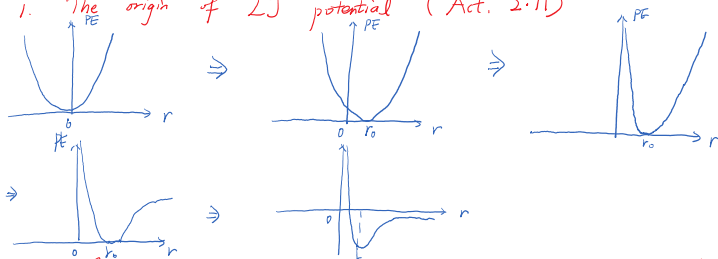


Supplimental materials for Quiz 4 (DL7 ~ DL 11)

Sunday, November 5, 2017 6:00 PM

Important ideas and equations

1. The origin of LJ potential (Act. 2.11)



2. The meaning of σ , r_0 , ϵ (Act. 3.2 3)

σ - diameter of atom

$$r_0 = 1.12\sigma$$

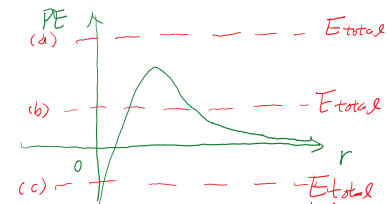
ϵ = magnitude of the most negative value of PE (always positive)

3. how to obtain PE with different distance r (practice by yourself)

4. bonded or unbonded (FNT 8 & 9)

Given total energy and PE curve, you should know the type of motion and range of motion.

Quick check: Bounded or unbounded?



5. Bond energy definition

$$BE \stackrel{\text{def}}{=} \sum (PE_{\text{pair-wise}})$$

For nearest neighbors: $r = r_0$, $PE_{\text{pair-wise}} = -\epsilon$

$$BE = \# NN \times (-\epsilon)$$

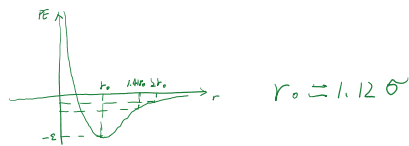
6. bond energy calculation

a). When particles are in small amount:

Count $\# NN$ (nearest neighbors) and $\# NNN$ (next nearest neighbors), calculate PE pair-wise separately.

$$BE = \# NN \times (-\epsilon) + \# NNN \times (-\epsilon')$$

ϵ' is found by PE curve.

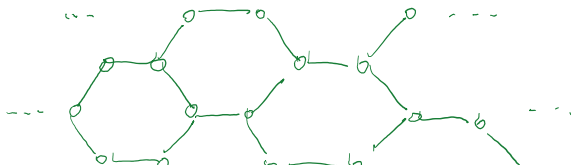
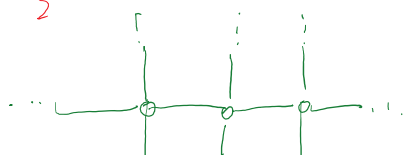


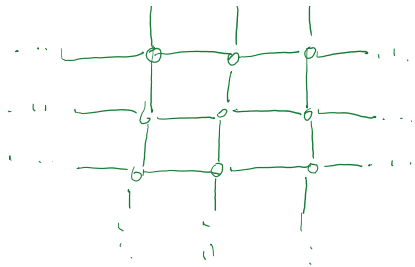
b). in huge amount:

As an approximation:

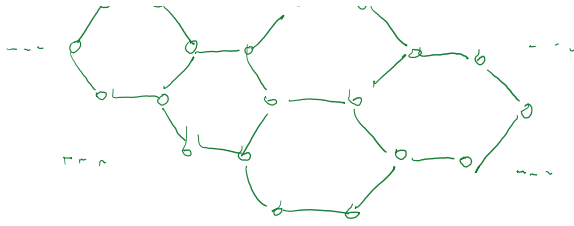
$$BE \approx \frac{1}{2} \times \# NN \times \# \text{ particles} \times (-\epsilon)$$

$\frac{\# NN}{2}$ is the average number of bonds for each particle.





$$\frac{\#NN}{\Sigma} = \frac{4}{2} = 2$$



$$\frac{\#NN}{\Sigma} = \frac{3}{2} = 1.5$$

c). edge effect

7. energy modes & temperature

thermal equilibrium means same temperature. 

$$T_A = T_B$$

(For energy: Thermal energy of A & B might not be the same)

Supplimental readings:

Your textbook chapter 3: P 66 - 68

DL workbook foldout: Particle model of thermal energy

Equipartition theorem from Wikipedia