PHY 514 Homework 3

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1 Molecular Dynamics

1.1 Code

I used the lj_start.py code from canvas. The Lennard-Jones potential used in the code is given by,

$$U(r) = \frac{-4}{r^6}\left(1 - \frac{1}{r^6}\right). \tag{1}$$

The force is then given by,

$$F(r) = -\frac{dU}{dr} = 24r^{-7} - 48r^{-13} = \frac{24}{r^7}\left(1 - \frac{2}{r^6}\right). \tag{2}$$

This is the "missing force calculation" that I will be inserting into the given code.

1.2 Integrator

I implemented the velocity Verlet algorithm under a function called "verlet" that I added to lj_start.py. The function works as follows: * Advance the positions one time step using equation (1). * Calculate the force on the particles using the "compute_forces" function using the new positions. Temporarily save the old forces for use in equation (2). * Advance the velocities one time step using equation (2).

```
In [1]: import numpy as np
        import matplotlib.pyplot as plt
        from numpy import genfromtxt
        import lj
        %matplotlib inline
```

```
In [40]: Nx = 6
         Ny = 6
         L = 5.
         rcut = 2.5
         Nstep = 10000
         lj.run(Nx,Ny,L,rcut,Nstep)
```

```
In [41]: xpos = genfromtxt("xpositions.dat",delimiter=",")
         ypos = genfromtxt("ypositions.dat",delimiter=",")
         xvel = genfromtxt("xvelocities.dat",delimiter=",")
```

```
yvel = genfromtxt("yvelocities.dat",delimiter=",")
energy = genfromtxt("energies.dat",delimiter=",")
solid_corr=genfromtxt("correlation.dat",delimiter=",")
```

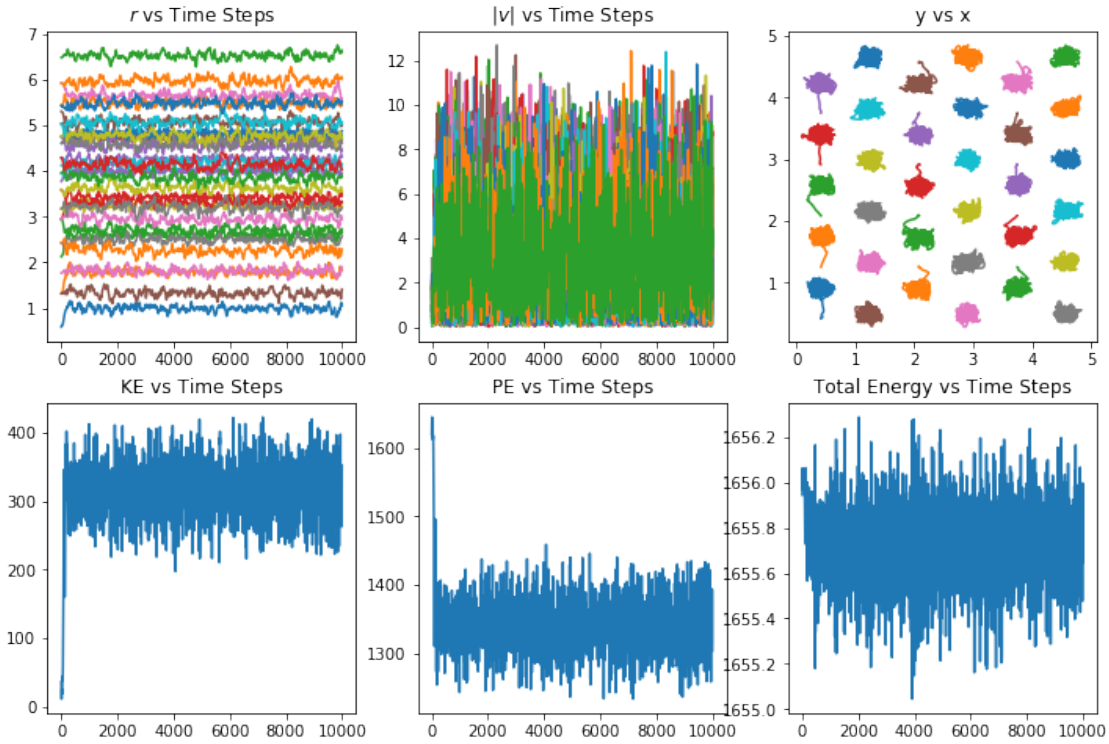
In [58]:
```
particle = [0,1,2,3,4,6,7,8,9,10,11,13,14,15,16,17,18,19,20,21,22,23,25,26,27,28,29,30,
start = 0
N = 9999
step = np.arange(len(xpos[start:N,particle[0]]))

# initialize figures
fig, axes = plt.subplots(nrows=2,ncols=3,figsize=(12,8))

# plot coordinates
for i in range(len(particle)):
    axes[0][0].plot(step,np.sqrt(xpos[start:N,particle[i]]**2\
                    +ypos[start:N,particle[i]]**2))
for i in range(len(particle)):
    axes[0][1].plot(step,np.sqrt(xvel[start:N,particle[i]]**2\
                    +yvel[start:N,particle[i]]**2))
for i in range(len(particle)):
    axes[0][2].plot(xpos[start:N,particle[i]],ypos[start:N,particle[i]])
for i in range(3):
    axes[1][i].plot(step,energy[start:N,i])

# Titles
axes[0][0].set_title("$r$ vs Time Steps")
axes[0][1].set_title("$|v|$ vs Time Steps")
axes[0][2].set_title("y vs x")
axes[1][0].set_title("KE vs Time Steps")
axes[1][1].set_title("PE vs Time Steps")
axes[1][2].set_title("Total Energy vs Time Steps")
```

