Name: _____

Student number: _____

1. Compute the derivative of the function: $f(x) = \cos(nx+n)$, with respect to x; n is an integer number.

   Solution. Chain rule with inner function $u = nx + n$, $\dfrac{du}{dx} = n$:

   $$f'(x) = -\sin(nx+n)\cdot n = -n\sin(nx+n).$$

Answer: _____

2. Compute the **total derivative** (or **total differential**) of the following state function,

   $$f(T,P) = w_0 + w_1 P + (w_2 + w_3 P)T + (w_4 + w_5 P)T^{-2},$$

   where w_i are virial coefficients.

   Solution.

   $$\left(\frac{\partial f}{\partial T}\right)_P = (w_2 + w_3 P) - \frac{2(w_4 + w_5 P)}{T^3}, \qquad \left(\frac{\partial f}{\partial P}\right)_T = w_1 + w_3 T + \frac{w_5}{T^2}$$

   $$df = \left[(w_2 + w_3 P) - \frac{2(w_4 + w_5 P)}{T^3}\right] dT + \left[w_1 + w_3 T + \frac{w_5}{T^2}\right] dP$$

Answer: _____

3. What is the value of the following integral?

$$\int \texttt{ELU}(x)\, dx$$

The ELU function is defined as,

$$\texttt{ELU}(x) = \begin{cases} x & \text{if} \quad x \geq 0 \\ \alpha(e^x - 1) & \text{if} \quad x < 0 \end{cases}$$

where α is a constant.
• (Tip) Integrals can be split into multiple ones each with a different integration range.

Solution. Integrate each branch:

$$x \geq 0: \quad \int x\, dx = \frac{x^2}{2} + C_1, \qquad x < 0: \quad \int \alpha(e^x - 1)\, dx = \alpha(e^x - x) + C_2.$$

Since ELU is continuous, the antiderivative must also be continuous at $x = 0$:

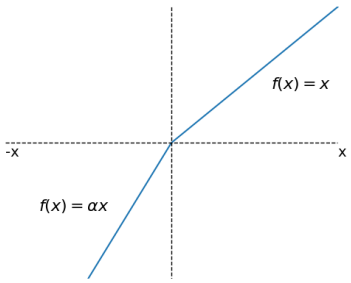
$$\lim_{x \to 0^-} F(x) = \alpha + C_2 \;=\; F(0) = C_1 \qquad \Longrightarrow \qquad C_2 = C_1 - \alpha.$$

Hence, with a single constant C,

$$\int \texttt{ELU}(x)\, dx = \begin{cases} \dfrac{x^2}{2} + C & \text{if } x \geq 0 \\ \alpha\,(e^x - x - 1) + C & \text{if } x < 0 \end{cases}$$

Answer:_____

4. In class, we computed the derivative of the so-called function ReLU (rectified linear unit) using the definition of a derivative through the limit. Some of the more modern AI models use a modified version of the ReLU named Parametric ReLU function (PReLU(x)), defined as,



$$\texttt{PReLU}(x) = \max(\alpha\, x, x) = \begin{cases} \alpha\, x & \text{if} \quad x < 0 \\ x & \text{if} \quad x \geq 0 \end{cases}$$

where α is the slope parameter for negative values.
Compute the derivative of PReLU using the limit definition when,

(a) Δx is negative and $x = 0$

Solution. Here $\texttt{PReLU}(0) = 0$ (the $x \geq 0$ branch). Since $\Delta x < 0$, the point $0 + \Delta x = \Delta x$ is negative, so $\texttt{PReLU}(\Delta x) = \alpha\, \Delta x$:

$$\lim_{\Delta x \to 0^-} \frac{\alpha \Delta x - 0}{\Delta x} = \lim_{\Delta x \to 0^-} \alpha = \alpha.$$

This is the *left-hand* derivative at the origin.

Answer:_____

Cont.

