_{ij,y}\mathbf{j}+r_{ij,z}\mathbf{k})\\
&= \frac{\mathbf{r}_{ij}}{r_{ij}}
\end{aligned}$$

(iii) The Hamiltonian equations of motion are:

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{p}_i \text{ and } \frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i.$$

The total system momentum is

$$\mathbf{p}_{tot} = \sum_i \mathbf{p}_i$$

and we want to show that $\frac{d\mathbf{p}_{tot}}{dt} = \mathbf{0}$. The solution is as follows:

$$\begin{aligned} \frac{d\mathbf{p}_{tot}}{dt} &= \frac{d}{dt}\sum_i \mathbf{p}_i \\ &= \sum_i \frac{d\mathbf{p}_i}{dt} \\ &= \sum_i \mathbf{F}_i. \end{aligned}$$

If there are no external forces acting on the system, then by Newton's 3rd law, all the forces must balance so that

$$\frac{d\mathbf{p}_{tot}}{dt} = \sum_i \mathbf{F}_i = \mathbf{0}.$$

(b) Consider a Taylor series expansion around $v_{i,x}(t+\Delta t)$ with a step of $(-\Delta t/2)$:

$$v_{i,x}(t+\Delta t/2) = v_{i,x}(t+\Delta t) + \left.\frac{dv_{i,x}}{dt}\right|_{t+\Delta t}\left(-\frac{\Delta t}{2}\right).$$

Subbing in $\frac{dv_{i,x}}{dt} = \frac{F_{i,x}}{m_i}$ gives

$$v_{i,x}(t+\Delta t/2) = v_{i,x}(t+\Delta t) - \frac{F_{i,x}(t+\Delta t)}{m_i}\left(\frac{\Delta t}{2}\right),$$

which can be rearranged to

$$v_{i,x}(t+\Delta t) = v_{i,x}(t+\Delta t/2) + \frac{F_{i,x}(t+\Delta t)}{m_i}\left(\frac{\Delta t}{2}\right).$$

2. (20 points) (a) The Hamiltonian is

$$H = U + K \quad = \quad U_s + \frac{p^2}{2m} = U_s + \frac{p^2}{2}.$$

The x equation of motion is

$$\dot{x} = \frac{\partial H}{\partial p} = p.$$

The p equation of motion is

$$\dot{p} = -\frac{\partial H}{\partial x} = -\frac{\partial U_s}{\partial x}.$$

Taking the time derivative of the x equation and substituting into the p equation gives the second order equation

$$\ddot{x} = -\frac{\partial U_s}{\partial x}.$$

(b) The equation of motion is

$$\ddot{x} + x = 0,$$

which has a general solution of the form

$$x(t) = A\cos t + B\sin t.$$

With initial conditions x_0 and v_0, the solution will be

$$x(t) = x(0)\cos t + v(0)\sin t,$$

which for the given initial conditions reduces to

$$\begin{aligned} x(t) &= \sqrt{2}\sin t \\ v(t) &= \sqrt{2}\cos t. \end{aligned}$$

See the attached plot.

The total energy of the system is

$$E = \Phi + K = \frac{x^2}{2} + \frac{v^2}{2} = \frac{2\sin^2 t}{2} + \frac{2\cos^2 t}{2} = \sin^2 t + \cos^2 t = 1,$$

