

Unit 13 - Week 8

Course outline
How does an NPTEL online course work?
MATLAB
MATLAB_SCRIPTS
LAMMPS_SCRIPTS
Installation_Procedure
Week 1
Week 2
Week 3
Week 4
Week 5
Week 6
Week 7
Week 8
<input checked="" type="radio"/> Introduction to phase space
<input type="radio"/> Introduction to phase average and time average
<input checked="" type="radio"/> Canonical ensemble; Partition function
<input checked="" type="radio"/> Week 8 Lecture materials
<input type="radio"/> Quiz : Assignment 8
<input type="radio"/> Week 8 Feedback : Foundations of Computational Materials Modelling
Week 9
Week 10
Week 11
Week 12
Additional Documents
Download videos
Text Transcripts

Assignment 8

The due date for submitting this assignment has passed. Due on 2020-03-25, 23:59 IST.
 As per our records you have not submitted this assignment.

- 1) The phase average of a quantity 'A' is $\langle A \rangle = \frac{\int A(q, p) \rho(q, p, t) dp dq}{\int \rho(q, p, t) dp dq}$ 2 points
- True
 False
- No, the answer is incorrect.
 Score: 0
 Accepted Answers:
 True
- 2) The time average properties of a quantity 'A' is 2 points
- $\lim_{\Delta t \rightarrow \infty} \Delta t \int_{t_0}^{t_0 + \Delta t} A(q(t), p(t)) dt$

 $\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{t_0}^{t_0 + \Delta t} A(q(t), p(t)) dt$

 $\lim_{\Delta t \rightarrow 0} \Delta t \int_{t_0}^{t_0 + \Delta t} A(q(t), p(t)) dt$

 $\lim_{\Delta t \rightarrow \infty} \frac{1}{\Delta t} \int_{t_0}^{t_0 + \Delta t} A(q(t), p(t)) dt$
- No, the answer is incorrect.
 Score: 0
 Accepted Answers:
 $\lim_{\Delta t \rightarrow \infty} \frac{1}{\Delta t} \int_{t_0}^{t_0 + \Delta t} A(q(t), p(t)) dt$
- 3) Which of the following is not true for microcanonical ensemble? 2 points
- E, V, N constant
 System is isolated.
 It has a specific total Energy
 The temperature of the system is fixed
- No, the answer is incorrect.
 Score: 0
 Accepted Answers:
 The temperature of the system is fixed
- 4) The average kinetic energy of gas molecules with known temperature is? 2 points
- kT
 $3kT$
 $\frac{3}{2}kT$
 $\frac{2}{3}kT$
- No, the answer is incorrect.
 Score: 0
 Accepted Answers:
 $\frac{3}{2}kT$
- 5) For an isolated system, every microstate is equally probable 2 points
- True
 False
- No, the answer is incorrect.
 Score: 0
 Accepted Answers:
 True
- 6) For canonical ensemble, which of the following is true? 2 points
- $\rho \propto \exp\left(\frac{-H(p, q)}{k_b T}\right)$

 $\rho \propto \exp\left(\frac{-k_b T}{H(p, q)}\right)$

 $\rho > \exp\left(\frac{-k_b T}{H(p, q)}\right)$

 $\rho < \exp\left(\frac{-k_b T}{H(p, q)}\right)$
- No, the answer is incorrect.
 Score: 0
 Accepted Answers:
 $\rho \propto \exp\left(\frac{-H(p, q)}{k_b T}\right)$
- 7) The relation between the number of microstates $\Omega(E)$ for an ideal gas of N monoatomic molecules in a volume V is related to energy E :? 2 points
- $\Omega(E) \propto E$
 $\Omega(E) \propto E^N$
 $\Omega(E) \propto E^{\frac{N}{2}}$
 $\Omega(E) \propto E^{\frac{3N}{2}}$
- No, the answer is incorrect.
 Score: 0
 Accepted Answers:
 $\Omega(E) \propto E^{\frac{3N}{2}}$
- 8) In a canonical ensemble, a system A of fixed volume is in contact with a large reservoir B. Then ____ 2 points
- A can exchange only energy with B
 A can exchange only particles with B
 A can exchange neither energy nor particles with B
 A can exchange both energy and particles with B
- No, the answer is incorrect.
 Score: 0
 Accepted Answers:
 A can exchange only energy with B
- 9) In classical statistical mechanics, when the system is in thermal equilibrium, the equipartition theorem relates the temperature of a system to its average energies. 2 points
- True
 False
- No, the answer is incorrect.
 Score: 0
 Accepted Answers:
 True
- 10) In the following expression, P_r is 2 points
- $$P_r = \frac{\exp(-\beta E_r)}{\sum_r \exp(-\beta E_r)}$$
- the pressure at temperature r
 the probability that the system evolves from the current energy to the energy E_r
 the probability of finding the temperature so that the energy is E_r
 the probability of finding the system with energy E_r
- No, the answer is incorrect.
 Score: 0
 Accepted Answers:
 the probability of finding the system with energy E_r
- 11) $\ln(N!)$ for large N is 2 points
- $N \ln(N) - N$
 $N \ln(N)$
 N
 0
- No, the answer is incorrect.
 Score: 0
 Accepted Answers:
 $N \ln(N) - N$
- 12) If the Helmholtz energy is written as 1 point
- $$A = -k_b T \ln(Q_N(V, T))$$
- Then Q
- is called the Quotient
 is the ratio of the Energy of the system to the maximum energy it can attain
 is called the Partition function
 Is a constant with temperature
- No, the answer is incorrect.
 Score: 0
 Accepted Answers:
 is called the Partition function