

Outline of 7A

Zeppelin Wang

Phase change and energy conservation

Two important models

1. three phase model
x-axis, y-axis, $E_{thermal}$, E_{Bond} , slope, turning points, heat capacity C_v , specific heat C_{vm} , change of enthalpy ΔH
2. energy interaction model
open vs close system, different indicators, energy equation (energy conservation), definition of heat and work, the meaning of Δ , different convey by initial and final state

Typical questions

1-4, 2-5, 3-1, 3-4

Mechanical energy system

Types of mechanical energy

1. gravitational potential energy
constant g , position dependence, change of energy $\Delta PE = mg\Delta h$, the choose of 'zero'
2. kinetic energy
velocity quadratic dependence, change of energy $\Delta KE = \frac{1}{2}m\Delta(v^2)$, when reaches max and min, translation and rotation(*)
3. spring mass potential energy
distance quadratic dependence (distance to zero Δx), spring constant k , energy transfer between spring and mass (Act. 2.4 B, Act. 2.7 3), change of energy $\Delta SE = \frac{1}{2}k\Delta(\Delta x)^2$

Input and output(or dissipation)

1. work W
could do to your system or be done by system(sign of work), definition $W = \int Fdx$ (the work done by force F), another form $W = - \int pdV$, determined by process
2. heat Q
could throw to your system or be released by system(sign of heat), the result of frictions, definition $Q = \int CdT = n \int C_{molar}dT = m \int C_{mass}dT$, determined by process

Typical questions

4-2, Act. 2.4, 5-2, 5-3, 5-5, 5-6, Act. 2.7, Act. 2.8, 6-3

Microscopic interaction and energy system

LJ potential

1. transfer from spring mass potential to LJ potential
the relationship between force and potential $F = -|\frac{dPE}{dr}|$
Act. 2.11
why curve goes flat when distance is so large
why we set energy to be zero when distance is so large
2. meaning of σ , r_0 and ϵ
 σ is the distance of two atoms when they are touched
 $r_0 = 1.12\sigma$, which is the equilibrium position(minimum LJ potential)
 ϵ is the value of minimum LJ potential
3. bonded or unbonded
Given the total energy and potential energy curve, you shall know whether the object can reach the infinite distance or not

Microscopic energy

1. definition of bond energy
energy for single bond: $E_{single\ bond} + W = 0$. W is the work you need to separate two atoms to infinity. 0 is the total energy when two atoms reach infinity distance
always have negative values
 $E_{bond} = \sum(PE_{pair-wise})$
2. bond energy calculation
nearest neighbor(NN), next nearest neighbor(NNN)

$E_{bond} = Total\ number\ of\ bonds * PE_{single\ bond}$

Approximation: $E_{bond} \approx NN(nearest\ neighbor)\ bonds * PE_1 + NNN\ bonds * PE_2$, where PE_1 and PE_2 are single bond energy when two atoms are NN and NNN (Here we neglect part of bond energy when two atoms are further than NNN).

Further approximation: $E_{bond} \approx \frac{\#Total\ atoms}{2} (\#NN * PE_1 + \#NNN * PE_2)$. Here we neglect the atoms who are on the edge. $\#NN$ means number of nearest neighbors for one atom in the bulk, and so does $\#NNN$.

edge effect

3. thermal energy and bond energy (Act. 3.9)

When temperature is rising, E_{bond} does not change, $E_{thermal}$ increases.

$$PE = E_{bond} + \frac{1}{2}E_{thermal}$$

$$KE = \frac{1}{2}E_{thermal}$$

Potential and translation motion bisect total modes

For gas the situation will be different

Energy modes

1. meaning of modes

Degree of freedom

equipartition principle: each mode gets energy $E = \frac{1}{2}k_B T$

$$E_{th} = Total\ \#\ of\ modes * \frac{1}{2}k_B T = \# atoms * \frac{\# modes\ per\ atom}{2} k_B T$$

monatomic, diatomic and complex (more than 2 atoms) gas

frozen modes: temperature dependence, vibrational modes

2. constant-volume molar heat capacity C_{vm}

when $\Delta E_{bond} = 0, W = 0, Q = \Delta E_{th}$

$$\text{heat capacity } C = \frac{C}{\Delta T} = \frac{\Delta E_{th}}{\Delta T} = \# atoms * \frac{\# modes\ per\ atom}{2} k_B$$

$$\# atoms = N_A * \# moles = N_A * n$$

$$\text{molar heat capacity } C_{vm} = \frac{C}{n} = N_A * \frac{\# modes\ per\ atom}{2} k_B = \frac{\# modes\ per\ atom}{2} R$$

Typical questions

7-3, 8-3, 8-4, 10-5, 11-7, 12-4, Act. 3.13, 13-1

1st and 2nd law of thermodynamics

State functions and P-V diagram

1. state function

Only depends on initial and final states, no matter how the process in between goes

2. process variable
depends on the path from initial to final(example: the direction of path, the area under the path)
3. internal energy
Basically, $U = E_{th} + E_{bond}$
4. ideal gas equation of state
 $Pressure * Volume = \# moles * R * Temperature$
5. P-V diagram for ideal gas
The initial and final pressure and volume could be read. Temperature could be interpreted by ideal gas equation of state.
 $\Delta U = \Delta E_{th} = \# atoms * \frac{\# modes per atom}{2} k_B \Delta T$
magnitude of work: area under the path
sign of work: + when final volume is smaller than initial; - when final volume is bigger than initial

1st law of thermodynamics

1. description: energy conservation
 $\Delta U = Q + W$
Q is + when heat is absorbed by system, - when heat is released
W is + when work is done to system, - when done by system
2. constant-pressure molar heat capacity C_{pm}
 $C_{pm} = C_{vm} + R$
3. Enthalpy
 $\Delta H = \Delta(U + PV) = \Delta U + P\Delta V = \Delta U - W = Q$

Probability and microstates

1. definition of states and microstates
microstate a specific orientation of your system(one specific orientation for 100 coins)
state: a series of microstates who attribute to same macroscopic property(all the orientations which have 50 heads for 100 coins)
2. equiprobability
all the microstates have the same possibility to occur
3. maximum probability
The state which has highest possibility(biggest number of microstates) is the state shown in reality in equilibrium
4. multiplication or addition

Entropy and T-S diagram

1. definition

description: the randomness of the system (the number of microstates)

statistic expression: $S = k_B \ln \Omega$

classic expression: $\Delta S = \frac{Q}{T_{avg}}$ ($dS = \frac{\bar{d}Q}{T}$)

2. T-S diagram for ideal gas

The initial and final temperature could be read. ΔU could be interpreted.

magnitude of heat: area under the curve

sign of heat: + when final entropy is bigger than initial; - when final entropy is smaller than initial

2nd law of thermodynamics

1. reversible and irreversible process

reversible: $\Delta S = 0$

irreversible: $\Delta S > 0$

2. 2nd law of thermodynamics

description: All the processes happening in the universe should obey

$\Delta S \geq 0$

Typical questions

14-2, 15-4, 16-1, 17-2, all the relating questions in practical quizzes