Name: ____

Student number: ______________________

1. Compute the derivative of the function: $f(x) = \cos(nx + n)$, with respect to x; n is an integer number.
Using chain rule: $\frac{d}{dx}[\cos(u)] = -\sin(u) \cdot \frac{du}{dx}$ where $u = nx + n$

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

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.
Total differential: $df = \left(\frac{\partial f}{\partial T}\right)_P dT + \left(\frac{\partial f}{\partial P}\right)_T dP$

$$\frac{\partial f}{\partial T} = (w_2 + w_3 P) - 2(w_4 + w_5 P)T^{-3}, \quad \frac{\partial f}{\partial P} = w_1 + w_3 T + w_5 T^{-2}$$

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

3. What is the value of the following integral?

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

The `ELU` function is defined as,

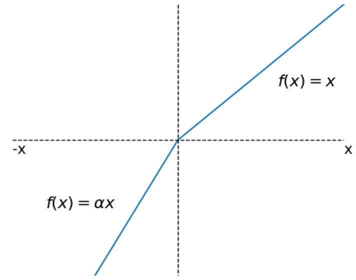
$$\texttt{ELU}(x) = \begin{cases} x & \text{if} \quad x \geq 0 \\ \alpha(e^x - 1) & \text{if} \quad x < 0 \end{cases}$$

where α is a constant.
• (Tip) Integrals can be split into multiple ones each with a different integration range.
Split by range: For $x \geq 0$: $\int x dx = \frac{1}{2}x^2 + C_1$ For $x < 0$: $\int \alpha(e^x - 1)dx = \alpha(e^x - x) + C_2$

$$\int \texttt{ELU}(x)dx = \begin{cases} \frac{1}{2}x^2 + C_1 & \text{if } x \geq 0 \\ \alpha(e^x - x) + C_2 & \text{if } x < 0 \end{cases}$$

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 ($\texttt{PReLU}(x)$), 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 $x = 0$

Limit definition: $f'(0) = \lim_{\Delta x \to 0^-} \frac{\texttt{PReLU}(0+\Delta x) - \texttt{PReLU}(0)}{\Delta x}$

For $\Delta x < 0$: $\texttt{PReLU}(\Delta x) = \alpha \Delta x$, $\texttt{PReLU}(0) = 0$

$$f'(0) = \lim_{\Delta x \to 0^-} \frac{\alpha \Delta x - 0}{\Delta x} = \alpha$$

(b) Δx and x are both positives

Limit definition: $f'(x) = \lim_{\Delta x \to 0^+} \frac{\texttt{PReLU}(x+\Delta x) - \texttt{PReLU}(x)}{\Delta x}$

For $x > 0$ and $\Delta x > 0$: $\texttt{PReLU}(x) = x$, $\texttt{PReLU}(x + \Delta x) = x + \Delta x$

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

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

$$a) \quad \frac{\partial f(x,y)}{\partial x}, \quad b) \quad \frac{\partial f(x,y)}{\partial y}, \quad c) \quad \frac{\partial^2 f(x,y)}{\partial x \partial y}, \quad d) \quad \frac{\partial^2 f(x,y)}{\partial x^2}$$

$$\frac{\partial f(x,y)}{\partial x} = 1 + 2x + 3x^2$$

$$\frac{\partial f(x,y)}{\partial y} = -1 + 2y \exp(y^2)$$

$$\frac{\partial^2 f(x,y)}{\partial x^2} = 2 + 6x$$

$$\frac{\partial^2 f(x,y)}{\partial x \partial y} = 0$$

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 $p(T, V) = \frac{RT}{V-b} - \frac{a}{V^2}$.

