MechE 416 HW 1

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1 Data analysis and property calculation

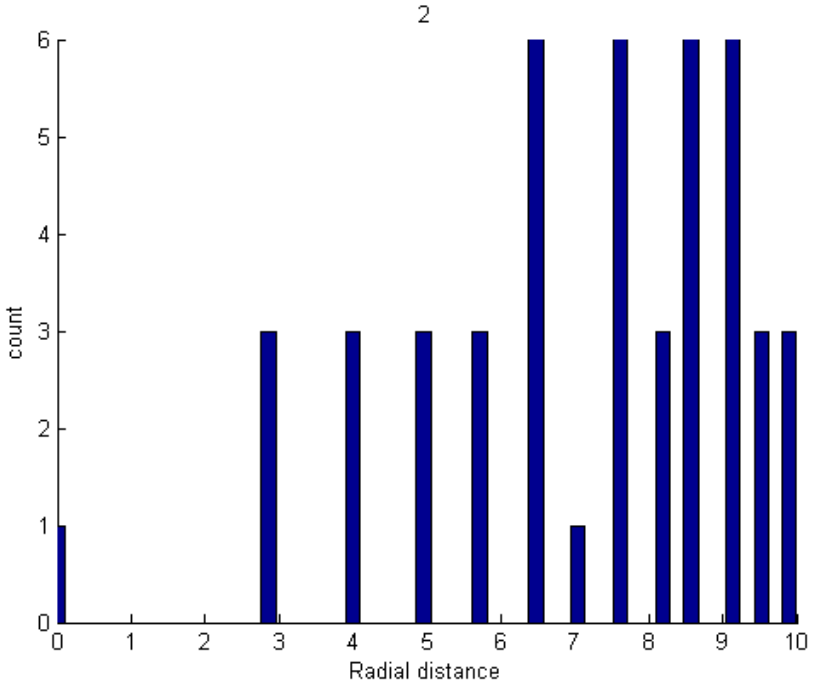

Figure 1.1: a) Solid b) FCC c) Gold

R = [1,1.4,1.73] N = [3,3,3]

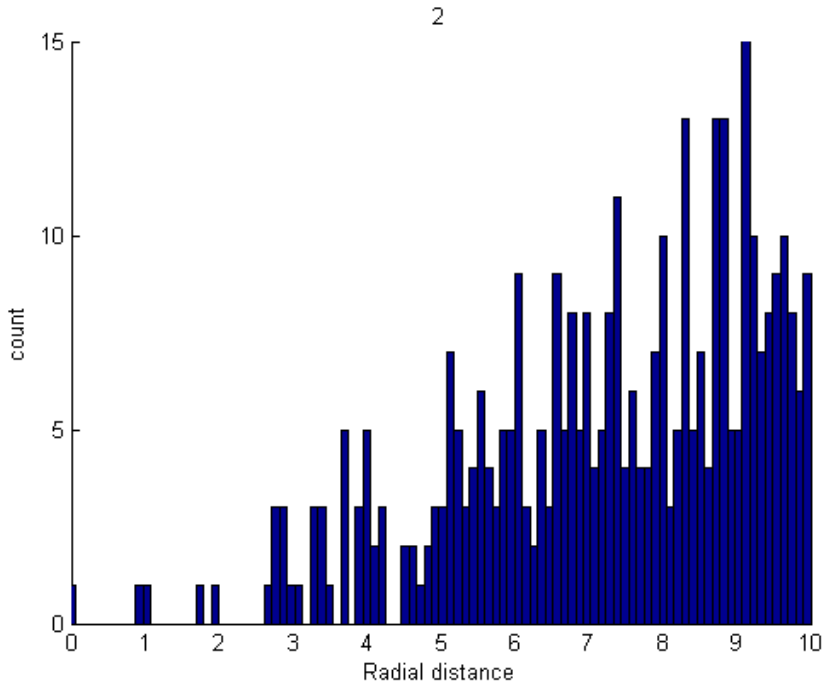

Figure 1.2: a) liquid b) none c) water

R = [1,1.11,1.88] N = [1,1,1]