(b) Δx and x are both positives

Solution. Both x and $x + \Delta x$ are positive, so both use the branch $\texttt{PReLU}(x) = x$:

$$\lim_{\Delta x \to 0^+} \frac{(x + \Delta x) - x}{\Delta x} = \lim_{\Delta x \to 0^+} \frac{\Delta x}{\Delta x} = 1.$$

Since the two one-sided derivatives at $x = 0$ are α and 1, PReLU is differentiable at the origin only if $\alpha = 1$.

Answer:

5. Compute the Hessian for $f(x, y) = x + x^2 + x^3 - y + \exp(y^2)$.

Solution. First derivatives: $f_x = 1 + 2x + 3x^2, \quad f_y = -1 + 2y\, e^{y^2}$. Then

$$f_{xx} = 2 + 6x, \qquad f_{yy} = 2e^{y^2}\left(1 + 2y^2\right), \qquad f_{xy} = f_{yx} = 0$$

(the mixed partials vanish because the function is a sum of a term in x only and a term in y only). Hence

$$\mathbf{H} = \begin{bmatrix} 2 + 6x & 0 \\ 0 & 2e^{y^2}\left(1 + 2y^2\right) \end{bmatrix}$$

Answer:

6. Isothermal compressibility is defined by

$$\kappa = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T.$$

Determine κ for van der Waals gas, where $p(T, V) = \frac{RT}{V-b} - \frac{a}{V^2}$.

Hint: You can use the **reciprocity relation**, $\left(\frac{\partial z}{\partial x}\right)_y = \frac{1}{\left(\frac{\partial x}{\partial z}\right)_y}$

Solution. The equation of state gives p explicitly, so differentiate it and invert:

$$\left(\frac{\partial p}{\partial V}\right)_T = -\frac{RT}{(V-b)^2} + \frac{2a}{V^3}$$

By reciprocity, $\left(\frac{\partial V}{\partial p}\right)_T = \left[-\frac{RT}{(V-b)^2} + \frac{2a}{V^3}\right]^{-1}$, so

$$\kappa = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T = \frac{1}{V\left[\frac{RT}{(V-b)^2} - \frac{2a}{V^3}\right]} = \frac{V^2(V-b)^2}{RT\,V^3 - 2a(V-b)^2}$$

Check: with $a = b = 0$ this reduces to $\kappa = V/(RT) = 1/p$, the ideal-gas result.

Answer:

7. Let's assume the molar enthalpy ($\bar{H}$) is a state function of T and P.

Cont.

(a) For a gas obeying the equation of state,

$$\bar{V} = \frac{RT}{P} - \frac{a}{RT}P + b,$$

where a and b are constants. The **total differential** of $\bar{H}$ can be written as,

$$d\bar{H} = \bar{C}_P dT + \left(-T\left(\frac{\partial \bar{V}}{\partial T}\right)_P + \bar{V}\right) dP.$$

Determine an expression for $(\partial \bar{H}/\partial P)_T$

Solution. Reading off the coefficient of dP,

$$\left(\frac{\partial \bar{H}}{\partial P}\right)_T = -T\left(\frac{\partial \bar{V}}{\partial T}\right)_P + \bar{V}.$$

From the equation of state,

$$\left(\frac{\partial \bar{V}}{\partial T}\right)_P = \frac{R}{P} + \frac{aP}{RT^2}.$$

Substituting, the RT/P terms cancel:

$$\left(\frac{\partial \bar{H}}{\partial P}\right)_T = -\frac{RT}{P} - \frac{aP}{RT} + \frac{RT}{P} - \frac{aP}{RT} + b = b - \frac{2aP}{RT}$$

Answer:_____

(b) Get an expression for $(\partial \bar{C}_P/\partial P)_T$.
Hints:

- Remember that for a multivariate function, e.g., $f(x_1, x_2)$, $\frac{\partial^2 f(x_1,x_2)}{\partial x_1 \partial x_2} = \frac{\partial^2 f(x_1,x_2)}{\partial x_2 \partial x_1}$.
- Check the total differential definition for $\bar{H}$.