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

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

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

$$= \left(\frac{VRT}{(V-b)^2} - \frac{2a}{V^2}\right)^{-1}$$

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

(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 $(\partial \bar{H}/\partial P)_T$

From the given equation for $d\bar{H}$,

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

$$= -T\left(\frac{\partial}{\partial T}\right)_P\left(\frac{RT}{P} - \frac{a}{RT}P + b\right) + \frac{RT}{P} - \frac{a}{RT}P + b$$

using given equation of state

$$= -T\left(\frac{R}{P} + \frac{a}{RT^2}P\right) + \frac{RT}{P} - \frac{a}{RT}P + b$$

$$= -\frac{2a}{RT}P + b$$

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

- 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 $\bar{H}$.

Equality of mixed second partial derivatives of $\bar{H}$, we get

$$\left(\frac{\partial}{\partial P}\right)_T \left(\frac{\partial \bar{H}}{\partial T}\right)_P = \left(\frac{\partial}{\partial T}\right)_P \left(\frac{\partial \bar{H}}{\partial P}\right)_T,$$

or

$$\left(\frac{\partial}{\partial P}\right)_T \bar{C}_P = \left(\frac{\partial}{\partial T}\right)_P \left(-\frac{2a}{RT}P + b\right)$$

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

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

Since $f(x, y)$ separates as $f_0(x) + f_1(y)$, the mixed partial derivatives are zero.

Answer: **A**

9. The **trace** of a matrix, is defined as $\mathrm{Tr}(\mathbf{A}) = \sum_{i=1}^{n} A_{ii}$.
Compute $\mathrm{Tr}(\mathbf{A})$ for,

$$\mathbf{A} = \begin{bmatrix} 2 & -3 & -2 & 0 & -2 \\ -2 & -2 & 2 & 1 & -3 \\ -2 & 0 & -2 & -1 & 0 \\ -1 & 2 & 2 & 0 & -3 \\ -3 & -2 & 2 & 2 & -2 \end{bmatrix}$$

Trace is sum of diagonal elements: $2 + (-2) + (-2) + 0 + (-2) = -4$

10. Compute $\mathbf{v}_1 \cdot (\mathbf{v}_2 \times \mathbf{v}_3)$ for,

$$\mathbf{v}_1 = \frac{1}{\sqrt{3}}\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{v}_2 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}, \quad \mathbf{v}_3 = \frac{1}{\sqrt{6}}\begin{bmatrix} 1 \\ 1 \\ -2 \end{bmatrix}.$$

$$\mathbf{v}_2 \times \mathbf{v}_3 = \frac{1}{\sqrt{2}\sqrt{6}}\begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 1 & -1 & 0 \\ 1 & 1 & -2 \end{vmatrix} = \frac{1}{\sqrt{12}}[(2-0)\mathbf{i} - (-2-0)\mathbf{j} + (1+1)\mathbf{k}] = \frac{1}{\sqrt{12}}[2\mathbf{i} + 2\mathbf{j} + 2\mathbf{k}] = \frac{1}{\sqrt{12}}\begin{bmatrix} 2 \\ 2 \\ 2 \end{bmatrix}$$

$$\mathbf{v}_1 \cdot (\mathbf{v}_2 \times \mathbf{v}_3) = \frac{1}{\sqrt{3}} \cdot \frac{1}{\sqrt{12}}(1 \cdot 2 + 1 \cdot 2 + 1 \cdot 2) = \frac{6}{\sqrt{36}} = 1$$

11. Compute $\mathbf{u}\mathbf{v}^\top$, given

$$\mathbf{u} = \begin{bmatrix} 5 \\ 10 \end{bmatrix} \quad \mathbf{v} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

$$\mathbf{u}\mathbf{v}^\top = \begin{bmatrix} 5 & 10 & 15 \\ 10 & 20 & 30 \end{bmatrix}$$

12. Let the matrix $\mathbf{A}$ be defined as:

$$\mathbf{A} = \begin{bmatrix} 2 & 4 & 0 \\ 1 & 0 & 5 \end{bmatrix}$$

Answer the following,

(a) What is $\mathbf{A}^\top$ and its number of rows and columns? $\mathbf{A}^\top = \begin{bmatrix} 2 & 1 \\ 4 & 0 \\ 0 & 5 \end{bmatrix}$, 3 rows $\times$ 2 columns