Out[58]:
```
<matplotlib.text.Text at 0x13fad6908>
```



We can see from the energy plot that the Verlet algorithm is doing is indeed keeping the total energy relatively constant. Over 10^4 time steps, the energy stays at 1655.7 ± 0.7.

1.3 Measurements

We can see that the system above is clearly a solid from the "y vs x" plot. All of the particles stay near their relative positions, never straying far from their lattice points. Note that I have excluded a few points that were crossing over the boundary because their connecting lines were blocking the other points. To reduce the density of the system, I will reduce the number of particles (making it less computationally intensive as I move away from a solid).

```
In [5]: Nx = 3
        Ny = 4
        L = 5.
        rcut = 2.5
        Nstep = 10000
        lj.run(Nx,Ny,L,rcut,Nstep)

In [6]: xpos = genfromtxt("xpositions.dat",delimiter=",")
        ypos = genfromtxt("ypositions.dat",delimiter=",")
        xvel = genfromtxt("xvelocities.dat",delimiter=",")
        yvel = genfromtxt("yvelocities.dat",delimiter=",")
        energy = genfromtxt("energies.dat",delimiter=",")
        fluid_corr=genfromtxt("correlation.dat",delimiter=",")
```

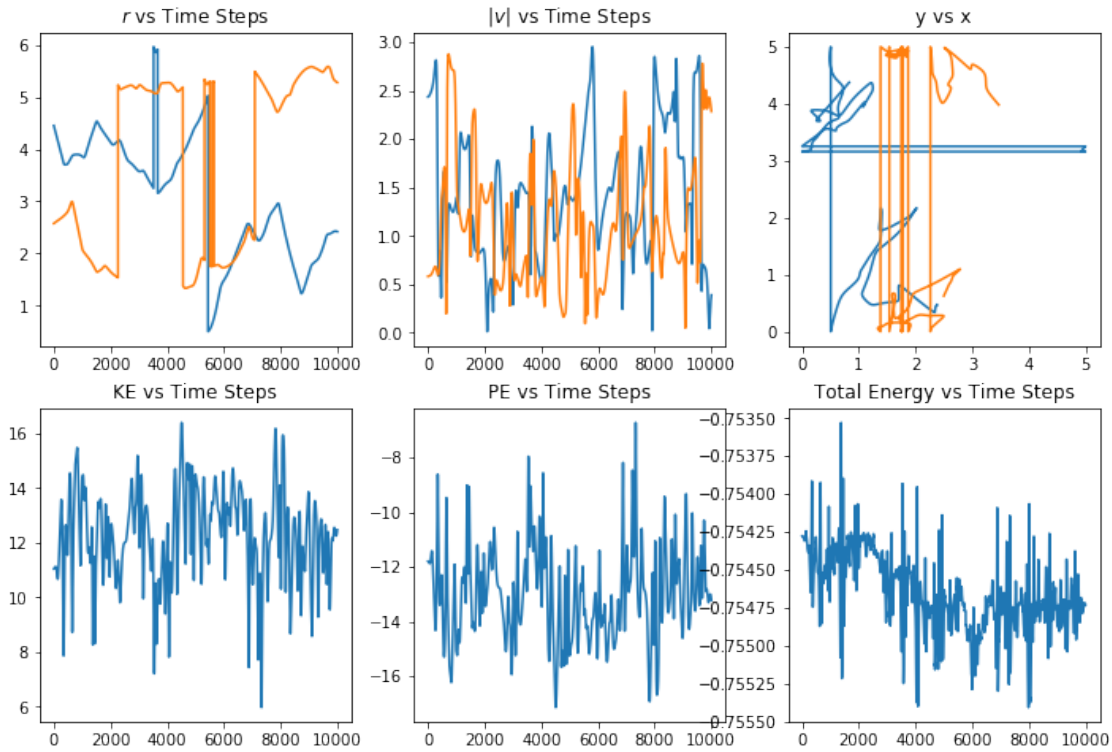
In [7]:
```
particle = [3,4]
start = 0
N = 9999
step = np.arange(len(xpos[start:N,particle[0]]))

# initialize figures
fig, axes = plt.subplots(nrows=2,ncols=3,figsize=(12,8))

# plot coordinates
for i in range(len(particle)):
    axes[0][0].plot(step,np.sqrt(xpos[start:N,particle[i]]**2\
                    +ypos[start:N,particle[i]]**2))
for i in range(len(particle)):
    axes[0][1].plot(step,np.sqrt(xvel[start:N,particle[i]]**2\
                    +yvel[start:N,particle[i]]**2))
for i in range(len(particle)):
    axes[0][2].plot(xpos[start:N,particle[i]],ypos[start:N,particle[i]])
for i in range(3):
    axes[1][i].plot(step,energy[start:N,i])

# Titles
axes[0][0].set_title("$r$ vs Time Steps")
axes[0][1].set_title("$|v|$ vs Time Steps")
axes[0][2].set_title("y vs x")
axes[1][0].set_title("KE vs Time Steps")
axes[1][1].set_title("PE vs Time Steps")
axes[1][2].set_title("Total Energy vs Time Steps")
```