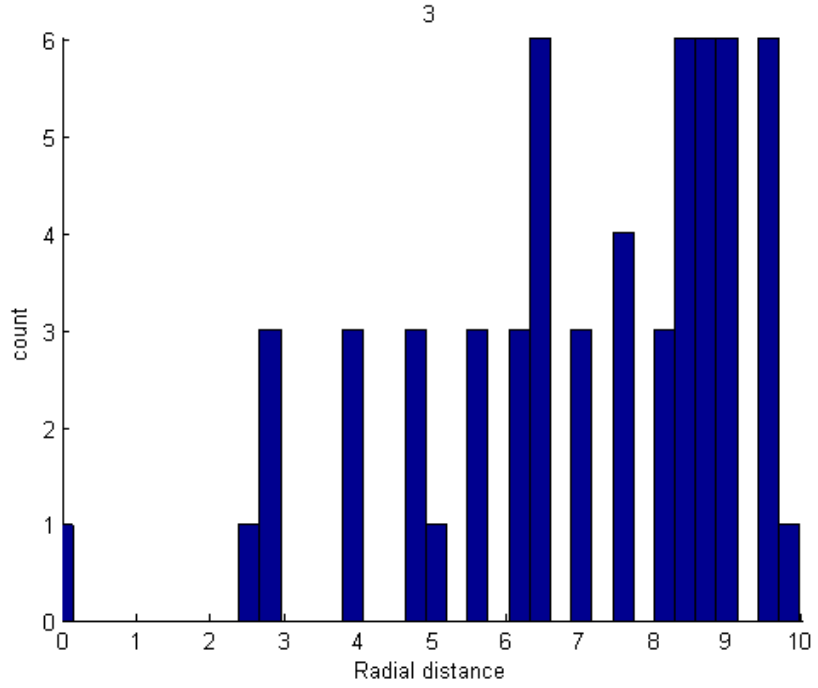

Figure 1.3: a) Solid b) BCC c) Fe

R = [1,1.25,1.75] N = [1,3,3]

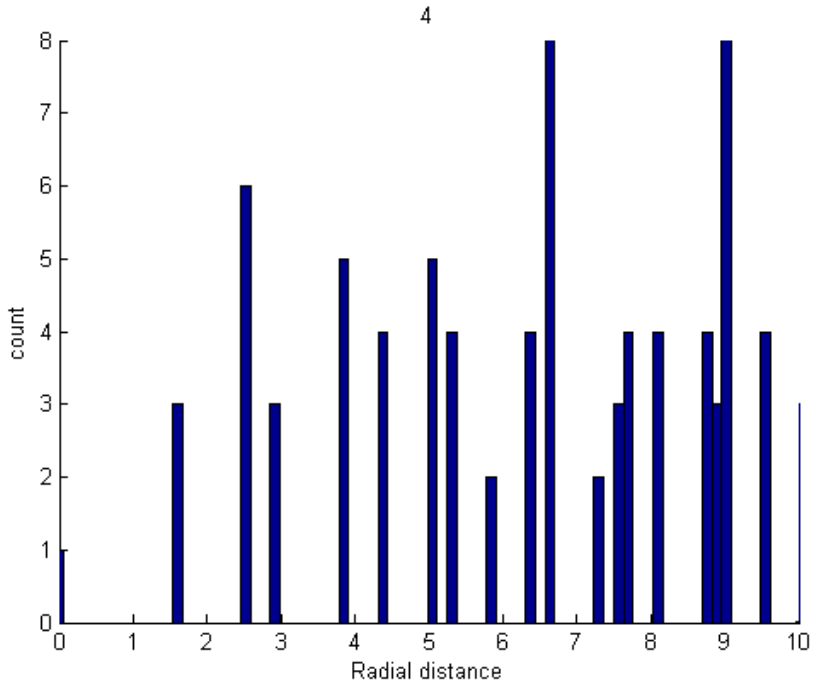

Figure 1.4: a) Solid b) Hexagonal c) Graphene

R = [1,1.63,2] N = [3,6,3]

