# Physics 212 - Problem Set #3

## Solution

1.) (a.)

$$Z_n = \frac{1}{n!} \prod_j \int \frac{d^3x \, d^3p}{(2\pi\hbar)^3} e^{-\beta p^2/2m}$$

$$= \frac{1}{n!} V^n \left[ \frac{1}{(2\pi\hbar)^3} (2\pi m T)^{3/2} \right]^n$$

(b.)

$$F = -\frac{1}{\beta}\left[ n \log V + \frac{3n}{2} \log\left(\frac{mT}{2\pi\hbar^2}\right) - \log n! \right]$$

$$P = -\left.\frac{\partial F}{\partial V}\right|_{n,T} = \frac{n}{\beta V} = \frac{nT}{V} \text{ or } \frac{n k_B T}{V}$$

Using $\log n! = n \log n - n$

$$\frac{d}{dn} \log n! = \log n$$

$$\mu = \left.\frac{\partial F}{\partial n}\right|_{V,T} = T \left[ \log \frac{n}{V} \left(\frac{mT}{2\pi\hbar^2}\right)^{-3/2} \right]$$

(c.)

$$\Xi = \sum_n \frac{1}{n!}(n! Z_n) e^{\beta\mu n}$$

$$= \exp\left[ V\left(\frac{mT}{2\pi\hbar^2}\right)^{3/2} e^{\beta\mu} \right]$$

$$\Phi = -T\left( V\left(\frac{mT}{2\pi\hbar^2}\right)^{3/2} e^{\beta\mu} \right)$$

(d.) $$\frac{\partial \Phi}{\partial \mu}\Big|_{V,T} = \frac{\partial F}{\partial n}\Big|_{V,T} \frac{\partial n}{\partial \mu}\Big|_{V,T} - n - \mu \frac{\partial n}{\partial \mu}\Big|_{V,T}$$

$$= -n \quad \text{since} \quad \frac{\partial F}{\partial n}\Big|_{V,T} = \mu$$

$$\frac{\partial \Phi}{\partial V}\Big|_{\mu,T} = \frac{\partial F}{\partial V}\Big|_{n,T} + \frac{\partial F}{\partial n}\Big|_{V,T} \frac{\partial n}{\partial V}\Big|_{\mu,T} - \mu \frac{\partial n}{\partial V}\Big|_{\mu,T}$$

$$= \frac{\partial F}{\partial V}\Big|_{n,T} = -P$$

$\Phi(T, \mu, V)$ is extensive, but the only extensive variable that it depends on is $V$. Thus.

$$\Phi(T,\mu,V) = f(T,\mu) \cdot V$$

$$\frac{\partial \Phi}{\partial V}\Big|_{\mu,T} = f(T,\mu) = -p$$

so $$\Phi = -p(T,\mu) \cdot V$$

For the ideal gas.

$$p = T \left(\frac{mT}{2\pi\hbar^2}\right)^{3/2} e^{\beta\mu}$$

But, we must still determine $\mu$. $\mu$ is given by solving

$$n = -\frac{\partial \Phi}{\partial \mu}\Big|_{V,T} = +T \cdot \beta \cdot V \left(\frac{mT}{2\pi\hbar^2}\right)^{3/2} e^{\beta\mu}$$

$$= V\left(\frac{mT}{2\pi\hbar^2}\right)^{3/2} e^{\beta\mu}$$

so $$P = \frac{nT}{V} \quad \checkmark$$

(e.) In the calculation of $F$ or $\Phi$, the integral over the $\vec{p}_i$ always gives the factor

$$\left(mT/2\pi\hbar^2\right)^{3/2}$$

which is independent of $V$. If we work with $F$, this factor drops out when we compute $P$. If we work with $\Phi$ this factor always appears in the combination

$$\left(\frac{mT}{2\pi\hbar^2}\right)^{3/2} e^{\beta\mu}$$ and disappears

when we eliminate $\mu$ in favor of $n$.