Solution. From the total differential, $\left(\frac{\partial \bar{H}}{\partial T}\right)_P = \bar{C}_P$. Because $\bar{H}$ is a state function the mixed second partials are equal:

$$\left(\frac{\partial \bar{C}_P}{\partial P}\right)_T = \frac{\partial^2 \bar{H}}{\partial P\, \partial T} = \frac{\partial^2 \bar{H}}{\partial T\, \partial P} = \left(\frac{\partial}{\partial T}\left[-T\left(\frac{\partial \bar{V}}{\partial T}\right)_P + \bar{V}\right]\right)_P$$

Carrying out the T-derivative, two terms cancel:

$$-\left(\frac{\partial \bar{V}}{\partial T}\right)_P - T\left(\frac{\partial^2 \bar{V}}{\partial T^2}\right)_P + \left(\frac{\partial \bar{V}}{\partial T}\right)_P = -T\left(\frac{\partial^2 \bar{V}}{\partial T^2}\right)_P$$

This is the general result. For this equation of state, $\left(\frac{\partial^2 \bar{V}}{\partial T^2}\right)_P = -\frac{2aP}{RT^3}$, so

$$\left(\frac{\partial \bar{C}_P}{\partial P}\right)_T = \frac{2aP}{RT^2}$$

(the same result follows by differentiating the answer to part (a) with respect to T).

Answer:_____

Cont.

8. Consider an idealized liquid or solid whose volume is independent of temperature and pressure.

(a) Assume that its internal energy depends only on temperature, $U = U(T)$. Using the relationship

$$C_P = \left(\frac{\partial U}{\partial T}\right)_p + p\left(\frac{\partial V}{\partial T}\right)_p,$$

show that

$$C_P = C_V.$$

Hint: Consider how the volume changes when the system is heated at constant pressure.

Solution. From the first law, $dQ = dU + p\,dV$, expanded in the variables T and p:

$$dU = \left(\frac{\partial U}{\partial T}\right)_V dT + \left(\frac{\partial U}{\partial V}\right)_T dV, \qquad dV = \left(\frac{\partial V}{\partial T}\right)_p dT + \left(\frac{\partial V}{\partial p}\right)_T dp.$$

Collecting terms,

$$dQ = \left[C_V + \left(\left(\frac{\partial U}{\partial V}\right)_T + p\right)\left(\frac{\partial V}{\partial T}\right)_p\right] dT + \left[\left(\frac{\partial U}{\partial V}\right)_T + p\right]\left(\frac{\partial V}{\partial p}\right)_T dp,$$

so that $C_P = (dQ/dT)_p$ is the coefficient of dT.
For one mole of ideal gas, $(\partial U/\partial V)_T = 0$ and $V = RT/p$:

$$dQ = (C_V + R)\,dT - V\,dp \qquad \Longrightarrow \qquad C_P = C_V + R.$$

For the incompressible solid or liquid, $(\partial V/\partial T)_p = (\partial V/\partial p)_T = 0$, so the dp term vanishes and

$$dQ = C_V\,dT \qquad \Longrightarrow \qquad C_P = C_V.$$

Answer:_____

(b) Explain physically why the heat capacities are equal, referring to the first law and pressure–volume work.

Solution. Heating the solid or liquid at constant pressure produces no expansion, so it performs no pressure–volume work, $W = -p\int dV = 0$. By the first law $\Delta U = q + W = q$, so every joule of heat goes directly into internal energy — exactly as in a constant-volume process, where no work is possible either. Since neither path diverts energy into pushing back the surroundings, the heat required per degree is the same and $C_P = C_V$. For a gas the difference nR is precisely that expansion work, which here is zero.

Cont.

9. Let's consider a function of two variables, $f(xy) = c_0\, f_0(x) + c_1\, f_1(y)$, where c_0 and c_1 are some coefficients. Select the option that contains the second-order partial derivatives that **are non-zero**.