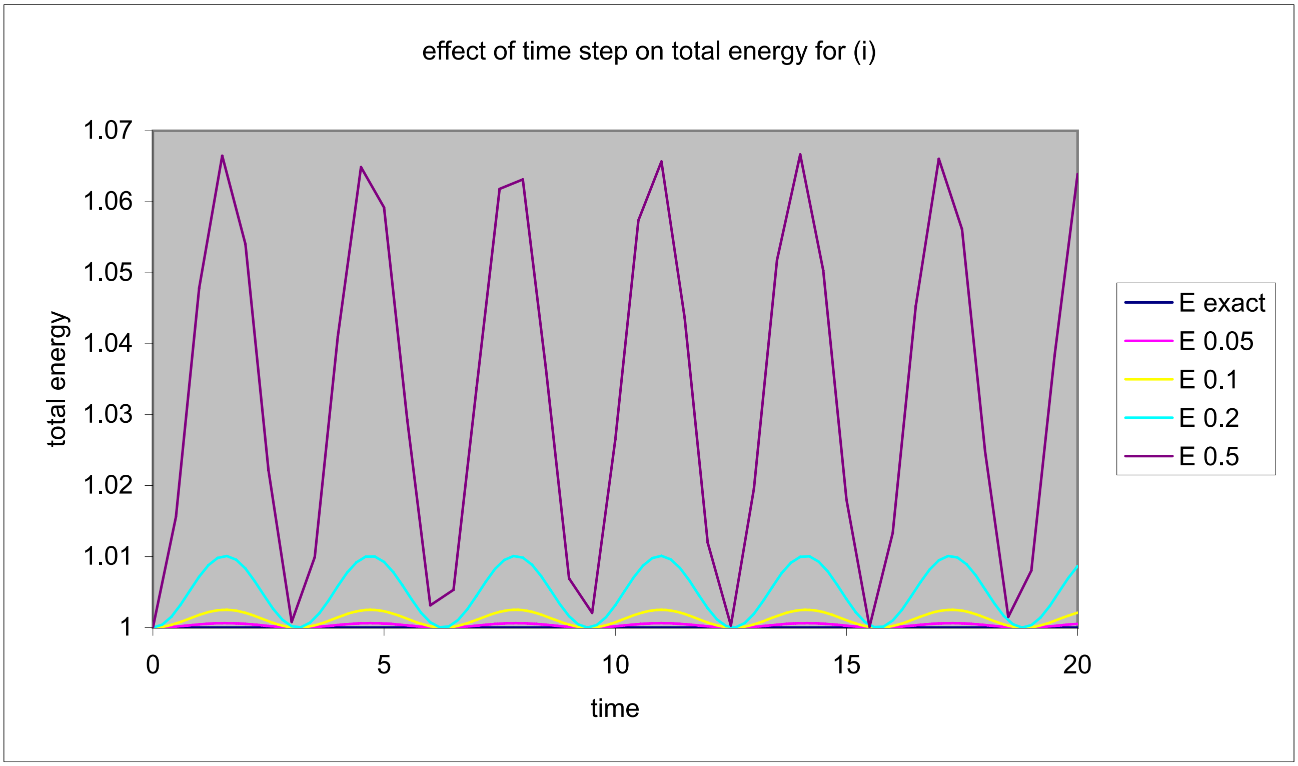
which is a constant.