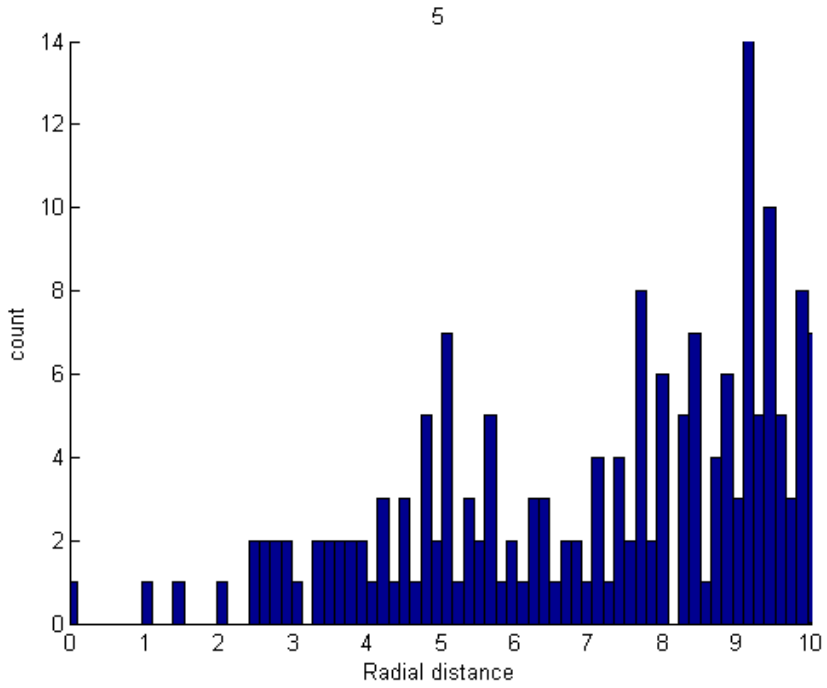

Figure 1.5: a) Solid/liquid? b) none c) Protein

R = [1,1.5,2.33] N = [1,1,1] I calculated the Ratios for the different crystal systems. To get a vector of values I use histc(). This gives me a vector of values. By using a bin width algorithm I can calculate the crystal distances. I then run an algorithm to calculate the number and location of the atoms. after this I divide the ratios R by my calculated values and where there is a small deviation the the resulting vector i determine that to be the crystal system I am looking for.

2 Elastic properties of crystals modeled using a LJ pair potential

a) Assuming a 12:6 Lennard-Jones potential in an FCC lattice write out the expression for the equilibrium position between pairs of atoms. Using the unit lattice properties of copper, express the LJ length parameter σ as a function of the lattice parameter $a0$

$$U(R) = 4\epsilon\left[\frac{\sigma^{12}}{r^{12}} + \frac{\sigma^{6}}{r^{6}}\right]$$

$$\Sigma\frac{1}{r^{6}} = \frac{14.45}{R^{6}}$$

$$\Sigma\frac{1}{r^{12}} = \frac{12.23}{R^{12}}$$

$$U(R) = 4\epsilon\left[\frac{\sigma^{12}}{R^{12}} + \frac{\sigma^{6}}{R^{6}}\right]$$

$$\frac{dU(R)}{dR} = 4\epsilon\left[\frac{12(12.13)\sigma^{12}}{R^{13}} - \frac{6(14.45)\sigma^{6}}{R^{7}}\right]$$

$$\frac{dU(R)}{dR} = 0; 4\epsilon \frac{12(12.13)\sigma^{12}}{R^{13}} = 4\epsilon \frac{6(14.45)\sigma^{6}}{R^{7}}$$

$$\frac{12(12.13)\sigma^{12}}{6(14.45)\sigma^{6}} = \frac{R^{13}}{R^{7}}$$

$$\frac{6(12.13)\sigma^{6}}{14.45} = R^{6}$$

$$6(0.839)\sigma^{6} = R^{6}$$

$$\sqrt[6]{6(0.839)\sigma^{6}} = \sqrt[6]{R^{6}}$$

$$R = \frac{a_0}{\sqrt{2}}$$

$$1.3\sqrt{2}\sigma = a_0$$

$$\boxed{\sigma = \frac{a_0}{1.3\sqrt{2}}} \quad \boxed{a_0 = 3.97\dot{A}} \quad \boxed{a_0 = 1.83\sigma}$$

B) Determine an expression for the minimum potential well of the LJ potential,corresponding to the maximum energy stored in each bond using the expression for bulk modulus and experimental values for the obtained bulk modulus.

$$K = -V\frac{\partial p}{\partial U}$$

$$p = -\frac{\partial U}{\partial V}$$

$\mu = \frac{U}{N}; V_c = \frac{V}{N}$

$$K = V_C \frac{\partial^2 \mu}{\partial V_c^2}$$

$$\frac{\partial}{\partial V_c} = \frac{\sqrt{2}}{3R^2}\frac{\partial}{\partial R}$$

