ASEN6519: Molecular Simulation of Materials
Spring 2019

Exam # 1

Instructor: Sanghamitra Neogi

Assigned: March 5, 2019
Due: March 5, 2019, 11:59 PM to Canvas

Total points: 70

Name: TY STERLING

Time taken to finish the exam: START: 8:51 AM → ~9 HR 45 MIN
END: 6:18 PM

– NOTE: I SPENT SEVERAL HOURS DOING OTHER THINGS DURING THIS INTERVAL

Instructions

- This exam has **three questions** with several parts in each. Read the instructions for each question and each sub-part carefully.
- You may attempt each question and the sub-parts within each question in any order you like, but you must clearly label your solutions.
- Answer each question thoroughly and make sure to explain your thought process. Please write clearly so that I can follow the steps.
- You should show each step of your solution and justify any assumptions made in your analysis.
- **You may lose points if the steps are not clear.**
- **Please separate the equations from the text. Do not write as a paragraph.**
- Explanations and answers should be in terms of variables used to define the problem. (**Please do not redefine the problem.**)

1

$$U(x) = -\frac{\omega^2}{8a^2}(x^2-a^2)^2$$

a)

HAMILTON'S EQ. $\dot{x} = \frac{\partial \mathcal{H}}{\partial p}$, $\dot{p} = -\frac{\partial \mathcal{H}}{\partial x}$ FOR SINGLE 1D PARTICLE

$$\mathcal{H} = \frac{p^2}{2m} - \frac{\omega^2}{8a^2}(x^2-a^2)^2 \quad , \quad \frac{\partial \mathcal{H}}{\partial p} = \frac{p}{m} = \dot{x}$$

$$-\frac{\partial \mathcal{H}}{\partial x} = \frac{\omega^2}{8a}\cdot\frac{\partial}{\partial x}(x^2-a)^2 = \boxed{\frac{\omega^2}{2a}x(x^2-a^2) = \dot{p}}$$

$\dot{p} = F = ma = m\ddot{x} = \ddot{x}$ FOR UNIT MASS.

$$a\frac{d}{dt}\left(\frac{d}{dt}\tanh\left(\frac{(t-t_0)\omega}{2}\right)\right) = a\frac{\omega}{2}\frac{d}{dt}\left(\operatorname{sech}^2\left(\frac{(t-t_0)\omega}{2}\right)\right)$$

$$= -\frac{a\omega^2}{2}\tanh\left(\frac{(t-t_0)\omega}{2}\right)\operatorname{sech}^2\left(\frac{(t-t_0)\omega}{2}\right) = \ddot{x}$$

DOES $\ddot{x} = \dot{p}$?

$$-\frac{\cancel{a}\omega^2}{\cancel{2}}\cancel{\tanh\left(\frac{(t-t_0)\omega}{2}\right)}\operatorname{sech}^2\left(\frac{(t-t_0)\omega}{2}\right) = \frac{\omega^{\cancel{2}}}{\cancel{2a^2}}\cancel{a\tanh\left(\frac{(t-t_0)\omega}{2}\right)}\left[\left(\cancel{a}\tanh\left(\frac{(t-t_0)\omega}{2}\right)\right)^2 - \cancel{a^2}\right]$$

$$-\operatorname{sech}^2\left(\frac{(t-t_0)\omega}{2}\right) = \tanh^2\left(\frac{(t-t_0)\omega}{2}\right) - 1$$

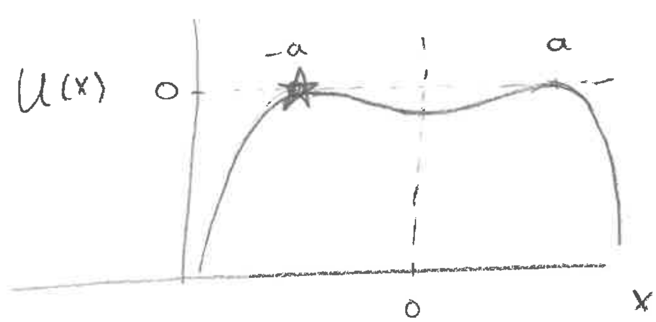
TRIG IDENTITY $\tanh^2(x) + \operatorname{sech}^2(x) = 1 \rightarrow \underline{\tanh^2(x) - 1 = -\operatorname{sech}^2(x)!}$

$x(t) = a\tanh\left(\frac{(t-t_0)\omega}{2}\right)$ IS A SOLUTION.