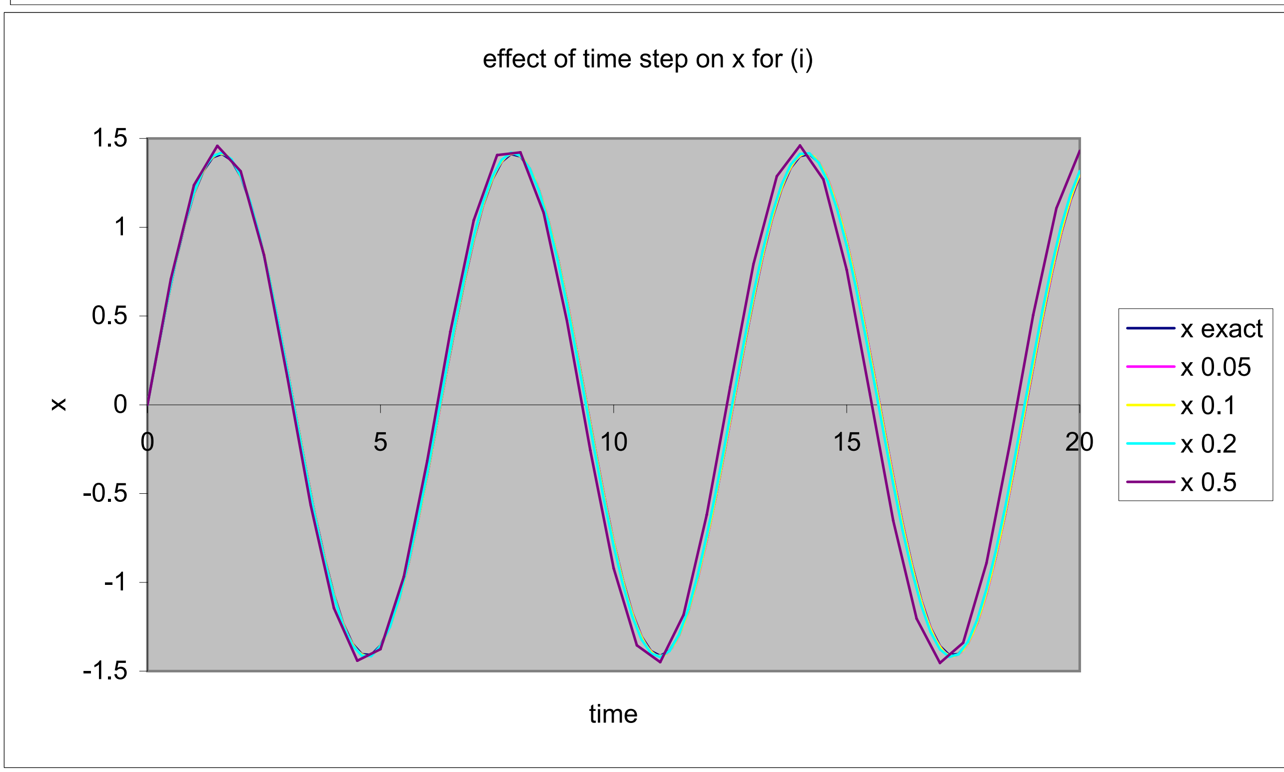
Momentum is not conserved because while we are considering forces on the wall, we are not modeling its dynamics (it is assumed to have infinite mass and be stationary).

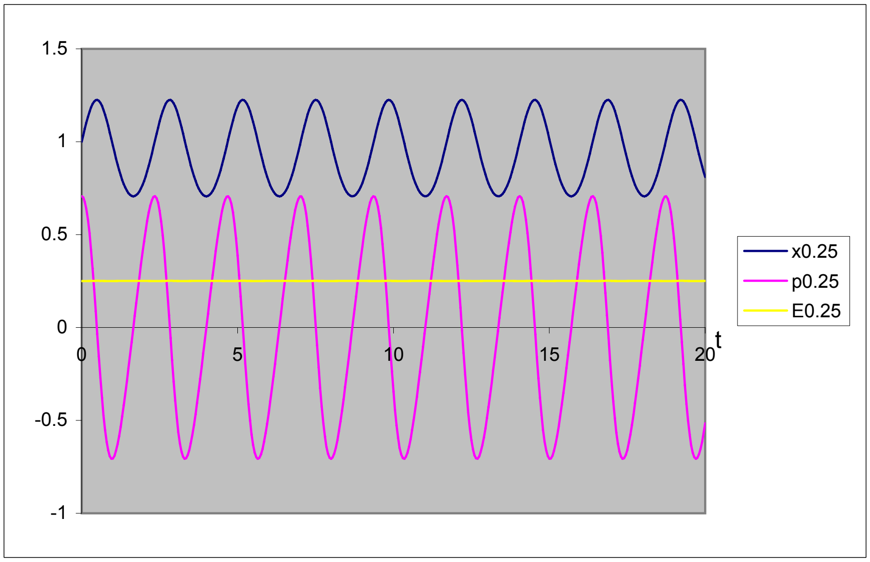
(c) See the attached plots. In one of the plots, the effect of the time step is shown. I chose 0.05 to be a suitable step (1/20 of the period of oscillation). For this time step, energy is conserved to within less than 0.1% of the total value and the numerical solution lies on top of the analytical solution.

(d) See the attached plots. I found that 0.05 was still a suitable time step. For all cases, the solution is periodic, although the motion is more complicated that the simple oscillator of (i). Note that we can only access one side of the energy surface when $E = 0.25$ for a given initial condition. To fully explore the $E = 0.25$ energy surface, more than one initial condition must be considered. By plotting the solutions points for one period of oscillation with the potential, we can see the extent of the potential well explored for each of the different energies.