$$K = \frac{\sqrt{2}}{9R}\frac{\partial^2 U}{\partial R^2}$$

$$K = \frac{75\epsilon}{\sigma^3}$$

$$\sigma = \sqrt[3]{\frac{75\epsilon}{K}}$$

$$\epsilon = 0.167eV; K = 123Gpa$$

$$\boxed{\sigma = 2.16 * 10^{-10} m}$$

COMPARE THE RESULTING VALUES WITH THE LJ COPPER POTENTIAL REPORTED BY CLERI AND COWORKERS

Cleri

$$\sigma = 2.314\dot{A}; a_0 = 1.56\sigma$$

Me

$$\sigma = 2.16\dot{A}; a_0 = 1.83\sigma$$

3 THERMAL EXPANSION

A) OBTAIN A HARMONIC APPROXIMATION FOR THIS POTENTIAL, VL. OBTAIN AN EXPRESSION FOR THE EQUIVALENT SPRING CONSTANT

$$\boxed{\frac{1}{2}Kx^2}$$

$$V_L(r) = \frac{1}{2}V_N''(0)x^2$$

$$V_N''(r) = D_0\alpha^2 e^{-\alpha r}$$

$$V_N''(0) = K = D_0\alpha^2$$

$$\boxed{K = D_0\alpha^2} \quad \boxed{V_L(r) = \frac{1}{2}D_0\alpha^2 K r^2}$$

B) OBTAIN AN EXPRESSION FOR THE UNNORMALIZED PROBABILITY DISTRIBUTION OF THE POSITION OF THE PARTICLE, FOLLOWING P(R) = EXP (-V(R)/KBT) FOR VN AND VL

$$p(r) = exp(\frac{-\frac{1}{2}D_0\alpha^2 K r^2}{kbT})$$
$$p(r) = exp(\frac{-D_0(1-e^{-\alpha r}}{kbT})$$

C)WHERE IS THE MOST LIKELY POSITION FOR THE PARTICLE AT ANY ARBITRARY TEMPERATURE FOR VN AND VL?

$$\boxed{r = 0}$$

D) APPROXIMATE THE MEAN (AVERAGE) POSITION OF THE PARTICLE AT ANY TEMPERATURE FOR VL. FOR VN, CALCULATE THE AVERAGE AS A SIMPLE AVERAGE BETWEEN THE POSITIVE AND NEGATIVE R VALUES FOR WHICH VN=KT.

In code

$$avg = \frac{r^- + r^+}{2}$$

E) OBTAIN A GRAPH ILLUSTRATING THE RELATIONSHIP BETWEEN MEAN POSITION VS. TEMPERATURE FOR THE TWO POTENTIALS. HOW DO THE CURVES LOOK DIFFERENT FOR VN AND VL? COMMENT ON THE RELEVANCE OF THIS FOR THERMAL EXPANSION OF THE MATERIAL.

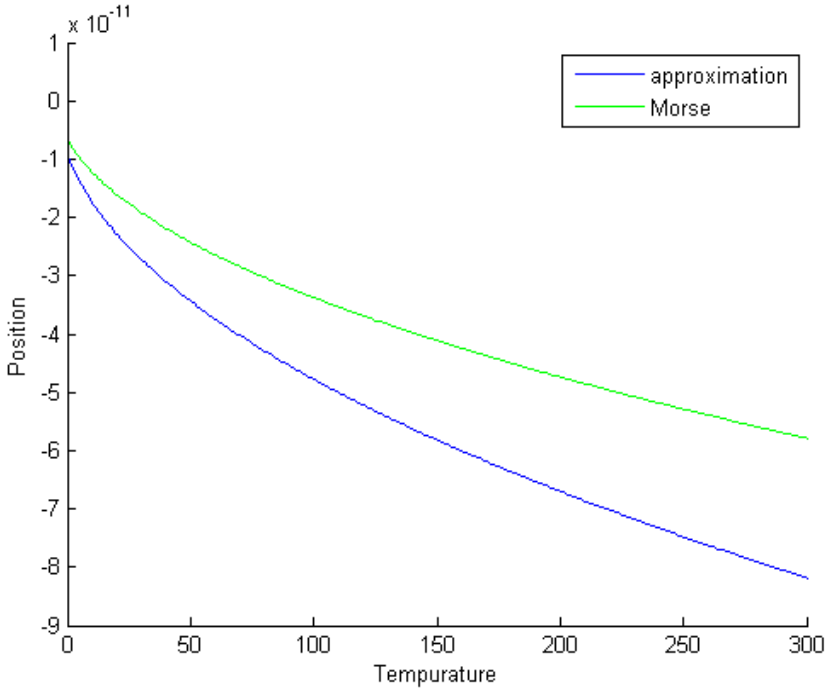

Figure 3.1: thermal dependence

As temperature increases, the lattice vibrates more and the position of the particle moves further away from zero on average. The curves look the same but diverge as temperature increases

A) PLOT OF THE POTENTIAL FUNCTION V(X) VS. X. HOW MANY EQUILIBRIUM POINTS CAN YOU IDENTIFY IF THE PARTICLE MOVES ACCORDING TO THIS POTENTIAL? WHICH ONES ARE STABLE EQUILIBRIUM POSITIONS (E.G. PARTICLE WILL RETURN TO THIS POSITION IF PERTURBED SLIGHTLY).