b) Well, $\tanh(-\infty) = -1$, so $x(t) = a\tanh\left(\frac{(-\infty - t_0)\omega}{2}\right)$

$$x(t) = a\tanh(-\infty) = -a$$

→ THIS INITIAL CONDITION WITH $t = -\infty$ CORRESPONDS TO A PARTICLE INITIALLY AT REST ON TOP OF THE PEAK AT $x = -a$



1 CONT

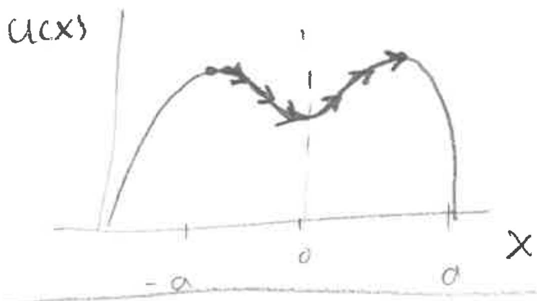
c) AS $t \to \infty$ (FOR INITIAL CONDITION $t = -\infty$, WHICH IS HOW I INTERPRET "this solution")

$$X(t) = a \tanh\left(\frac{(t - t_0)\omega}{2}\right) \quad \& \quad V(t) = \frac{a\omega}{2} \operatorname{sech}^2\left(\frac{(t-t_0)\omega}{2}\right)$$

INITIALLY, $X = -\infty$ & $V = 0$, i.e. PARTICLE IS AT REST ON PEAK AT $X = -a$.

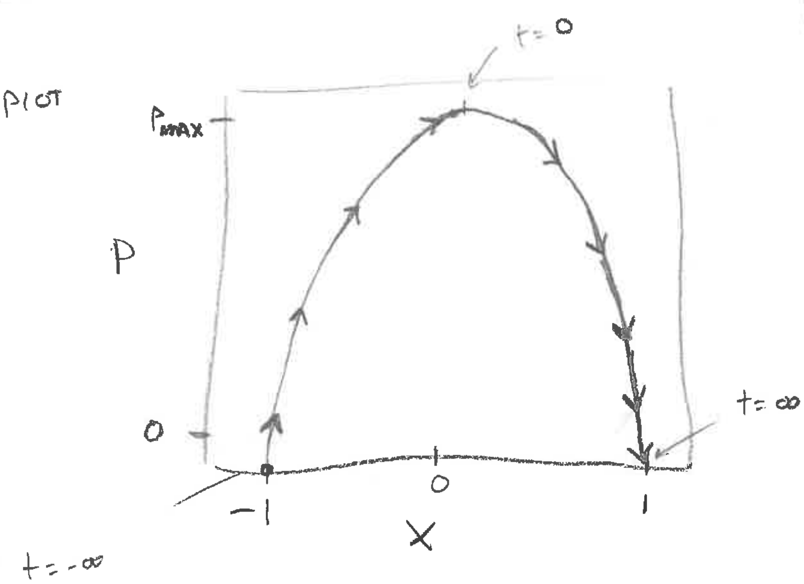
AS $t \to 0$, PARTICLE APPROACHES BOTTOM OF WELL i.e. $X \to 0$ & ATTAINS MAX VELOCITY.

AS $t \to \infty$, PARTICLE CLIMBS UP THE OTHER HUMP AND COMES TO REST AT $X \to a$, $V \to 0$.



d)

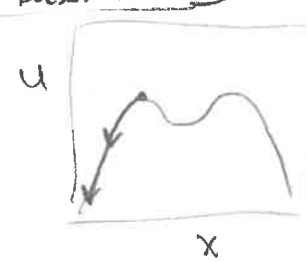
PHASE PLOT

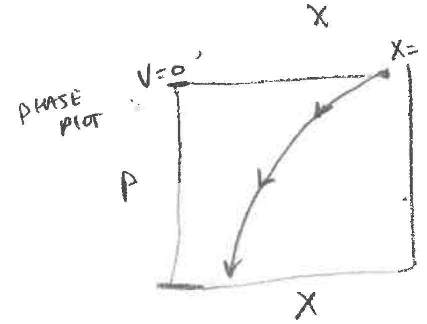


* POSSIBLE ALTERNATIVE?

FROM $t = -\infty$, PARTICLE MOVES TO LEFT INSTEAD OF TO RIGHT, i.e. INSTEAD OF TRAVELING THROUGH THE WELL, THE PARTICLE FALLS OFF TO INFINITY...

(THIS SOLT'N DOESN'T ALLOW IT)





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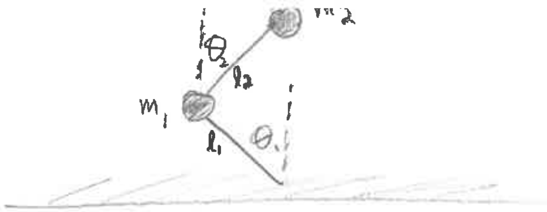
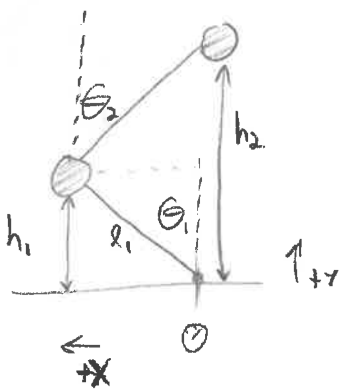