Out[7]:
```
<matplotlib.text.Text at 0x10f06c2b0>
```



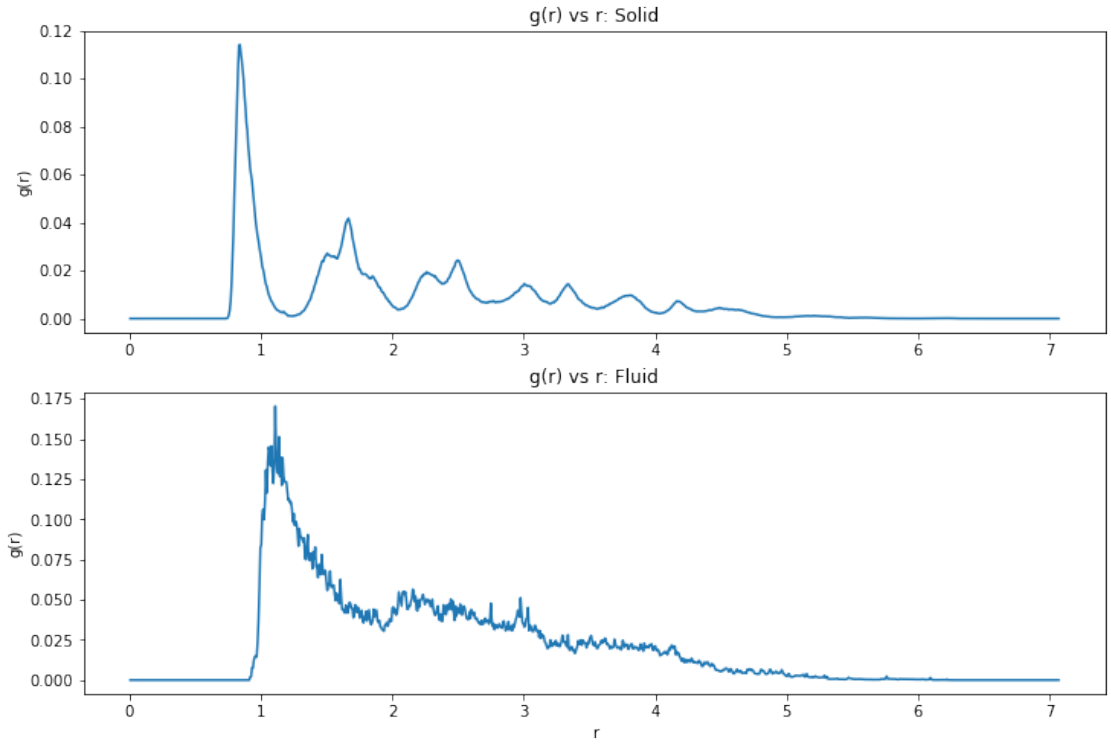
Above, we can observe two of the particles to see that they are no longer restricted to their lattice sites. By reducing the number of particles from 36 to 12, we have seen the phase change to a fluid.

1.4 Measurements(II)

The angle integrated pair correlation functions for both cases above were saved. They are compared below.

```
In [59]: fig, axes = plt.subplots(nrows=2,ncols=1,figsize=(12,8))
         axes[0].plot(solid_corr[0],solid_corr[1])
         axes[0].set_title("g(r) vs r: Solid")
         axes[0].set_ylabel("g(r)")
         axes[1].plot(fluid_corr[0],fluid_corr[1])
         axes[1].set_title("g(r) vs r: Fluid")
         axes[1].set_xlabel("r")
         axes[1].set_ylabel("g(r)")

Out[59]: <matplotlib.text.Text at 0x1405d1d30>
```



Note that these are time averaged over all time steps. The correlation function measures the average density of particles in an annulus of width dr from any particle. With this understanding, we can make sense of the correlation functions above. Both exhibit strong repulsion at short distances since $g(r) = 0$ for values less than about 1. However, the solid correlation function (top) exhibits periodic density peaks due to its lattice structure. The fluid correlation function does not exhibit such behavior, and has a more or less monotonic decrease as r increases. This shows the homogenous structure of the fluid.