A) $\left[\frac{\partial^2 f(xy)}{\partial^2 x^2}, \frac{\partial^2 f(xy)}{\partial^2 y^2}\right]$

B) $\left[\frac{\partial^2 f(xy)}{\partial^2 y^2}, \frac{\partial^2 f(xy)}{\partial x \partial y}, \frac{\partial^2 f(xy)}{\partial y \partial x}\right]$

C) $\left[\frac{\partial^2 f(xy)}{\partial y \partial x}, \frac{\partial^2 f(xy)}{\partial^2 y^2}, \frac{\partial^2 f(xy)}{\partial^2 x^2}\right]$

D) $\left[\frac{\partial^2 f(xy)}{\partial^2 y^2}, \frac{\partial^2 f(xy)}{\partial x \partial y}, \frac{\partial^2 f(xy)}{\partial^2 x^2}, \frac{\partial^2 f(xy)}{\partial y \partial x}\right]$

Solution. **A)**. Since $\frac{\partial f}{\partial x} = c_0 f_0'(x)$ contains no y, the mixed partials vanish: $\frac{\partial^2 f}{\partial y\, \partial x} = \frac{\partial^2 f}{\partial x\, \partial y} = 0$. Only the pure second derivatives $c_0 f_0''(x)$ and $c_1 f_1''(y)$ survive.

Answer:_____

For the next 10 questions, circle the correct answer.

10. The $\lim_{x\to 1} \frac{x^2-1}{x-1}$ does **NOT** exist.

A) True **B)** False

Solution. **B) False.** Factor: $\frac{(x-1)(x+1)}{x-1} = x+1 \to 2$. The limit exists; only the *value* $f(1)$ is undefined (removable discontinuity).

Answer:_____

11. If f is differentiable at $x = a$, then f is continuous at $x = a$.

A) True **B)** False

Solution. **A) True.** Differentiability implies continuity. (The converse is false: $|x|$ at $x = 0$.)

Answer:_____

12. $\frac{d}{dx}[\ln(3x)] = \frac{1}{x}$.

A) True **B)** False

Solution. **A) True.** Either $\ln(3x) = \ln 3 + \ln x$, whose derivative is $1/x$, or by the chain rule $\frac{3}{3x} = \frac{1}{x}$. The constant 3 does not survive.

Answer:_____

Cont.

13. $\dfrac{d}{dx}[x^x] = x\,x^{x-1}$.

A) True **B)** False

Solution. **B) False.** The power rule requires a *constant* exponent. By logarithmic differentiation, $\ln y = x \ln x \Rightarrow y'/y = \ln x + 1$, so $\dfrac{d}{dx}x^x = x^x\,(\ln x + 1)$. (Note the stated answer simplifies to x^x, which would make the function its own derivative.)

Answer:_____

14. $\dfrac{d}{dx}\left[e^{x^2}\right] = e^{x^2}$.

A) True **B)** False

Solution. **B) False.** The chain rule gives $\dfrac{d}{dx}e^{x^2} = 2x\,e^{x^2}$.

Answer:_____

15. The change in the state function is always lower than than zero if the system returns to its initial state during the processes.

A) True **B)** False

Solution. **B) False.** A state function depends only on the state, so over any cycle its change is exactly *zero*, $\oint dF = 0$ — not negative.

Answer:_____

16. According to the second law of thermodynamics, which of the following must be true for a process to be spontaneous? **A)** $\Delta S_{\text{system}} > 0$ **B)** $\Delta S_{\text{surroundings}} > 0$ **C)** $\Delta S_{\text{universe}} > 0$ **D)** $\Delta S_{\text{system}} = 0$

Solution. **C)** $\Delta S_{\text{universe}} > 0$. The system's entropy may decrease (e.g. freezing) provided the surroundings increase by more.

Answer:_____

17. Which of the following thermodynamic quantities are **not** state functions?

A) H (Enthalpy)
B) G (Gibbs free energy)
C) T (Temperature)
D) q (Heat)
E) S (Entropy)
F) P (Pressure)
G) W (Work)
H) U (Internal energy)
I) V (Volume)

Cont.