(f.) $$n_i = \frac{S_i+1}{2} = \begin{cases} 1 & \text{site has a molecule} \\ 0 & \text{site has \underline{no} molecule} \end{cases}$$

then $$n = \sum_i n_i = \sum_i \frac{S_i+1}{2}$$

(g) Starting from

$$\mathcal{H} = -J\sum_{i,\nu} S_i S_{i+\nu} - H\sum_i S_i$$

$$\mathcal{H} = -J\sum_{i,\nu} (2n_i-1)\underbrace{(2n_{i+\nu}-1)}_{\text{for each site, there are } d=3 \text{ terms.}} - H\sum_i (2n_i-1)$$

$$\mathcal{H} = -4J \sum_{i\nu} n_i n_{i+\nu} + J \cdot 2 \cdot 2 \cdot d \sum_i n_i$$
$$- 2H \sum_i n_i + N(-dJ + H)$$

$$= -4J \sum_{i\nu} n_i n_{i+\nu} - (2H - 12J)\, n$$
$$+ N(H - dJ)$$

then

$$Z_{\text{Ising}} = e^{\beta N(dJ - H)} \cdot \sum_{n_i = \pm 1} e^{-\beta \mathcal{V}} e^{+\beta \mu n}$$

for $\mu = 2H - 12J$

or

$$\Xi = e^{-\beta \Phi} = e^{-\beta N(3J - H)} Z_{\text{Ising}}$$

(h) Our approximate expression for $\Phi$, using mean field theory, is

$$\Phi = N\Big\{ -T \log 2\cosh \beta h_* - 3J \tanh^2 \beta h_*$$
$$- (H - h_*) \tanh \beta h_* + (3J - H) \Big\}$$

where $h_*$ minimizes the Ising free energy

$n$ is given by

$$n = -\frac{\partial \Phi}{\partial \mu} = -\frac{1}{2}\frac{\partial \Phi}{\partial H}$$

$$= \frac{N}{2}\left(\tanh \beta h_* + 1\right)$$

Recall that, in the Ising model, $s_* = \tanh \beta h_*$ is the expectation value of a spin. Since

$$n_i = \frac{s_i + 1}{2} \qquad n = \sum_i \frac{\langle s_i \rangle + 1}{2} = \frac{N(s_* + 1)}{2}$$

so this is just right.

(i) Let $\mu$ or $H$ be large and negative. Minimize $\Phi(h)$

$$0 = \frac{\partial \Phi}{\partial h} = N\Big\{ \cancel{-T\beta \frac{\sinh \beta h}{\cosh \beta h}} - 6\beta J \frac{\tanh \beta h}{\cosh^2 \beta h}$$
$$+ \cancel{\tanh \beta h} - (H-h)\,\beta \frac{1}{\cosh^2 \beta h} \Big]$$

for for $(-H) \gg J$ the solution is very close to

$$h = H$$

For large and negative $h$

$$\log 2\cosh \beta h = \log\left(e^{-\beta h} + e^{\beta h}\right) = -\beta h + e^{2\beta h}$$

$$\tanh \beta h = -1\,\frac{(1 - e^{2\beta h})}{1 + e^{2\beta h}} = (-1)\left(1 - 2e^{2\beta h}\right)$$

so

$$\frac{n}{N} = \frac{1}{2}\left(\tanh \beta h + 1\right) \cong e^{2\beta h} = e^{-2\beta |h|}$$

the value of $\Phi$ for $h = H$ is

$$\Phi = N\{ -T(-\beta H + e^{2\beta H}) - \cancel{3J}$$
$$- 0 + (\cancel{3J} - H) \}$$
$$= N ( H - H - T e^{2\beta H} )$$
$$= -NT \frac{n}{N} = -nT$$

so $$P = \frac{nT}{V}$$ as we had hoped.

(j) The Ising model critical point is $T_c = 6J$, $h_* = 0$, $H=0$

Then

$$\Phi = N\{ -T_c \log 2\cosh(0) - 0$$
$$- 0 + 3J \}$$
$$= N\{ -(6J \log 2 - 3J) \}$$
$$= -3J(2\log 2 - 1) \cdot V$$

or $$P = +3J(2\log 2 - 1)$$

(k) Below $T_c$, in the mean field Ising model, at $H=0$

the equation for $h_*$ is

$$h_* = 6J \tanh \beta h_*$$

$$h_* = 6J\beta h_* - \frac{1}{3} 6J(\beta h_*)^3 + \cdots$$

$$h_* \simeq \frac{T_c}{T} h_* - \frac{1}{3}\frac{1}{T_c^2} h_*^3 + \cdots$$

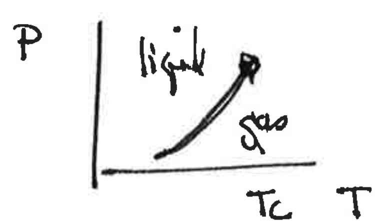
$$\left(\frac{T_c - T}{T}\right) = \frac{1}{3}\frac{1}{T_c^2} h_*^2$$