$m_1 \to q_1 \qquad m_2 \to q_2$

$V(h_i) = q_i E h_i$



(X_1, Y_1) & (X_2, Y_2)

$X_1 = l_1 \sin\theta_1 \quad , \quad Y_1 = l_1 \cos\theta_1$

$X_2 = X_1 - l_2 \sin\theta_2 = l_1 \sin\theta_1 - l_2 \sin\theta_2$

$Y_2 = Y_1 + l_2\cos\theta_2 = l_1\cos\theta_1 + l_2 \cos\theta_2$

DEF $\theta_1(X_1, Y_1; X_2, Y_2)$ & $\theta_2(X_1, Y_1; X_2, Y_2)$

X_1, Y_1 & X_2, Y_2 $\equiv$ INV. TRANSFORM i.e. $X_1(\theta_1, \theta_2)$
$Y_1(\theta_1, \theta_2)$

$X_2(\theta_1, \theta_2)$ $Y_2(\theta_1, \theta_2)$ IN GENERAL

$\therefore$ COORDINATES DEFINED BY INVERSE TRANSFORM FROM θ_1 & θ_2;
IN GENERAL EACH X & Y DEPEND ON θ_1 & θ_2

$$\frac{dX_i}{dt} = \frac{\partial X_i}{\partial\theta_1}\dot\theta_1 + \frac{\partial X_i}{\partial\theta_2}\dot\theta_2 \quad ; \quad \frac{dY_i}{dt} = \frac{\partial Y_i}{\partial\theta_1}\dot\theta_1 + \frac{\partial Y_i}{\partial\theta_2}\dot\theta_2$$

$$KE = \frac{1}{2}\sum_k m_k (\vec{V}_k)^2 = \frac{1}{2}\sum_k m_k\left(\left(\frac{dX_k}{dt}\right)^2 + \left(\frac{dY_k}{dt}\right)^2\right)$$

$$\left(\frac{dX_k}{dt}\right)^2 = \left(\frac{\partial X_k}{\partial\theta_1}\dot\theta_1 + \frac{\partial X_k}{\partial\theta_2}\dot\theta_2\right)\left(\frac{\partial X_k}{\partial\theta_1}\dot\theta_1 + \frac{\partial X_k}{\partial\theta_2}\dot\theta_2\right) = \frac{\partial X_k}{\partial\theta_1}\frac{\partial X_k}{\partial\theta_1}\dot\theta_1\dot\theta_1$$

$$+ \frac{\partial X_k}{\partial\theta_1}\frac{\partial X_k}{\partial\theta_2}\dot\theta_1\dot\theta_2 + \frac{\partial X_k}{\partial\theta_2}\frac{\partial X_k}{\partial\theta_1}\dot\theta_2\dot\theta_1 + \frac{\partial X_k}{\partial\theta_2}\frac{\partial X_k}{\partial\theta_2}\dot\theta_2\dot\theta_2$$

$$\left(\frac{dX_k}{dt}\right)^2 \equiv \frac{1}{2}\sum_i\sum_j\left[\sum_k m_k \frac{\partial X_k}{\partial\theta_i}\frac{\partial X_k}{\partial\theta_j}\right]\dot\theta_i\dot\theta_j \to \left(\frac{dY_k}{dt}\right) \equiv \frac{1}{2}\sum_i\sum_j\left[\sum_k \frac{\partial Y_k}{\partial\theta_i}\frac{\partial Y_k}{\partial\theta_j}\right]\dot\theta_i\dot\theta_j$$

"MASS METRIC TENSOR" $\equiv G_{ij} \equiv \sum_k m_k \frac{\partial\vec{r}_k}{\partial\theta_i}\frac{\partial\vec{r}_k}{\partial\theta_j}$

$$G_{11}^{K=1} = m_1\left(\frac{\partial \vec{r}_1}{\partial \theta_1}\cdot\frac{\partial \vec{r}_1}{\partial \theta_1}\right) = m_1\left[\left(\frac{\partial x_1}{\partial \theta_1}\hat{\imath} + \frac{\partial y_1}{\partial \theta_1}\hat{\jmath}\right)\cdot\left(\frac{\partial x_1}{\partial \theta_1}\hat{\imath} + \frac{\partial y_1}{\partial \theta_1}\hat{\jmath}\right)\right]$$

$$= m_1\left[\left(\frac{\partial x_1}{\partial \theta_1}\right)^2 + \left(\frac{\partial y_1}{\partial \theta_1}\right)^2\right] = \ldots$$

$$G_{11} = m_1\left[\left(\frac{\partial x_1}{\partial \theta_1}\right)^2 + \left(\frac{\partial y_1}{\partial \theta_1}\right)^2\right] + m_2\left[\left(\frac{\partial x_2}{\partial \theta_1}\right)^2 + \left(\frac{\partial y_2}{\partial \theta_1}\right)^2\right] =$$