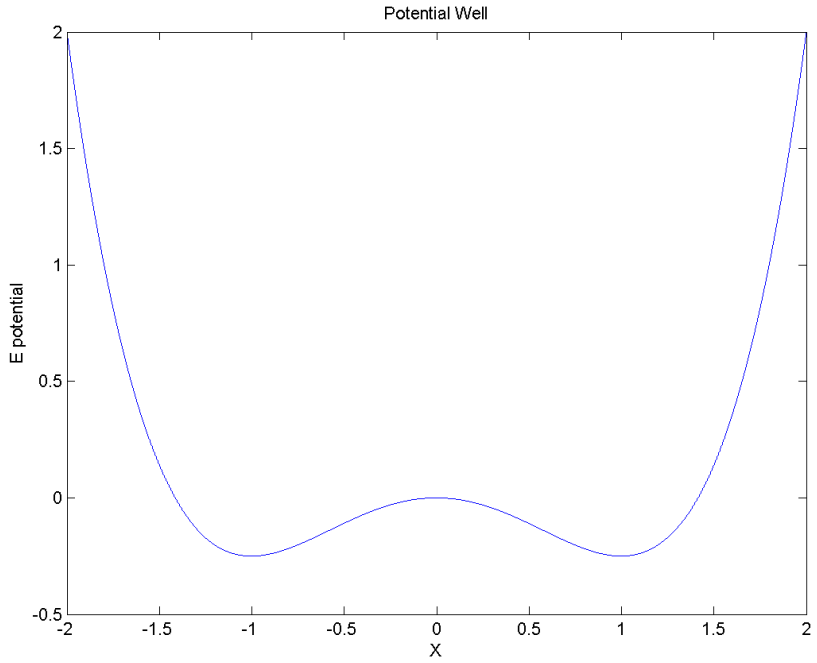

Figure 4.1: Well potential

3 equilibrium points. 2 stable equilibrium points.

B) WRITE DOWN THE EQUATION OF MOTION FOR THIS PARTICLE UNDER THE GIVEN POTENTIAL AND DISSIPATIVE FORCE USING NEWTONÂĂŹS SECOND LAW.

$$V(x) = -\frac{x^2}{2} + \frac{x^4}{4}$$

$$F(x) = -\frac{\partial V(x)}{\partial x}$$

$$F(x) = x + x^3$$

$$\boxed{F(x) = x - x^3}$$

C) NUMERIC INTEGRATION

i) ii)

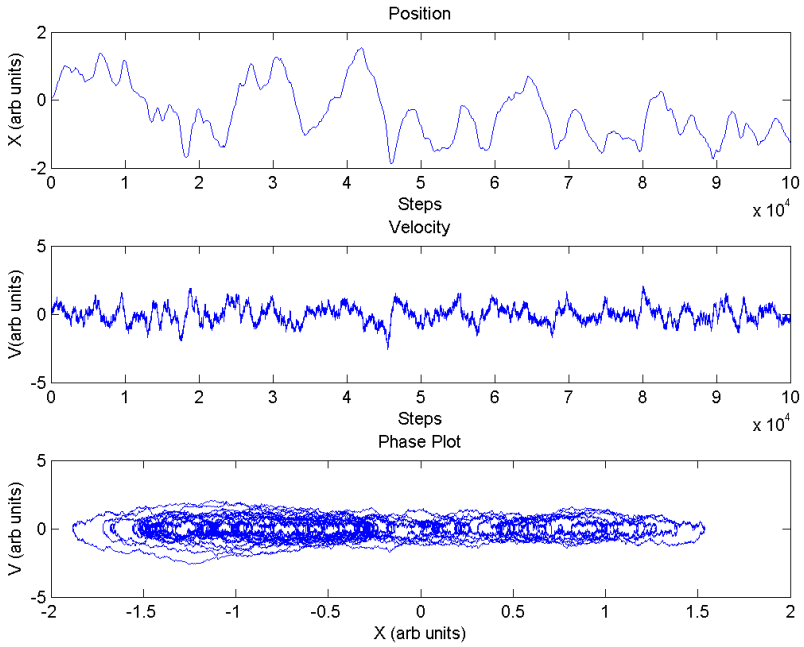

Figure 4.2: A) Position B) Velocity C) Phase

iii)