Solution. **D) q and G) W.** Heat and work are *path* functions — they describe energy in transit and depend on how the change is carried out, so δq and δW are inexact differentials. All the others depend only on the state of the system.

Answer:_____

18. Which of the following statements about isobaric, isochoric, and isothermal processes is **True**?

A) In an isobaric process, the pressure remains constant while the volume changes.

B) In an isochoric process, both temperature and pressure remain constant.

C) In an isothermal process, the volume remains constant and temperature changes.

D) In an isobaric process, the internal energy of the system does not change.

Solution. **A)**. Isobaric means constant p. B) is wrong (isochoric fixes V), C) is wrong (isothermal fixes T), and D) is wrong ($\Delta U \neq 0$ in general at constant pressure).

Answer:_____

19. Which of the following is true for a **reversible adiabatic process**?

The first law of thermodynamics is given by $\Delta U = q + w$, where ΔU is the change in internal energy, q is the heat added to the system, and w is the work done on the system.

A) $q = 0$, so $\Delta U = w$

B) $w = 0$, so $\Delta U = q$

C) $\Delta U = 0$, so $q = -w$

D) $\Delta U = q + w$, as both heat and work are nonzero

Solution. **A)**. Adiabatic means no heat exchange, $q = 0$, so the first law reduces to $\Delta U = w$. (Option C describes an *isothermal* process of an ideal gas.)

Answer:_____

Cont.

20. In class, we learned that the state function **entropy** (S) is related to the number of possible microstates of a system. Consider a container divided into two sides, left (L) and right (R), containing N balls (atoms or particles). In our initial example, each ball had an equal probability of being on either side, $P_L(x_i) = P_R(x_i) = \frac{1}{2}$. For two particles, the probability of each microstate is the product of the individual probabilities—for example, the probability that both particles are on the left side is

$$P_{L_1L_2} = P_L(x_1)P_L(x_2) = \tfrac{1}{4}.$$

Recall that the entropy change between two states can be expressed in terms of probabilities as:

$$\Delta S = S_f - S_i = k \ln\left(\frac{P(S_f)}{P(S_i)}\right),$$

where $P(S_f)$ and $P(S_i)$ are the probabilities of the final and initial macrostates, respectively.

Now, let's consider a slightly different situation in which an external "magnet" on the right side of the container *repels* the balls, meaning $P_R(x_i) = \frac{1}{4}$.

*This question will only be marked if the correct procedure or logic argumentation is shown.

Solution. Normalisation gives $P_L(x_i) = 1 - \frac{1}{4} = \frac{3}{4}$. For two independent particles the *macrostate* probabilities are

$$P(\text{both } L) = \left(\tfrac{3}{4}\right)^2 = \tfrac{9}{16}, \qquad P(\text{both } R) = \left(\tfrac{1}{4}\right)^2 = \tfrac{1}{16},$$

$$P(\text{one each side}) = 2\,P_L P_R = 2 \cdot \tfrac{3}{4} \cdot \tfrac{1}{4} = \tfrac{6}{16},$$

where the factor 2 counts the two microstates (L_1R_2) and (R_1L_2). A process is spontaneous when $\Delta S > 0$.

(a) Will the process be spontaneous if the initial state has one ball on each side of the container and the final state has both on the left side?
A) TRUE **B)** FALSE

Solution. A) TRUE.

$$\Delta S = k \ln\left(\frac{9/16}{6/16}\right) = k \ln\left(\frac{3}{2}\right) \approx +0.41\,k > 0$$

The left side is favoured by the magnet, so crowding both balls there raises the entropy: the process is spontaneous.

Answer:_____

(b) Will the process be spontaneous if the initial state has both balls on the left side and the final state has both on the right side?
A) TRUE **B)** FALSE

Solution. B) FALSE.

$$\Delta S = k \ln\left(\frac{1/16}{9/16}\right) = k \ln\left(\frac{1}{9}\right) = -k \ln 9 \approx -2.2\,k < 0$$

Moving both balls into the repelled region lowers the entropy, so the process is not spontaneous.

Answer:_____

The End.