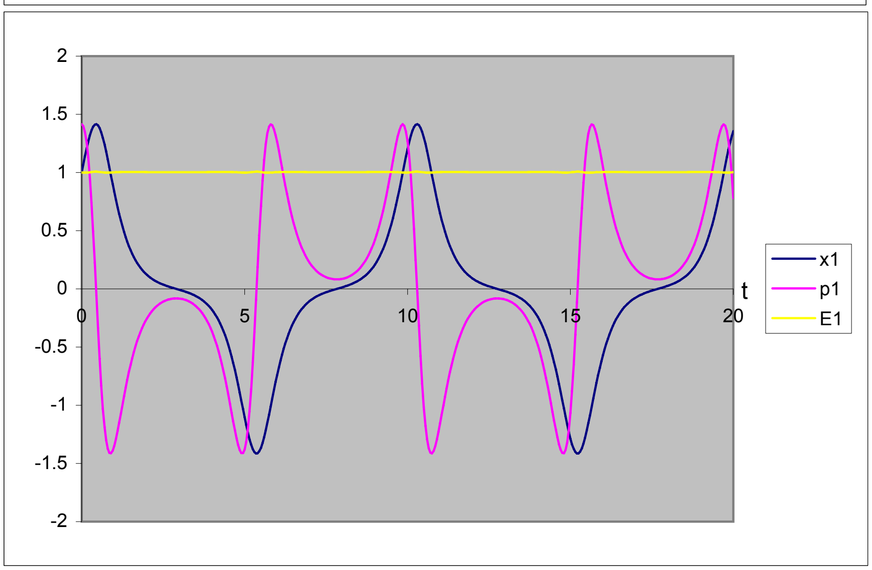
3. (20 points) See the attached plots of momenta and energies run over 2 units of dimensionless time.


effect of time step on total energy for (i)
total energy
1.07
1.06
1.05
1.04
1.03
1.02
1.01
1
0
5
10
15
20
time
E exact
E 0.05
E 0.1
E 0.2
E 0.5

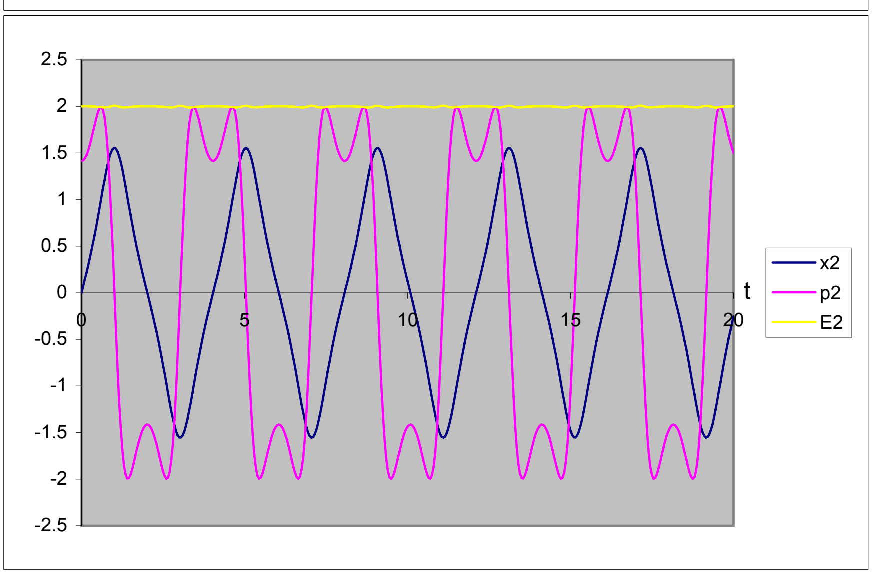

effect of time step on x for (i)
x
1.5
1
0.5
0
-0.5
-1
-1.5
0
5
10
15
20
time
x exact
x 0.05
x 0.1
x 0.2
x 0.5



