homework 1; van der Waals

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purpose: calculate molar volume of a gas using the van der Waals equation

2 a. i.

the program code is finding the zeros of the $f(V)$ equation to find the volume given all the other parameters. It's solving neumerically because the equation is not easily solvable by hand and possibly impossible to isolate the volume with algebra.

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

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

code from lobo's video:

In [ ]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import scipy.optimize as opt

# constants for van der waals equation

a = 0.3634 # Pa m^6/mol^2
b = 4.236e-5 # m^3/mol

# other params

R = 8.314 # J/(mol K) ; ideal gas constant
P = 5e5 # Pa ; pressure
T = 300 # K ; temperature

# van der waals equation

def vdW(V):
    return (R * T) - ((P + a / V**2) * (V - b))

volume = opt.fsolve(vdW, R*T/P)[0]

print(f'van der Waals volume: {volume:.5f} mol') # m^3/mol
```

```
van der Waals volume: 0.00488 mol
```

Comparing van der Waals with the ideal gas

In [ ]:
```
ideal = R * T / P
print(f'ideal gas volume: {ideal:.6f} mol') # m^3/mol

percent_diff = 100 * (ideal - volume) / volume
print(f'percent difference: {percent_diff:.2f}%')
```

```
ideal gas volume: 0.004988 mol
percent difference: 2.15%
```

2. a. ii.

first i'll setup another van der Waals function that also takes Temperature as an input

In [ ]:
```
def vdWT(V, T):
    return (R * T) - ((P + a / V**2) * (V - b))

temperatures = np.array([150,200,250,300,350])
vdw_volumes = [opt.fsolve(vdWT, R*T/P, args=(T))[0] for T in temperatures]
ideals = R * temperatures / P
diff = abs(ideals - vdw_volumes)

df = pd.DataFrame({'T (K)': temperatures,
                   'V (m^3/mol)': vdw_volumes,
                   'Ideal Gas': ideals,
                   'Difference (m^3/mol)': diff})
df.set_index('T (K)', inplace=True)
df
```

Out[ ]:

T (K)	V (m^3/mol)	Ideal Gas	Difference (m^3/mol)
150	0.002215	0.002494	0.000280
200	0.003140	0.003326	0.000186
250	0.004020	0.004157	0.000137
300	0.004883	0.004988	0.000105
350	0.005736	0.005820	0.000083

results for the 150K are somewhat different (~1%) though the rest are quite similar. then as temperature rises the ideal gas equation gets much more similar to the van der Waals equation. i.e. as temperature increases the difference decreases.