$$= m_1\left(\underbrace{(l_1\cos\theta_1)^2 + (l_1\sin\theta_1)^2}_{=l_1^2}\right) + m_2\left(\underbrace{(l_1\cos\theta_1)^2 + (l_1\sin\theta_1)^2}_{=l_1^2}\right)$$

$$G_{11} = l_1^2(m_1 + m_2)$$

$$G_{12} = m_1\left[\frac{\partial x_1}{\partial \theta_1}\underbrace{\cancel{\frac{\partial x_1}{\partial \theta_2}}}_{0} + \frac{\partial y_1}{\partial \theta_1}\underbrace{\cancel{\frac{\partial y_1}{\partial \theta_2}}}_{0}\right] + m_2\left[\frac{\partial x_2}{\partial \theta_1}\frac{\partial x_2}{\partial \theta_2} + \frac{\partial y_2}{\partial \theta_1}\frac{\partial y_2}{\partial \theta_2}\right]$$

$$= m_2\left[-l_1\cos\theta_1 l_2\cos\theta_2 + (-l_1\sin\theta_1)(-l_2\sin\theta_2)\right] = -m_2 l_1 l_2\left[\cos\theta_1\cos\theta_2 - \sin\theta_1\sin\theta_2\right]$$

$$G_{12} = -m_2 l_1 l_2\cos(\theta_1 + \theta_2) = G_{21}$$

$$G_{22} = m_1\left[\underbrace{\cancel{\left(\frac{\partial x_1}{\partial \theta_2}\right)^2}}_{0} + \underbrace{\cancel{\left(\frac{\partial y_1}{\partial \theta_2}\right)^2}}_{0}\right] + m_2\left[\left(\frac{\partial x_2}{\partial \theta_2}\right)^2 + \left(\frac{\partial y_2}{\partial \theta_2}\right)^2\right] = m_2\left[\underbrace{(l_2\cos\theta_2)^2 + (l_2\sin\theta_2)^2}_{l_2^2}\right]$$

$$G_{22} = m_2 l_2^2$$

$$KE = \frac{1}{2}\sum_i\sum_j G_{ij}\dot{\theta}_i\dot{\theta}_j = \frac{1}{2}\left[l_1^2(m_1+m_2)(\dot{\theta}_1)^2 - 2m_2 l_1 l_2\cos(\theta_1+\theta_2)\dot{\theta}_1\dot{\theta}_2 + m_2 l_2^2(\dot{\theta}_2)^2\right]$$

$U_i \equiv q_i E h_i \qquad U = \sum_i u_i = q_1 E h_1 + q_2 E h_2 = E(q_1 h_1 + q_2 h_2)$

IN GENERALIZED COORDS.

$$PE = U = E\left[q_1 \ell_1 \cos\theta_1 + q_2(\ell_1 \cos\theta_1 + \ell_2 \cos\theta_2)\right]$$

→ I DEFINED THE SURFACE AS $y = \varnothing$, SO $h_i = y_i$, & SUBSTITUTED $h_i(\theta_1, \theta_2)$ INTO U. → $U(\theta_1, \theta_2)$

THE LAGRANGIAN IS DEFINED AS KE − PE. THE LAGRANGIAN IN TERMS OF $(\theta_1 \text{ \& } \theta_2)$ IS THEN $KE(\theta_1, \theta_2) - U(\theta_1, \theta_2)$

$$\mathcal{L}(\theta_1, \theta_2) = \frac{1}{2}\sum_i^2 \sum_j^2 \left[\sum_k m_k \frac{\partial \vec{r}_k}{\partial \theta_i}\frac{\partial \vec{r}_k}{\partial \theta_j}\right]\dot{\theta}_i \dot{\theta}_j - E\sum_i^2 q_i h_i(\theta_1, \theta_2)$$

$$= \frac{1}{2}\left[\ell_1^2(m_1+m_2)\dot{\theta}_1^2 - 2m_2 \ell_1 \ell_2 \cos(\theta_1+\theta_2)\dot{\theta}_1\dot{\theta}_2 + m_2 \ell_2^2 \dot{\theta}_2^2\right]$$
$$- E\left[q_1 \ell_1 \cos\theta_1 + q_2(\ell_1 \cos\theta_1 + \ell_2 \cos\theta_2)\right]$$

EULER-LAGRANGE EQ. $\equiv \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}}\right) - \frac{\partial \mathcal{L}}{\partial x} = \varnothing$