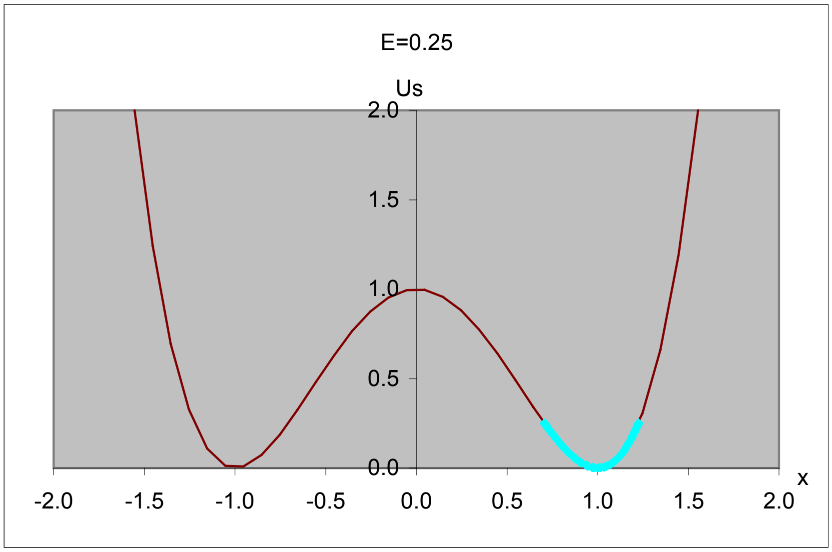
1.5
1
0.5
0
-0.5
-1
0
5
10
15
20
t
x0.25
p0.25
E0.25

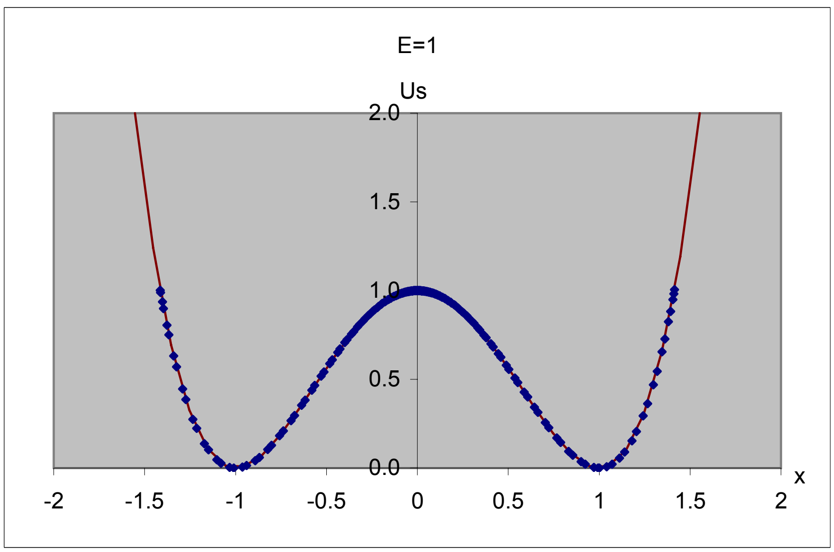


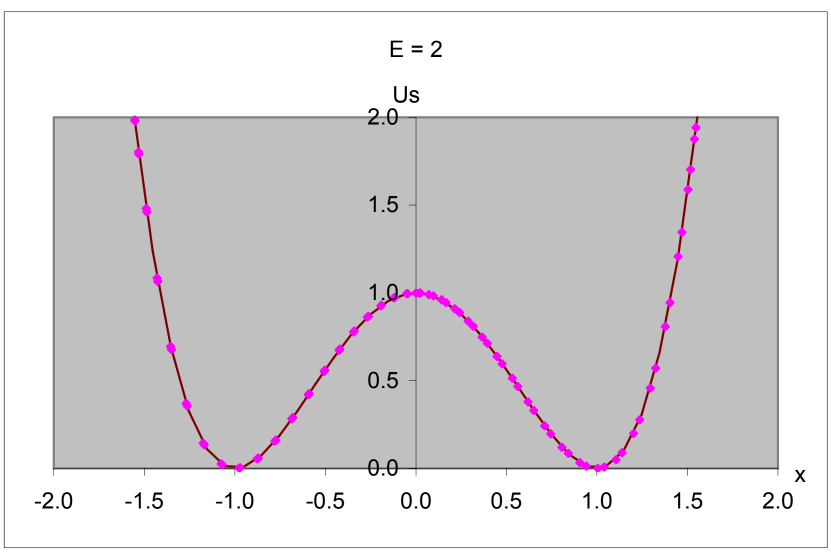
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
0
5
10
15
20
t
x1
p1
E1

