Homework Assignment #1

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ex=1 a) Please see provided python code.

b) V_{LJ} is minimum ~~at~~ when $\frac{\partial V}{\partial r} = \emptyset$ (ignoring the "ij" for the moment)

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$\frac{\partial r}{\partial r} = 4\varepsilon\left[\sigma^{12}\frac{\partial}{\partial r}\left(\frac{1}{r^{12}}\right) - \sigma^{6}\frac{\partial}{\partial r}\left(\frac{1}{r^{6}}\right)\right] = \emptyset$$

$$= 4\varepsilon\left[\sigma^{12}\cdot(-12)\cdot\frac{1}{r^{13}} - \sigma^{6}(-6)\cdot\frac{1}{r^{7}}\right] = \emptyset$$

$$\emptyset = 4\varepsilon\left[\frac{-12\sigma^{12}}{r^{13}} + \frac{6\sigma^{6}}{r^{7}}\right]$$

$\Rightarrow$ oxygen-oxygen

$\sigma = 0.295\ nm = 0.295\times10^{-9}\ m$

$\varepsilon = 61.6 \times k_B$

$\hookrightarrow 1.38\times10^{-23}\ \frac{m^2\,kg}{s^2 K}$

plug them in

$\therefore\ r = 3.31\times10^{-10}\ m = \underline{3.31\ \text{Angstrom}}$

$$F = -\frac{\partial V}{\partial r} = 4\varepsilon\left[\frac{12\sigma^{12}}{r^{13}} - \frac{6\sigma^{6}}{r^{7}}\right]$$

$$= 7.07885\times10^{-14}\ \underline{\text{Newtons}}$$

c) $$\sum_i^{2N-1} F_i(\vec{r}_1, \ldots \vec{r}_{2N+1}, \vec{v}_i) = \sum_i^{2N-1} m_i \frac{d^2\vec{r}_i}{dt^2}$$

d) Please see provided python code.

e) $\dfrac{6\cdot\binom{10^{23}}{2}\ \text{operations}}{10^{12}\ \text{operations}} \times \dfrac{\times\ \text{time}}{1\ \text{second}}$ → BuTinah

$\underline{10^{23}\text{ particles}}$

$$\frac{6\times\binom{10^{23}}{2}}{10^{12}} \times \frac{1\,min}{60\,sec} \times \frac{1\,h}{60\,min} \times \frac{1\,day}{24\,h} = \underline{3.47\times10^{29}\ \text{days}}$$

$\underline{10^{4}\text{ particles}}$

$$\frac{6\times\binom{10^{4}}{2}}{10^{12}} \times \frac{1\,min}{60\,sec} \times \frac{1\,h}{60\,min} \times \frac{1\,day}{24\,h} = \underline{3.47\times10^{-9}\ \text{days}}$$

$\boxed{ex=2}$

a) $\frac{d^2x}{dt^2} \Rightarrow x(t) = a\cos\omega t + b\sin\omega t$ $\longrightarrow$ general second-order differential solution

$x(0) = a\cos\phi + \cancel{b\sin\phi} = a\cos\phi = a = x(0).$

$v(0) = \frac{d\,x(0)}{dt} = -a\omega\sin\omega t + b\omega\cos\omega t \overset{t=\phi}{=} \cancel{-a\omega\sin\phi} + b\omega\cos\phi$

$= b\omega\cos\phi = b\omega = v(0)$

$b = \frac{v(0)}{\omega}$

Therefore, $x(t) = x(0)\cos\omega t + \frac{v(0)}{\omega}\sin\omega t$

$p(t) = m \cdot v(t) = m \cdot \left[-x(0)\,\omega\sin(\omega t) + \frac{v(0)}{\omega}\cos(\omega t)\right]$

$= \frac{m \cdot v(0)}{\omega}\cos\omega t - m \cdot x(0)\,\omega\sin\omega t$