SUBT. NEW COORD, θ_1 & θ_2 FOR x ↔

θ_1: $\quad \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\theta}_1}\right) - \frac{\partial \mathcal{L}}{\partial \theta_1} = \varnothing$

$$\frac{\partial \mathcal{L}}{\partial \dot{\theta}_1} = \frac{1}{2}\frac{\partial}{\partial \dot{\theta}_1}\left[\ell_1^2(m_1+m_2)\dot{\theta}_1^2 - 2m_2 \ell_1 \ell_2 \cos(\theta_1+\theta_2)\dot{\theta}_1\dot{\theta}_2 + \cancel{m_2 \ell_2^2 \dot{\theta}_2^2}^{\varnothing}\right]$$

$$\boxed{\frac{\partial \mathcal{L}}{\partial \dot{\theta}_1} = \ell_1^2(m_1+m_2)\dot{\theta}_1 - m_2 \ell_1 \ell_2 \cos(\theta_1+\theta_2)\dot{\theta}_2}$$

$$\frac{\partial \mathcal{L}}{\partial \theta_1} = \frac{1}{2}\frac{\partial}{\partial \theta_1}\left[-2m_1 l_1 l_2 \cos(\theta_1+\theta_2)\dot{\theta}_1\dot{\theta}_2\right] - \varepsilon\frac{\partial}{\partial \theta_1}\left[q_1 l_1\cos\theta_1 + q_2(l_1\cos\theta_1 + l_2\cos\theta_2)\right]$$

$$= \boxed{m_1 l_1 l_2 \dot{\theta}_1\dot{\theta}_2 \sin(\theta_1+\theta_2) + \varepsilon q_1 l_1 \sin\theta_1 + \varepsilon q_2 l_1 \sin\theta_1 = \frac{\partial \mathcal{L}}{\partial \theta_1}}$$

$$\frac{\partial \mathcal{L}}{\partial \dot{\theta}_2} = \frac{1}{2}\frac{\partial}{\partial \dot{\theta}_2}\left[l_1^2(m_1+\cancel{m_2})\dot{\theta}_1^2 - 2m_2 l_2 l_1\cos(\theta_1+\theta_2)\dot{\theta}_1\dot{\theta}_2 + l_2^2 m_2\dot{\theta}_2^2\right]$$

$$= \boxed{l_2^2 m_2\dot{\theta}_2 - m_2 l_2 l_1\cos(\theta_1+\theta_2)\dot{\theta}_1 = \frac{\partial \mathcal{L}}{\partial \dot{\theta}_2}}$$

$$\frac{\partial \mathcal{L}}{\partial \theta_2} = \frac{1}{2}\frac{\partial}{\partial \theta_2}\left[-2m_1 l_2 l_1\cos(\theta_1+\theta_2)\dot{\theta}_1\dot{\theta}_2\right] - \varepsilon\frac{\partial}{\partial \theta_2}\left[q_2(l_1\cos\theta_1 + l_2\cos\theta_2)\right]$$

$$\boxed{= m_1 l_2 l_1\dot{\theta}_1\dot{\theta}_2\sin(\theta_1+\theta_2) + \varepsilon q_2 l_2\sin\theta_2 = \frac{\partial \mathcal{L}}{\partial \theta_2}}$$

NOTE: I WONT WRITE DOWN THE $\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\theta}_i}\right) - \frac{\partial \mathcal{L}}{\partial \theta_i} = 0$

EQUATIONS SINCE, WITHOUT SOLVING FOR $\theta_i(t)$, I CAN'T EVALUATE $\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\theta}_i}\right)$ & WOULD JUST BE RECOPYING THE $\frac{\partial \mathcal{L}}{\partial \dot{\theta}_1}$, $\frac{\partial \mathcal{L}}{\partial \theta_1}$ & $\frac{\partial \mathcal{L}}{\partial \dot{\theta}_2}$, $\frac{\partial \mathcal{L}}{\partial \theta_2}$ INTO ANOTHER EQUATION THAT CAN'T REALLY BE SIMPLIFIED BY MUCH MORE.

c) THE "SMALL ANGLE APPROXIMATION" GIVES, FOR $\sin\theta$ & $\cos\theta$:

$$\sin\theta \approx \theta \qquad \text{AND} \qquad \cos\theta \approx 1 - \frac{\theta^2}{2}$$

$$\left.\frac{\partial L}{\partial \dot\theta_1}\right|_{\theta_1,\theta_2 \ll 1} \approx \boxed{l_1^2 (m_1+m_2)\dot\theta_1 - m_2 l_1 l_2 \dot\theta_2 \left(1 - \frac{\theta_1+\theta_2}{2}\right)}$$