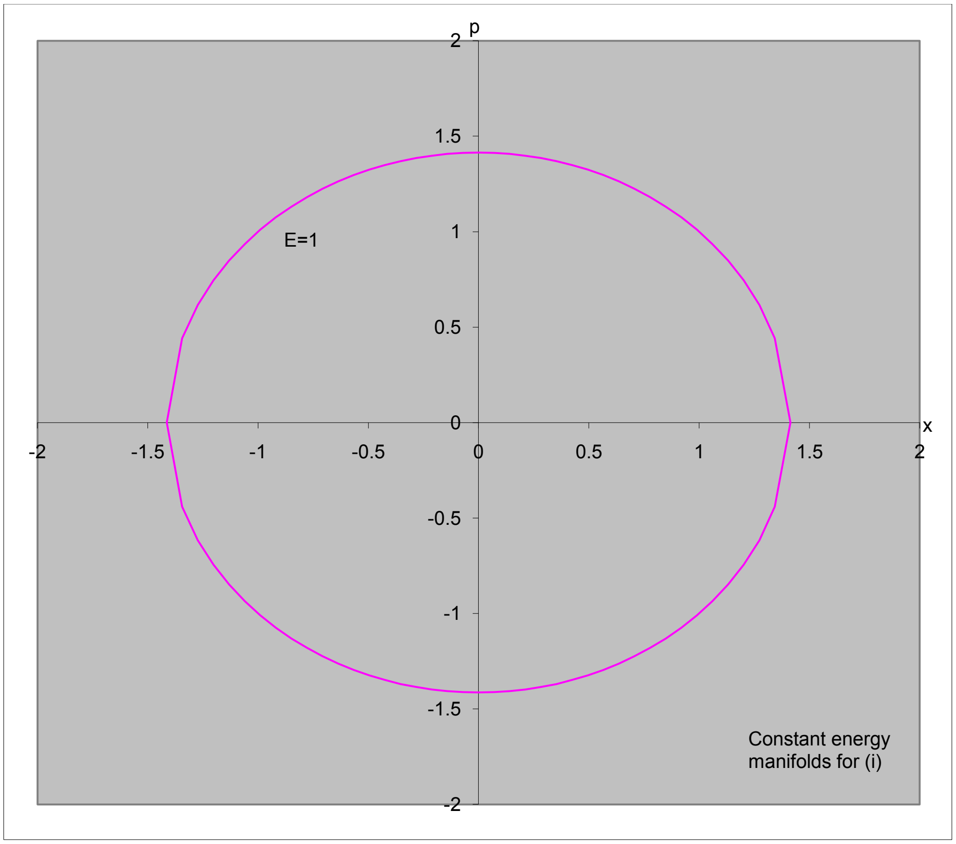


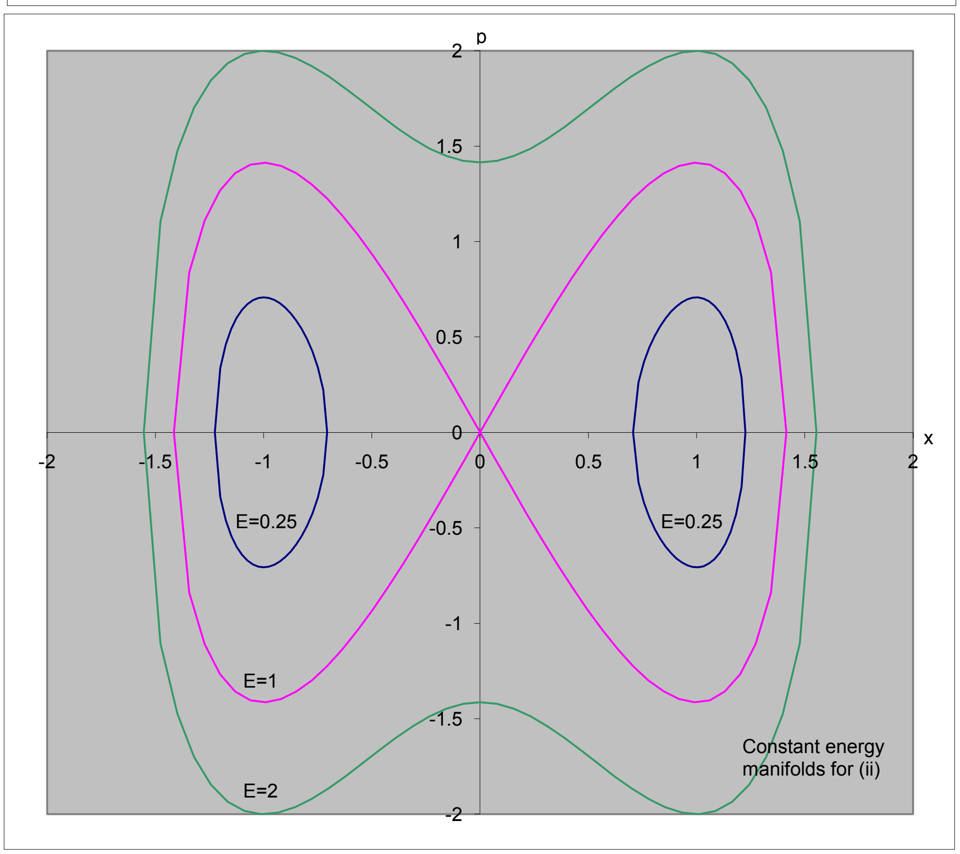
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
0
5
10
15
20
t
x2
p2
E2