$$h_* \approx \sqrt{3}\, T_c \left(1 - \frac{T}{T_c}\right)^{1/2}$$

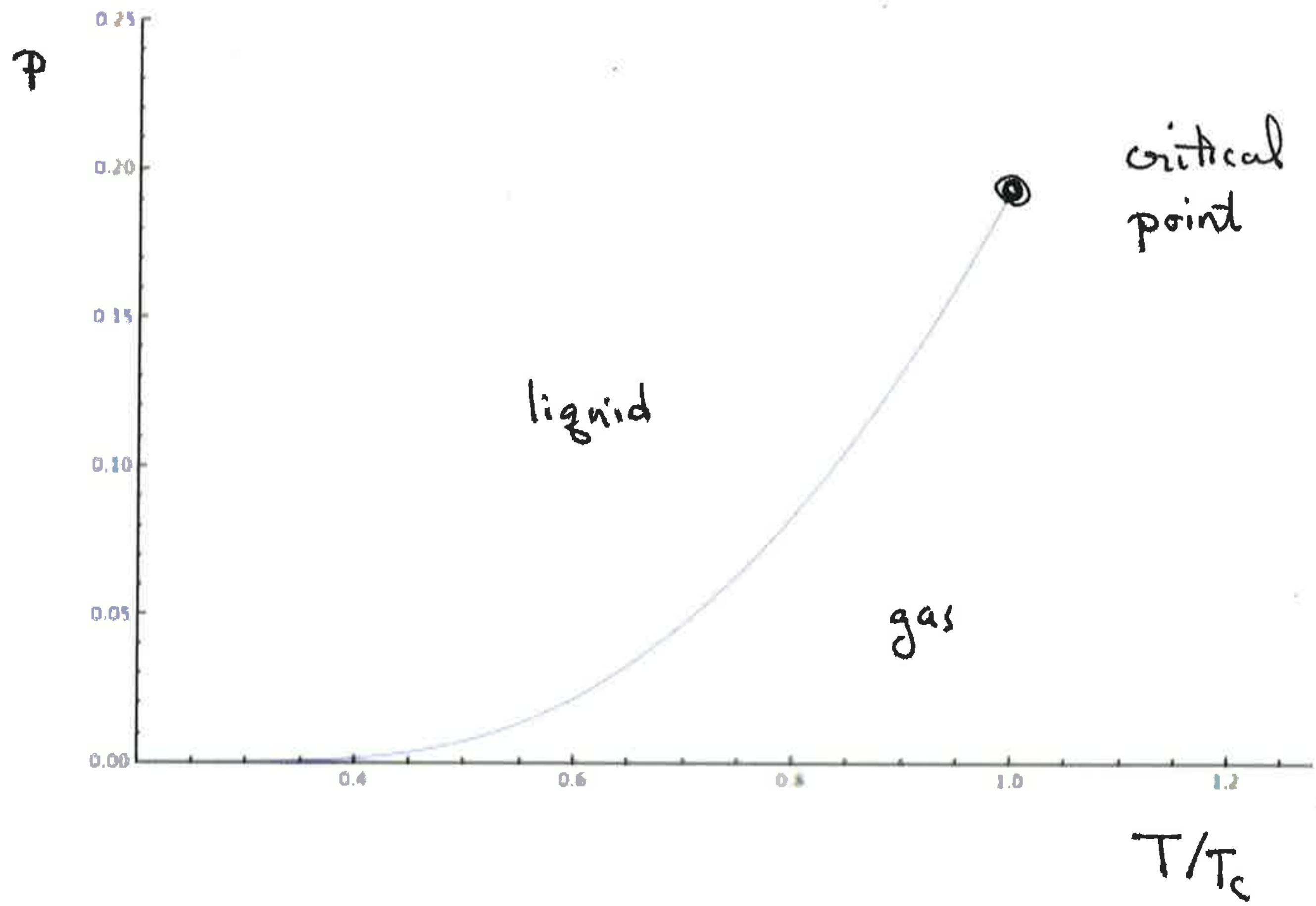
(l.) The liquid-gas coexistence curve will correspond to the coexistence curve in the Ising model, i.e. $H = 0$, $T < T_c$. With