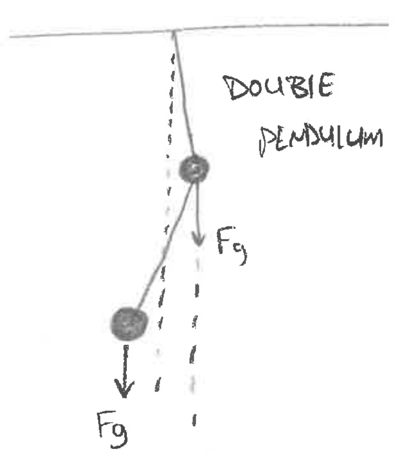
$$\left.\frac{\partial L}{\partial \theta_1}\right|_{\theta_1,\theta_2 \ll 1} \approx m_1 l_1 l_2 \dot\theta_1 \dot\theta_2 (\theta_1+\theta_2) + E q_1 l_1 \theta_1 + E q_2 l_1 \theta_1$$

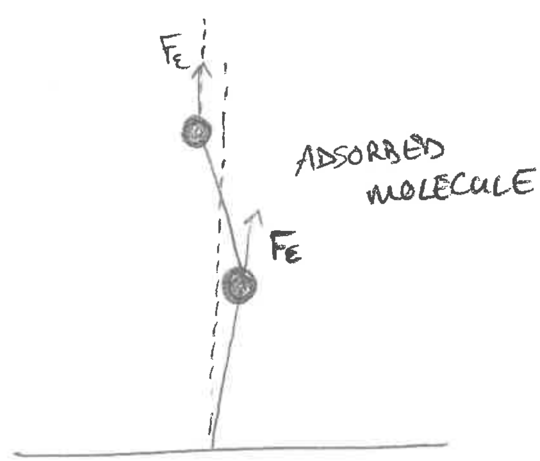
$$\approx \boxed{m_1 l_1 l_2 \dot\theta_1 \dot\theta_2 (\theta_1+\theta_2) + E l_1 \theta_1 (q_1+q_2)}$$

$$\left.\frac{\partial L}{\partial \dot\theta_2}\right|_{\theta_1,\theta_2 \ll 1} \approx \boxed{l_2^2 m_2 \dot\theta_2 - m_2 l_2 l_1 \dot\theta_1 \left(1 - \frac{\theta_1+\theta_2}{2}\right)}$$

$$\left.\frac{\partial L}{\partial \theta_2}\right|_{\theta_1,\theta_2 \ll 1} \approx \boxed{m_1 l_1 l_2 \dot\theta_1 \dot\theta_2 (\theta_1+\theta_2) + E l_2 \theta_2 q_2}$$

THESE LOOKS LIKE THE EQUATIONS FOR A DOUBLE PENDULUM WITH GRAVITY POINTING UP (IN THIS CASE, NO GRAVITY BUT E FIELD POINTS UP).





3)

$$f(v) = \left(\frac{m}{2\pi kT}\right)^{1/2} e^{-mv^2/2kT}$$

$$\rightarrow f(x) = \left(\frac{1}{2\pi\sigma^2}\right)^{1/2} e^{-x^2/2\sigma^2}$$

$$x \in (-\infty, X) \rightarrow P(X) = \left(\frac{1}{2\pi\sigma^2}\right)^{1/2} \int_{-\infty}^{X} dx\, e^{-x^2/2\sigma}$$

PROB OF RANDOM X BEING IN INTERVAL $(-\infty, X)$ IS $P(X)$

$P(X) = \xi$ → i.e. PICKING AN ξ & SOLVING

$P(X) = \xi$ WILL TELL US X FOR x THAT LIES IN THE INTERVAL $(-\infty, X]$.

$$\rightarrow P(X, Y) = \frac{1}{2\pi\sigma^2} \int_{-\infty}^{X} dx \int_{-\infty}^{Y} dy\; e^{-\frac{(x^2+y^2)}{2\sigma^2}}$$

$x = r\cos\phi \qquad y = r\sin\phi \qquad X = R\cos\Phi \qquad Y = R\sin\Phi$

$$P(R, \Phi) = \frac{1}{2\pi} \int_0^{\Phi} d\phi\; \frac{1}{\sigma^2} \int_0^{R} dr\; r\, e^{-r^2/2\sigma^2} = \left(\frac{\Phi}{2\pi}\right)\left(1 - e^{-R^2/2\sigma^2}\right)$$

$P(R, \Phi)$ IS PRODUCT OF 2 INDEPENDENT PROB'S. $\left(\frac{\Phi}{2\pi}\right)$ & $\left(1 - e^{-R^2/2\sigma^2}\right)$