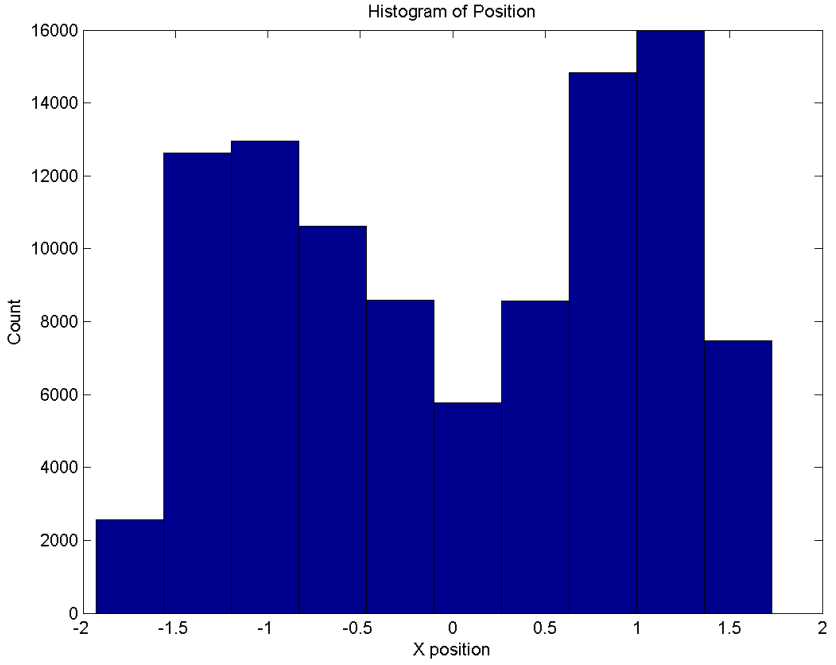

Figure 4.3: Histogram of position

Peaks are observed at the valleys of the potential. The dissipative force F_D controls the probability distribution of the peaks. iv)

$$\tau_{Dwell} = 10.63 seconds$$

v)

$$V''(\pm 1) = K$$

$$V''(x) = -1 + 3x^2$$

$$K = 2$$

vi)

D)Brownian Dynamics technique

i) I think that the particle will become trapped on one of the wells and stay there. τ_{Avg} is dependent on the relation between $K_b T$ and the barrier potential
ii) $\gamma = 0$
iii)

