Project 3: Phase coexistence of N_2 using MD and the van der Waals equation of state

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(Dated: October 30, 2017)

(a) Finding the pressure simply amounts to rewriting the van der Waals equation of state in terms of the pressure:

$$\left(P + \frac{aN^2}{V^2}\right)(V - Nb) = NkT$$
$$\left(P + \frac{aN^2}{V^2}\right) = \frac{NkT}{(V - Nb)}$$
$$P = \frac{NkT}{V - Nb} - \frac{aN^2}{V^2} \tag{1}$$

(b) The dimensionless quantities are solved for the variables they represent, and are inserted in equation 1. This yields

$$P_C\hat{P} = \frac{NkT_C\hat{T}}{V_C\hat{V} - Nb} - \frac{aN^2}{V_C^2\hat{V}^2}$$

After inserting the expressions for T_C, V_C and P_C, and some algebra, we arrive at

$$\hat{P} = \frac{8\hat{T}}{3\hat{V} - 1} - \frac{3}{\hat{V}^2} \tag{2}$$

which is what we wanted to show.

(c) See figure 1.

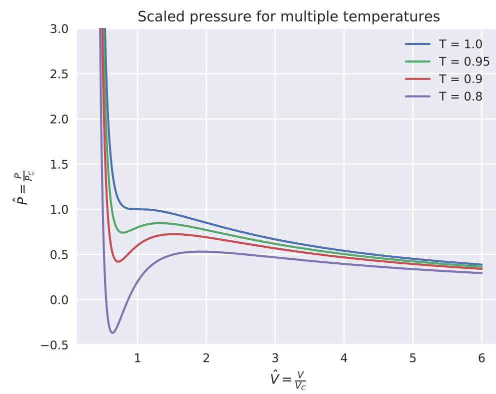

Figure 1: Pressure vs volume

(d) For the scaled quantities we have $\hat{\rho} = \frac{1}{\hat{V}}$. Inserting this in equation 2 yields

$$\hat{P} = \frac{8\hat{\rho}\hat{T}}{(3 - \hat{\rho})} - 3\hat{\rho}^2 \tag{3}$$

which is what we wanted to show.

(e) See figure 2.

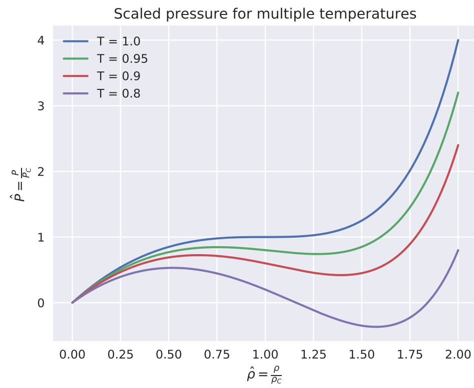

Figure 2: Pressure vs density

(f) Based on your plot, for what temperature does the density become non-unique function of the pressure?

(g) sumthin sumthing