$\frac{\Phi}{2\pi}$ IS PROB OF $\phi \leq \Phi$, $\left(1 - e^{-R^2/2\sigma^2}\right)$ IS PROB. $r \leq R$

$$\frac{\Phi}{2\pi} = \xi_1 \qquad 1 - e^{-R^2/2\sigma^2} = \xi_2 \rightarrow \xi_2' = 1 - \xi_2$$

$$\Phi = 2\pi\xi_1 \qquad R = \sigma\sqrt{-2\ln(\xi_2')} \qquad \therefore\ \xi_2' \in [0,1]$$

$$\ln \xi_2' \leq 0$$

$$X = \sigma\sqrt{-2\ln \xi_2'}\cos(2\pi\xi_1)$$

$$Y = \sigma\sqrt{-2\ln \xi_2'}\sin(2\pi\xi_1)$$

X & Y ARE GAUSSIAN RANDOM NO'S GENERATED BY INPUTING UNIFORMLY SAMPLED RANDOM NO'S ξ_1 & $\xi_2' \in [0,1]$

$$\sigma_{MB} = \sqrt{\frac{kT}{m}} \rightarrow Y_1 = \sqrt{\frac{kT}{m}}\sqrt{-2\ln \xi_2'}\cos(2\pi\xi_1)$$

$$Y_2 = \sqrt{\frac{kT}{m}}\sqrt{-2\ln \xi_2'}\sin(2\pi\xi_1)$$

Problem 3: Midterm Exam

10
NOTE about the version error: I am using python2.7… I use this version because it is the one with which I am most familiar, i.e. there are syntactical differences between 2.7 and 3x. Version 2.7 is still supported and developed same as 3.x, along with all the modules that go with it… Additionally, the IDE I use (Spyder) is built for python2.7 and changing would require uninstalling the whole package manager (Conda) and installing the newer version 3… as well as converting all my codes. Sorry! I will start using 3 in the future!
Note: I fixed my non-dimensional velocity problem since the HW assignment; this project works in true non dimensional LJ units.

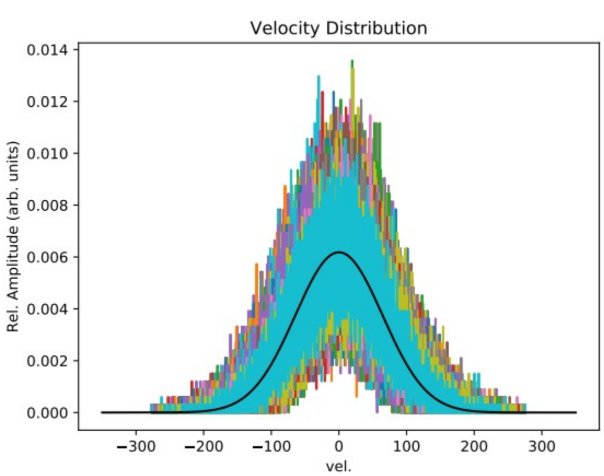
I randomly generate the initial velocities using the Box-Muller method, as done in class.

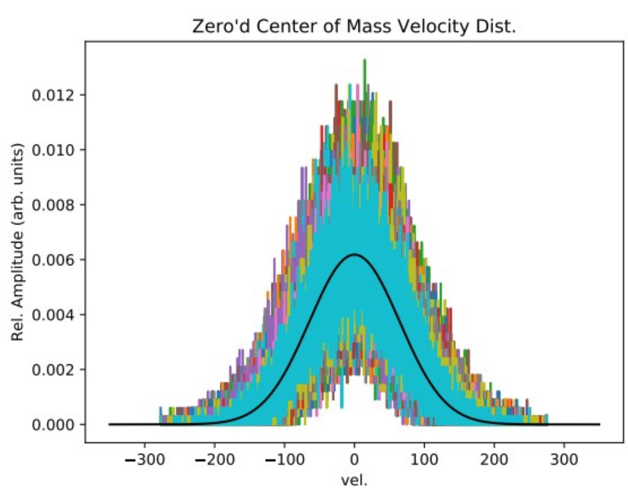
```
x1 = np.random.uniform(0,1,(num*3/2))
x2 = np.random.uniform(0,1,(num*3/2))
y1 = (kb*val/mass)**.5*(-2*np.log(x1))**.5*np.cos(2*np.pi*x2)
y2 = (kb*val/mass)**.5*(-2*np.log(x1))**.5*np.sin(2*np.pi*x2)
num = len(pos[:,0])
vels[:,2:5] = np.reshape(np.append(y1,y2),(num,3))[0:num,:]

cmv = (mass*vels[:,2:5]).sum(axis=0)/(mass*num)
vels[:,2:5] = vels[:,2:5]-cmv
```

x1 and x2 are random numbers sampled uniformly from [0,1). I sample num*3/2 random numbers each for x1 and x2, where num is the number of atoms.

x1 and x2 are then used to generate the two sets of random velocities, y1 and y2. The two arrays are concatenated to form an array num*3 elements long, then that array is reshaped into a (num,3) 2-d array that are the velocities. I then calculate the center of mass velocity vector for the whole distribution in x,y, and z and shift each component of the velocity vectors by that amount.