(b) Compute $\mathbf{A}^\top\,\mathbf{A}$, and state the number of rows and columns of this matrix-matrix multiplication.
$\mathbf{A}^\top\,\mathbf{A} = \begin{bmatrix} 5 & 8 & 5 \\ 8 & 16 & 0 \\ 5 & 0 & 25 \end{bmatrix}$, $3{\times}3$

(c) Compute $\mathbf{A}\;\mathbf{A}^\top$, and state the number of rows and columns of this matrix-matrix multiplication.
$\mathbf{A}\,\mathbf{A}^\top = \begin{bmatrix} 20 & 2 \\ 2 & 26 \end{bmatrix}$, $2{\times}2$

13. Consider the following matrices and vectors with their specified dimensions:

- $\mathbf{A}$ is a (3,2) matrix
- $\mathbf{B}$ is a (2,2) matrix
- $\mathbf{C}$ is a (4,3) matrix
- $\mathbf{v}$ is a column vector with 2 elements
- $\mathbf{w}$ is a column vector with 3 elements
- $\mathbf{u}$ is a column vector with 4 elements

Mark all expressions that are **valid operations** (multiplication, addition, or subtraction) based on their dimensions:

A) $\mathbf{A}\,\mathbf{v}$ B) $\mathbf{B}\,\mathbf{v} + \mathbf{w}$ C) $\mathbf{C}\,\mathbf{u}$ D) $\mathbf{A}\,\mathbf{v} - \mathbf{B}\,\mathbf{v}$ E) $\mathbf{w} + \mathbf{u}$

A: $(3,2)\times(2,1) = (3,1)$

B: $(2,2)\times(2,1) = (2,1)$ but $\mathbf{w}$ is (3,1) Dimension mismatch

C: $(4,3)\times(4,1)$ Inner dimensions don't match (3 4)

D: $\mathbf{A}\,\mathbf{v} = (3,1)$, $\mathbf{B}\,\mathbf{v} = (2,1)$ Dimension mismatch $(3 \neq 2)$

E: $(3,1) + (4,1)$ Dimension mismatch $(3 \neq 4)$

Answer: **A**

14. Select the correct answer. 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

State functions return to original value when system returns to initial state

Answer: **B) False**

15. 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)** $\Delta S_{\text{system}} = 0$

Second law requires $\Delta S_{\text{universe}} > 0$ for spontaneous process

Answer: **C**

16. 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)

Heat (q) and Work (W) are path-dependent, not state functions

Answer: **D, G**

17. 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.

Isobaric means constant pressure, volume can change Answer: **A**

18. 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

Adiabatic means $q = 0$, so $\Delta U = w$ Answer: **A**

19. 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

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

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.

(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

Given: $P_R = \frac{1}{4}$, so $P_L = 1 - \frac{1}{4} = \frac{3}{4}$

Initial: one ball on each side $P_i = 2 \times (P_L \times P_R) = 2 \times (\frac{3}{4} \times \frac{1}{4}) = \frac{6}{16}$

Final: both on left side $P_f = P_L \times P_L = \frac{3}{4} \times \frac{3}{4} = \frac{9}{16}$

$\Delta S = k\ln\left(\frac{9/16}{6/16}\right) = k\ln\left(\frac{3}{2}\right) > 0 \rightarrow$ Spontaneous

Answer: **A) TRUE**

(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

Initial: both on left side $P_i = P_L \times P_L = \frac{3}{4} \times \frac{3}{4} = \frac{9}{16}$

Final: both on right side $P_f = P_R \times P_R = \frac{1}{4} \times \frac{1}{4} = \frac{1}{16}$

$\Delta S = k\ln\left(\frac{1/16}{9/16}\right) = k\ln\left(\frac{1}{9}\right) < 0 \rightarrow$ Not spontaneous

Answer: **B) FALSE**

1 Extra space

Cont.

The End.