

Unit 12 - Week 7

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

● Statistical mechanics 2

● Basic introduction to mechanics

○ Quiz : Assignment 7

● Week 7 Lecture materials

○ Week 7 Feedback : Foundations of Computational Materials Modelling

Week 8

Week 9

Week 10

Week 11

Week 12

Additional Documents

Download videos

Text Transcripts

Assignment 7

The due date for submitting this assignment has passed.
As per our records you have not submitted this assignment.

Due on 2020-03-18, 23:59 IST.

- 1) In statistical mechanics, a semi-classical derivation of the entropy that does not take into account the indistinguishability of particles, yields an expression for the entropy which is not extensive. This leads to a paradox known as the Gibbs paradox. **2 points**

- True
 False

No, the answer is incorrect.
Score: 0

Accepted Answers:
True

- 2) The _____ of a system is defined to be the difference between the kinetic and potential energies of the system expressed as a function of positions and velocities. **2 points**

- Lagrangian
 Hamiltonian
 Total Energy
 None of the above

No, the answer is incorrect.
Score: 0

Accepted Answers:
Lagrangian

- 3) True or False:

For the Gamma (Γ) function,

$$x\Gamma(x) = \Gamma(x + 1)$$

- True
 False

No, the answer is incorrect.
Score: 0

Accepted Answers:
True

- 4) The total number of possible states for a single particle with an energy less than E^* is **2 points**

$$\phi_{<E^*} = \frac{\pi}{6} \left(\frac{E^* 8mV}{3 h^2} \right)^{\frac{2}{3}}$$

- True
 False

No, the answer is incorrect.
Score: 0

Accepted Answers:
False

- 5) The Lagrangian of a system is defined to be the sum of the kinetic and potential energies expressed as a function of positions and their conjugate momenta. **2 points**

- True
 False

No, the answer is incorrect.
Score: 0

Accepted Answers:
False

- 6) Complete the Hamilton's equations below: **2 points**

$$\frac{dp}{dt} = \text{_____}, \quad \frac{dq}{dt} = \text{_____}$$

- $-\frac{\partial H}{\partial q}, \frac{\partial H}{\partial p}$
 $-\frac{\partial H}{\partial q}, -\frac{\partial H}{\partial p}$
 $\frac{\partial H}{\partial q}, -\frac{\partial H}{\partial p}$
 $\frac{\partial H}{\partial q}, \frac{\partial H}{\partial p}$

No, the answer is incorrect.
Score: 0

Accepted Answers:
 $-\frac{\partial H}{\partial q}, \frac{\partial H}{\partial p}$

- 7) True or False:

$$\Gamma(x + 1) = \Gamma!$$

- True
 False

No, the answer is incorrect.
Score: 0

Accepted Answers:
True

- 8) What is the expression for hamiltonian formulation from the Lagrangian ? **2 points**

- $H(p, r) = \sum_{i=1}^N p_i \cdot \dot{r}_i + L(r, \dot{r})$
 $H(p, r) = \sum_{i=1}^N p_i \cdot \dot{r}_i - L(r, \dot{r})$
 $H(p, r) = \sum_{i=1}^N \dot{p}_i \cdot r_i - L(r, \dot{r})$
 $H(p, r) = \sum_{i=1}^N \dot{p}_i \cdot r_i + L(r, \dot{r})$

No, the answer is incorrect.
Score: 0

Accepted Answers:
 $H(p, r) = \sum_{i=1}^N p_i \cdot \dot{r}_i - L(r, \dot{r})$

- 9) A Legendre transform is used to switch between Lagrangian formulation and Hamiltonian formulation _____. **2 points**

- True
 False

No, the answer is incorrect.
Score: 0

Accepted Answers:
True

- 10) _____ ensemble represents an isolated system. **2 points**

- μVT
 NVT
 NVE
 NPT

No, the answer is incorrect.
Score: 0

Accepted Answers:
NVE

- 11) NVT ensemble is also called _____ ensemble **2 points**

- grand canonical
 isolated
 micro canonical
 canonical

No, the answer is incorrect.
Score: 0

Accepted Answers:
canonical