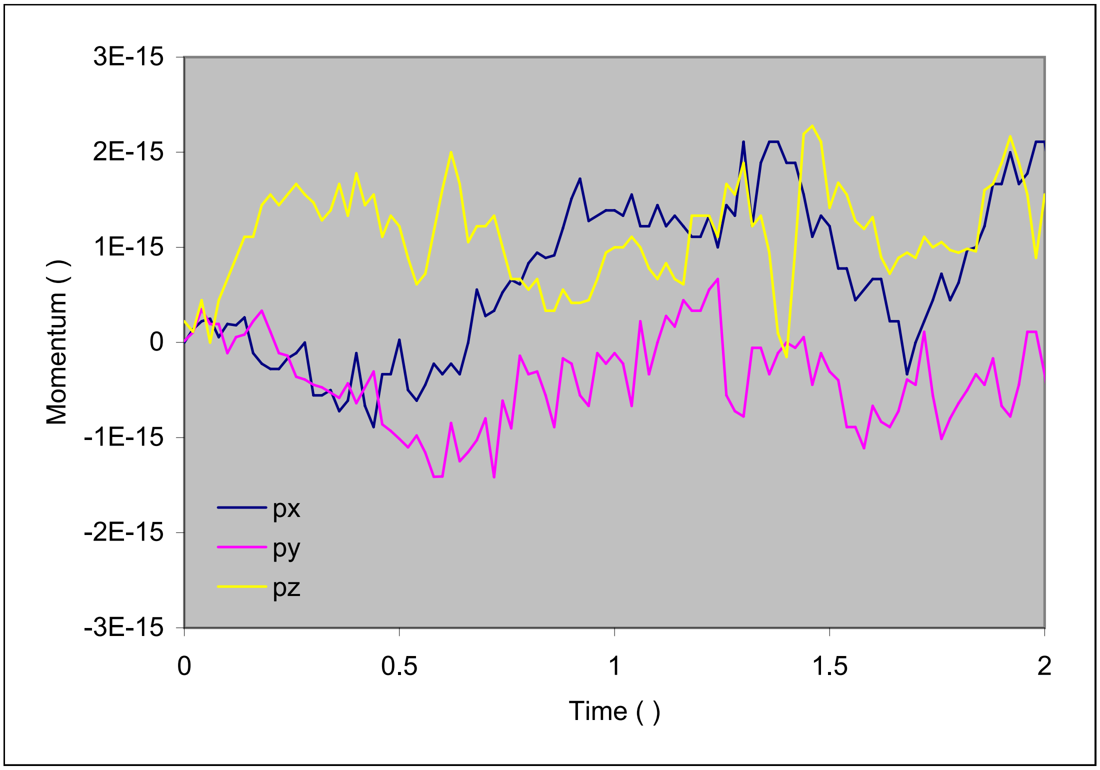

E=0.25
Us
2.0
1.5
1.0
0.5
0.0
x
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0

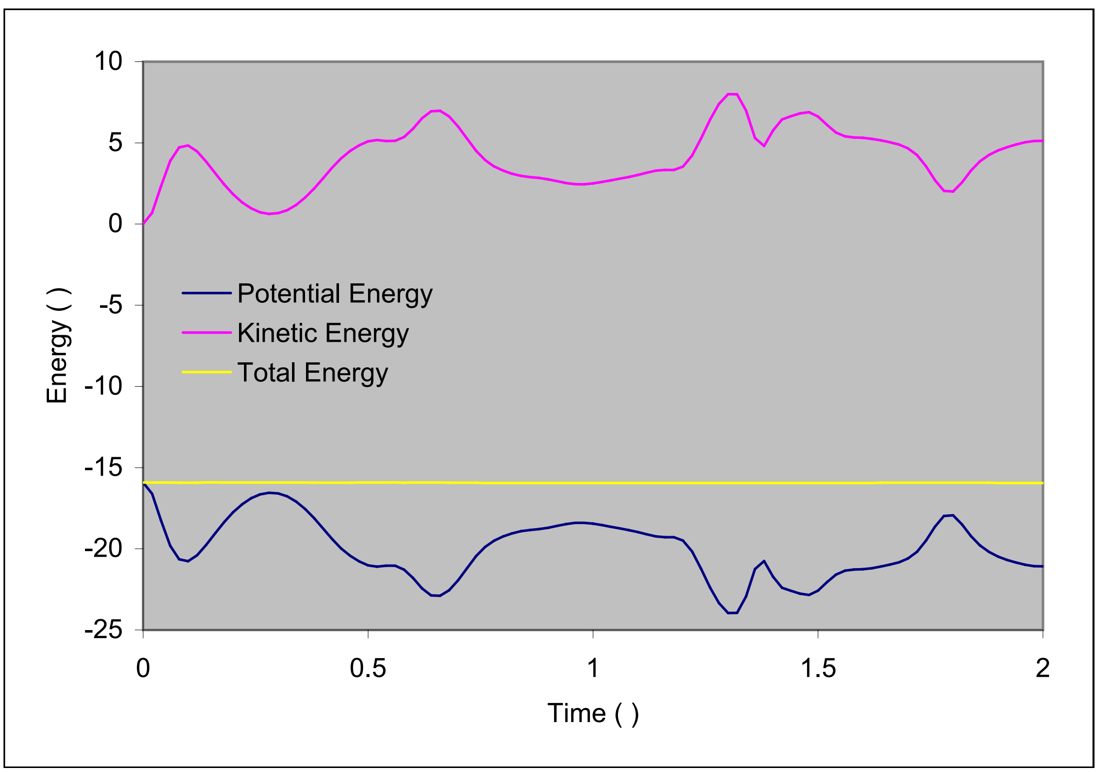

E=1
Us
2.0
1.5
1.0
0.5
0.0
x
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2


E = 2
Us
2.0
1.5
1.0
0.5
0.0
x
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0


p
x
E=1
Constant energy
manifolds for (i)


p
x
E=0.25
E=0.25
E=1
E=2
Constant energy
manifolds for (ii)


3E-15
2E-15
1E-15
0
-1E-15
-2E-15
-3E-15
Momentum ( )
px
py
pz
0
0.5
1
1.5
2
Time ( )


10
5
0
-5
-10
-15
-20
-25
Energy ( )
Potential Energy
Kinetic Energy
Total Energy
0
0.5
1
1.5
2
Time ( )