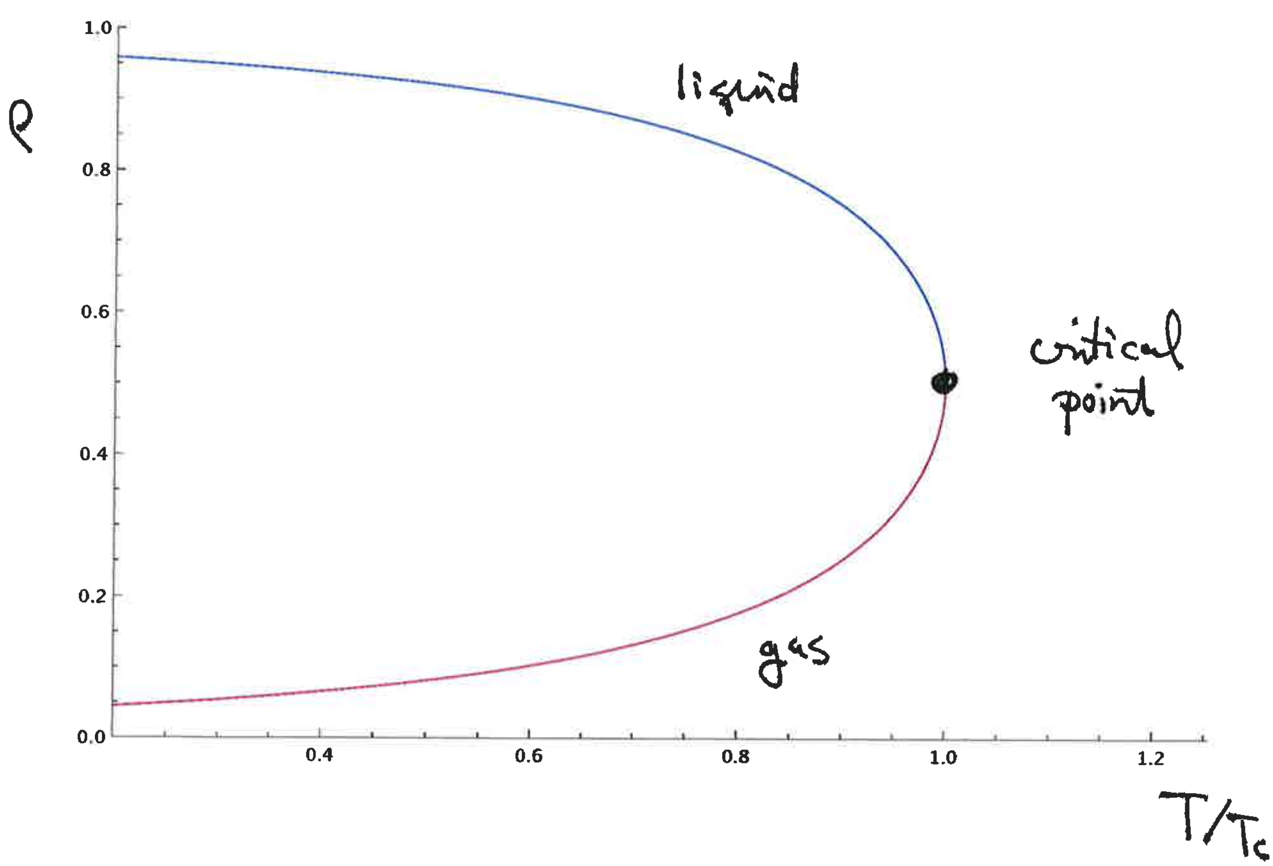
$$p = -\Phi/N$$

this is a curve at positive pressure that ends at $T/T_c = 1$, $p = \frac{1}{2} T_c (2 \ln 2 - 1)$




This curve and the curve in (m) are on the next page.


P
critical point
liquid
gas
0.00
0.05
0.10
0.15
0.20
0.25
0.4
0.6
1.0
1.2
T/Tc


ρ
liquid
critical point
gas
0.0
0.2
0.4
0.6
0.8
1.0
0.4
0.6
0.8
1.0
1.2
T/Tc