To validate that I am producing the right distribution, I plotted both the original and the zero'd center of mass velocity distributions versus the true Maxwell-Boltzann distribution for 100 iterations:

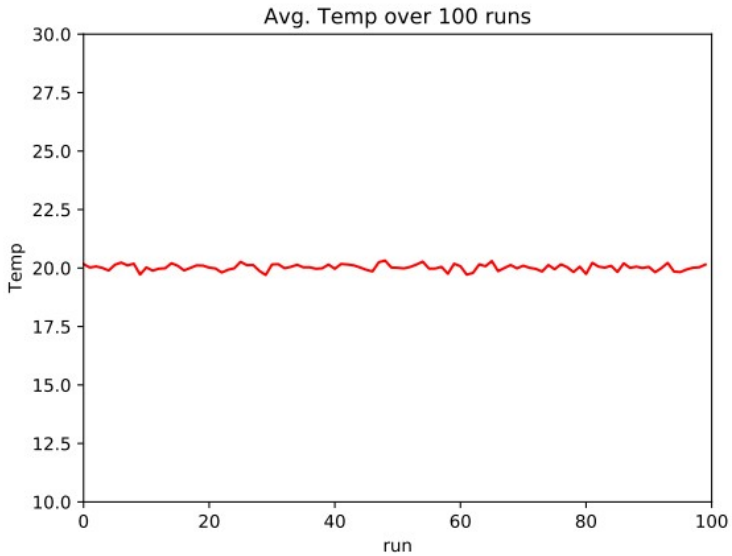




Problem 3: Midterm Exam

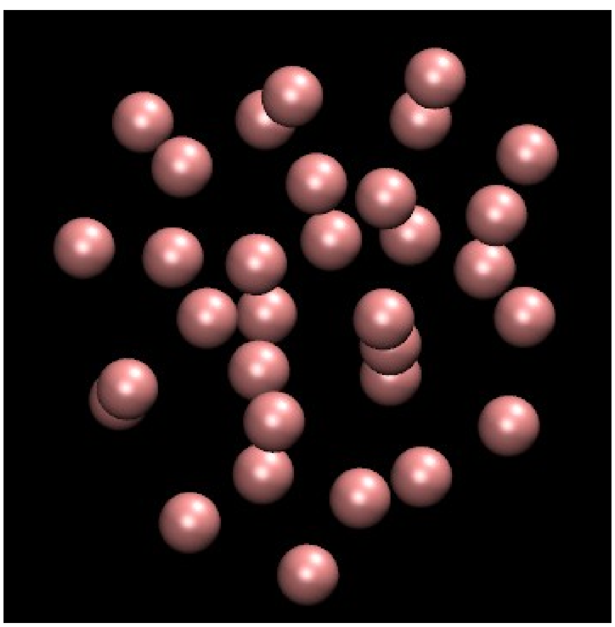
11

For each iteration, I also calculated the temperature from KE = 3/2 N Kb T, for each generated distribution. This ensures my velocities are scaled correctly:



The rest of the code is pretty much the same as before, except I minimized the number of arguments passed between functions. I do still work in dimensionless LJ units, but it’s done completely ‘behind the scenes.’

Here is a VMD snapshot of the cluster:



Problem 3: Midterm Exam

12

Finally, I updated my code to compute T, KE, and the x,y, and z components of total momentum, in addition to PE and total E that I provided before:

STEP	T	KE	PE	E	Px	Py	Pz
----	K	eV	eV	eV	pgA/ps	pgA/ps	pgA/ps
500	24.153	0.1	-1.333	-1.233	-0.001	0.0	-0.0
1000	21.669	0.09	-1.323	-1.233	-0.001	0.002	0.001
1500	22.456	0.093	-1.326	-1.233	-0.001	0.002	0.001
2000	21.27	0.088	-1.321	-1.233	0.0	0.003	0.001
2500	18.034	0.075	-1.308	-1.233	0.001	0.001	0.001
3000	28.707	0.119	-1.352	-1.233	0.0	0.001	0.001
3500	25.329	0.105	-1.338	-1.233	-0.0	0.0	0.001
4000	21.596	0.089	-1.322	-1.233	0.0	0.0	0.002
4500	18.552	0.077	-1.31	-1.233	0.001	-0.0	0.001
5000	20.926	0.087	-1.319	-1.232	0.0	-0.001	0.001
5500	22.791	0.094	-1.327	-1.233	0.0	-0.001	0.001
6000	22.794	0.094	-1.327	-1.233	0.0	-0.0	0.001
6500	21.504	0.089	-1.322	-1.233	0.0	0.001	0.002
7000	22.104	0.091	-1.324	-1.233	0.001	0.002	0.002
7500	18.745	0.078	-1.31	-1.232	0.001	0.001	0.001

Over the course of 15 ps, the temperature oscillates around 20 K as can be seen (and as is expected). The oscillations in T go with decreases in KE and increases in PE. However, total Energy, E, is conserved within 0.001 eV throughout the simulation.

Additionally, the total momentum vector (Px, Py, Pz) is very close to zero throughout the run, oscillating slightly one the order of 0.001 pg*ang/ps.