Thermodynamics (PHYS 425/525, APN 525) **Fall 2024**

Extra Credit Project I - Due Date: Oct 1, 2024 (Exam I date)

The points obtained in this project will be added towards Exam I. To obtain full credit, your computer source code + calculations done on paper MUST be provided along with the plots.

<u>Project IA:</u> **15 pts undergraduates, 10 pts graduates**

Use your preferred programming language (ideally, Python or C++ ROOT, etc.) to plot the reduced van der Waals equation of state (problem 2 of HW set 2), $p(v, t)$ versus v for isotherms, $t = 0.8, 0.9, 1.0, 1.10$ Set the y-axis plot range *p : [-1, 2.5],* x-axis plot range *v : [-0.1, 4]* for plot ranges

First, you will need to re-arrange the van der Waals equation to obtain $p(v, t)$. Then for each of the isotherms, you should have a different equation (curve) only in terms of *v*, e.g., $p(v, t = 0.8)$, $p(v, t = 0.9)$, $p(v, t = 1.0)$, $p(v, t = 1.1)$

How smooth the function *p(v, t)* comes out depends on the number of points (or states) assigned to the independent variable, *v*. For example, a range of *v = [v_min, 1.2, 100],* represents a range divided into 100 points. Since the denominator is zero for *v_min* = 1/3, I would suggest using a range starting from *v_min* = 1/3 + 1e-6, which is technically not zero for the denominator. Note that this range is different than the plot range. The *v_min* here a physical requirement imposed by the finite volume of the gas molecules, otherwise, you will end up with negative volumes.

Depending on which software/programming language you used, you can set an option to NOT use markers (data points), but rather use lines to connect the points. The result should look like multiple curves, which should be assigned a different color for each isotherm to distinguish them, and properly display a legend with the different isotherms, associated with each curve.

Project IB: **15 pts undergraduates, 10 pts graduates**

Compare the van der Waals (VDW) and Ideal Gas equations of states (EoS) for different isotherms using 1 mole of Argon gas. The VDW EoS has a pressure correction parameter (a) and volume correction parameter (b) for different gases, summarized here: VDW EoS Parameters

For Argon gas, $a = 1.355 * 100 = 135.5 \text{ kPa} \cdot \text{L}^2/\text{mol}^2$ and $b = 0.03201 \text{ L/mol}$.

To compare the Ideal Gas and VDW EoS, make an overlay plot of $P(V, T)$ vs. V for the isotherms: $T = 87.3,\ 100,\ 200,\ 300,\ 400 \text{ K}$. There should be five separate plots with proper labels and a legend comparing the Ideal Gas with the VDW at each temperature. Use a solid line for the Ideal Gas and a dashed line for VDW, to easily differentiate them.

Start by expressing the VDW EoS (Eq. 5.49) from the textbook (Schroeder, 1999) as $P(V, T)$. Similarly, express the Ideal Gas equation as $P(V, T)$. It is suggested to also re-express the EoS in terms of n moles rather than N molecules given that the parameters (a, b) are given in moles

What can you conclude about the comparison between Ideal and VDW gas ? Is the agreement better at higher or lower temperatures, and for a given temperature, is the agreement better for larger or smaller volumes ? Elaborate in a brief paragraph your answers.

This extra credit problem is a good opportunity to learn about or exercise your programming language skills, which are an essential part of doing scientific research. **If you don't understand, ASK ! There are NO SILLY questions. You are encouraged to ask questions regarding this extra credit exercise.**