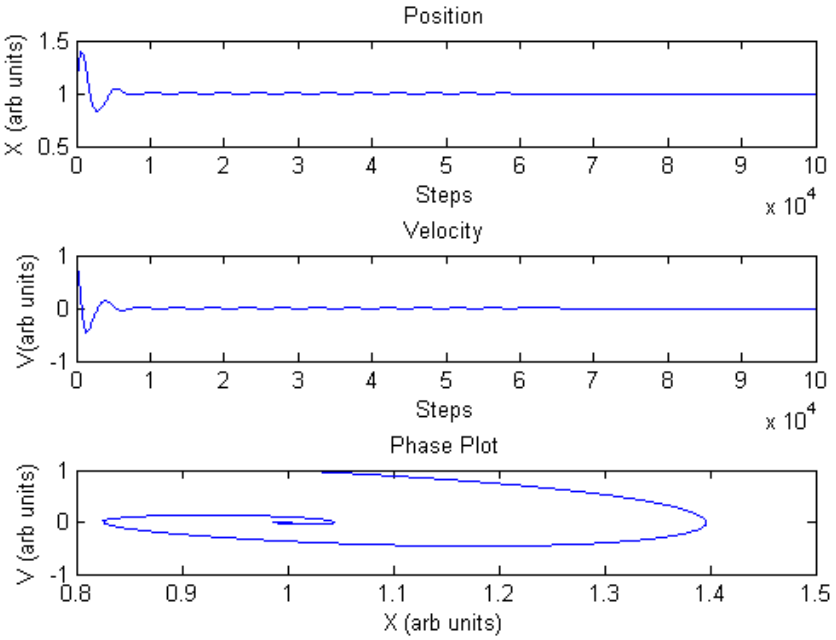

Figure 4.4: $\gamma = 1$

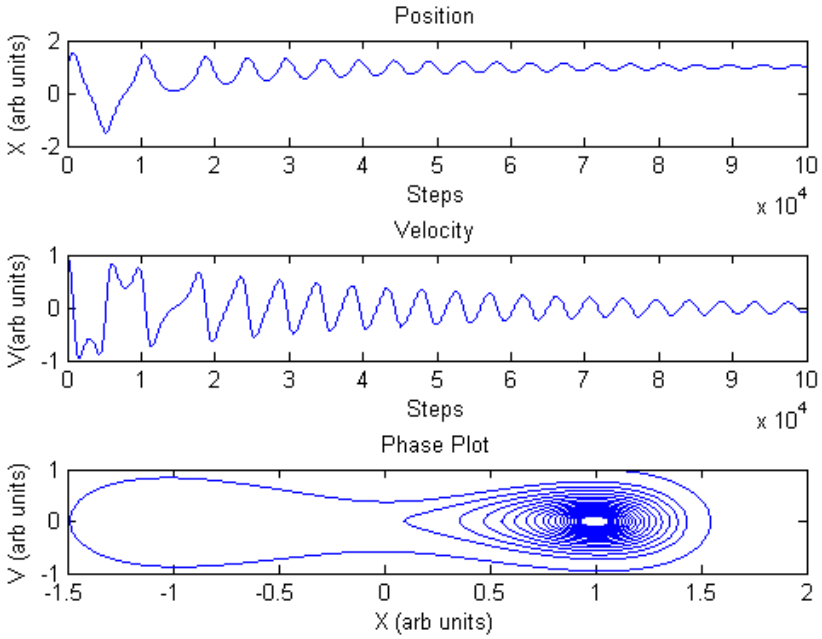

Figure 4.5: $\gamma = 0.05$

MATLAB CODE

```
clear all;clc;clf;
fid = fopen('4.xyz','r');
num = fscanf(fid,'%f',1);
header = fscanf(fid,'%s',3);
table = zeros(num,6);
% load Values
for i = 1:num-1
type= fscanf(fid,'%s',1); % read num of types
if size(type) == 1
  table(i,1:3) = [type,0,0];
elseif size(type) == 2
  table(i,1:3) = [type,0];
elseif size(table) == 3
    table(i,1:3) = type;
end
table(i,4:6) = fscanf(fid,'%f %f %f',3)';
end
fclose(fid);

%find max dx,dy,dz
x0 = table(round(num/2),4);
y0 = table(round(num/2),5);
z0 = table(round(num/2),6);
xmax = 0;ymax = 0;zmax = 0; % set max to zero
```

```
for i = 1:num-1
 x = abs(x0 - table(i,4));
    if x > xmax
xmax = x;
    end
y = abs(y0 - table(i,5));
if y > ymax
    ymax = y;
end
z = abs(z0 - table(i,6));
if z > zmax
zmax = z;
end
end
RadialMax = sqrt(xmax^2 + ymax^2 + zmax^2); % calculate radial max in spherical
NUM_BIN = 600; % number of Bins
BIN_Width = RadialMax/NUM_BIN; %Bin width

%Radial Distance
%find max dx,dy,dz
x0 = table(1,4);y0 = table(1,5);z0 = table(1,6);
xmax = 0;ymax = 0;zmax = 0; % set max to zero
Radial = 1:num-1;
for i = 1:num-1
x = abs(x0 - table(i,4));
y = abs(y0 - table(i,5));
z = abs(z0 - table(i,6));
Radial(i) = sqrt(x^2 + y^2 + z^2);
end
V = 0:BIN_Width:RadialMax;
figure(1)
hold on
title('5')
ylabel('count')
xlabel('Radial distance')
xlim([0,10])
hist(Radial,V)
hold off
figure(2)
n = histc(Radial,0:BIN_Width:RadialMax);
plot(V,n)
xlim([0,10])
Ratio = [0,0,0];
NUM = [0,0,0];
order = 0;
for i = 2:length(V)
    if (n(i) ~= 0) && (order == 0)
   Ratio(1) = V(i);
   NUM(1) = n(i);
   order = order+ 1;
    elseif (n(i) ~= 0) && (order == 1)
        Ratio(2) = V(i);
```

```
        NUM(2) = n(i);
        order = order+1;
        elseif (n(i) ~= 0) && (order == 2)
        Ratio(3) = V(i);
        NUM(3) = n(i);
        order = order+1;
    end
end
R = Ratio;
BCC = [sqrt(3)/2,1,sqrt(3)];
FCC = [sqrt(2)/2, 1,sqrt(2)];
Graphene = [0.5,sqrt(3)/2, 1];
Water = [1,2];
figure(3)
plot(NUM,Ratio)
```

HW1_416.m

```
clc;clear all;clf;
%%% Contants
KbT = 0.5;
N = 1000000;
M = 1;
gamma = 1;
dt = 0.001;
%%%%%%%%%%%%%%
%Potential Well
x =-2:0.000001:2 ;
V = -0.5*x.^2 + 0.25*x.^4;
figure(1)
plot(x,V);
title('Potential Well')
xlabel('X')
ylabel('E potential')
%print('-dpng','Well')
%%%%%%%%%%%%%%%
N = 100000;
X_0 = 0;
V_0 = KbT;
x = zeros(1,N);
v = zeros(1,N);
x(1) = X_0;
v(1) = V_0;
Dwell = 0;
Tau_Dwell = 0;
FirstTime = 0;
for T = 1:N-1
Dwell = Dwell + dt;
F_R = sqrt((2*M*KbT*gamma)/dt)*randn();
F_C = x(T) - x(T)^3;
x(T+1) = x(T) + v(T)*dt + 0.5*(-gamma*v(T) + (1/M)*(F_R + F_C))*(dt^2);
v(T+1) = v(T) + (-gamma*v(T) + (1/M)*(F_R + F_C))*dt;
if ((x(T) > 0 && x(T+1) < 0) || (x(T) < 0 && x(T+1) > 0))
```

```
    if (FirstTime == 0)
    Tau_Dwell = Dwell;
    FirstTime = FirstTime + 1;
    end
    if (FirstTime == 1)
    Tau_Dwell = (Tau_Dwell + Dwell)/2;
    end
    Dwell = 0;
end
end
figure(2)
subplot(3,1,1);plot(x)
title('Position')
ylabel('X (arb units)')
xlabel('Steps')
subplot(3,1,2);plot(v)
title('Velocity')
ylabel('V(arb units)')
xlabel('Steps')
subplot(3,1,3);plot(x,v)
title('Phase Plot')
ylabel('V (arb units)')
xlabel('X (arb units)')
%print('-dpng','ParticleMotion')
figure(3)
hist(x)
title('Histogram of Position')
xlabel('X position')
ylabel('Count')
%print('-dpng','HIST')
figure(4)
xlim([-2, 2])
plot(x,v)
title('Phase Plot')
ylabel('V (arb units)')
xlabel('X (arb units)')
```

molsim.m

```
clear all;clc;clf;
D = 5;
alpha = 0.5;
Kb = 1.38E-23;
R_max = 3E-10;
r = -R_max:R_max/10000:R_max;
T = 300;
C = Kb*T;
%%%%%%%%%%
%
%%%%%%%%%%
V_N = D*(1-exp(-alpha*r)).^2;
p_N = exp(-V_N/(Kb*T));
figure(1)
```

```
subplot(2,1,1);plot(r,V_N)
subplot(2,1,2);plot(r,p_N)
%%%%%%%%%%%%%%%
% Harmonic Approximation
%%%%%%%%%%%%%%%
K = D*alpha^2;
V_L = 0.5*K*r.^2;
P_L = exp(-V_L/(Kb*T));
figure(2)
subplot(2,1,1);plot(r,V_L);
title('Harmonic Approximation')
subplot(2,1,2);plot(r,P_L);
figure(3)
hold on
plot(r,V_L,'b');
plot(r,V_N,'r');
legend('Harmonic Approximation','Morse Potential')
hold off
e = 5E-23;
p_L = [];
p_N = [];
average_L = [];
average_N =[];
for T = 1:300
for i = 1:length(r)
  if((V_L(i) < Kb*T + e)&&(V_L(i) > Kb*T - e))
      p_L = [p_L,r(i)];
  end
   if((V_N(i) < Kb*T + e)&&(V_N(i) > Kb*T - e))
   p_N = [p_N,r(i)];
   end
end
average_L = [average_L,(p_L(1) + p_L(2))/2];
average_N = [average_N,(p_N(1) + p_N(2))/2];
p_L = [];
p_N = [];
end
figure(4)
hold on
plot(1:300,average_L,'b');
plot(1:300,average_N,'g');
legend('approximation','Morse')
xlabel('Tempurature')
ylabel('Position')
hold off
N = sum(average_L)/300;
L = sum(average_N)/300;
```

part3.m