HW 4

1) $\rho(\vec{r}) = \sum_{i=1}^{N} \delta(\vec{r} - \vec{r}_i)$

$$\rho(\vec{q}) = \int_V d\vec{r}\, \rho(\vec{r})\, e^{-i\vec{q}\cdot\vec{r}} = \int_V d\vec{r} \sum_{i=1} \delta(\vec{r}-\vec{r}_i)\, e^{-i\vec{q}\cdot\vec{r}}$$

$$= \sum_{i=1}^{N} \int d\vec{r}\, e^{-i\vec{q}\cdot\vec{r}}\, \delta(\vec{r}-\vec{r}_i) = \sum_{i=1}^{N} e^{-i\vec{q}\cdot\vec{r}_i}$$

$$\tfrac{1}{N}\langle \rho(\vec{q})\rho(-\vec{q})\rangle = \frac{1}{N}\left\langle \left(\sum_{i=1}^{N} e^{-i\vec{q}\cdot\vec{r}_i}\right)\left(\sum_{j=1}^{N} e^{+i\vec{q}\cdot\vec{r}_j}\right)\right\rangle$$

$$= \tfrac{1}{N}\left\langle \sum_{ij} e^{-i\vec{q}\cdot(\vec{r}_j - \vec{r}_i)} \right\rangle = S(\vec{q}) \checkmark$$

2) a) $\rho(\vec{q}) = \int d\vec{r}\, e^{-i\vec{q}\cdot\vec{r}} \left\langle \sum_{i=1}^{N} \delta(r - r_i) \right\rangle$

$$= \left\langle \int d\vec{r}\, e^{-i\vec{q}\cdot\vec{r}} \sum_{i=1}^{N} \delta(r - r_i) \right\rangle$$

we can prove later exchanging order is ok b/c brackets are integrals & sums where order can exchange

$$= \left\langle \sum_{i=1}^{N} e^{-i\vec{q}\cdot\vec{r}_i} \right\rangle$$

$$\rho(\vec{q} = \vec{0}) = \left\langle \sum_{i=1}^{N} 1 \right\rangle = \langle N \rangle$$

b) $S(\vec{q}) \simeq \frac{1}{\langle N \rangle} \langle \rho(\vec{q})\rho(-\vec{q}) \rangle$

$$= \tfrac{1}{\langle N \rangle} \left\langle \sum_{ij} e^{-i\vec{q}\cdot\vec{r}_{ij}} \right)$$

$$= \frac{1}{\langle N \rangle} \left\langle N + \sum_{i \neq j} e^{-i\vec{q}\cdot\vec{r}_{ij}} \right\rangle$$

$$= \frac{\langle N \rangle}{\langle N \rangle} + \frac{1}{\langle N \rangle} \left\langle \sum_{i \neq j} e^{-i\vec{q}\cdot\vec{r}_{ij}} \right\rangle$$

see class

$$= 1 + \frac{1}{\langle N \rangle} \cdot \left\langle N \cdot (N-1) e^{-i\vec{q}\cdot\vec{r}_{12}} \right\rangle \checkmark$$

and hence $S(0) = 1 + \frac{1}{\langle N \rangle} \langle N(N-1) \rangle \checkmark = \frac{\langle N^2 \rangle}{\langle N \rangle}$

c) $\rho k_B T \kappa_T = \frac{\mathrm{Var}(N)}{\langle N \rangle} = \frac{\langle N^2 \rangle - \langle N \rangle^2}{\langle N \rangle} = \frac{\langle N^2 \rangle}{\langle N \rangle} - \langle N \rangle = S(\vec{q}=0) - \rho(\vec{q}=0)$ ✓

d) now

$$S(\vec{q}) = 1 + \frac{\langle N \rangle}{V} \int_V d\vec{r}\, g(r) e^{-i\vec{q}\vec{r}}$$

$$\Rightarrow S(\vec{q}=0) = 1 + \langle N \rangle / V \int_V d\vec{r}\, g(r)$$

$$= 1 + \langle N \rangle / V \int_V d\vec{r} \left((g(r) - 1) + 1 \right)$$

$$= 1 + \langle N \rangle / V \int d\vec{r} \left(g(r) - 1 \right) + \frac{\langle N \rangle}{V} \overbrace{\int_V d\vec{r}}^{V}$$

$$= 1 + \rho \int d\vec{r} \left(g(r) - 1 \right) + \langle N \rangle$$

So $\rho k_B T \kappa_T = S(\vec{q}=0) - \underbrace{\rho(\vec{q}=0)}_{\langle N \rangle} = 1 + \rho \int d\vec{r} \left(g(r) - 1 \right)$

3) a) $u(r) = A/r^n = A r^{-n}$

low density $g(r) \approx e^{-\beta u(r)} = e^{-\beta A/r^n}$

$$\beta P = \rho - \frac{2\pi \rho^2}{3} \beta \underbrace{\int_0^\infty dr\, r^3 \frac{du}{dr} g(r)}_{I}$$

$$I = \int_0^\infty dr\, r^3 \left[-nAr^{-n-1} \right] e^{-\beta A/r^n}$$

$$= -nA \int_0^\infty dr\, r^{-n+2} e^{-\beta A r^{-n}}$$

$u(r=0) = \infty$
$u(r=\infty) = 0$

$$u = +\beta A r^{-n} \quad , \quad r = \left(\frac{u}{\beta A}\right)^{-1/n}$$

$$du = +\beta A \cdot (-n r^{-n-1}) dr$$

$$= +\frac{1}{\beta} \int_\infty^0 du\, r^3 e^{-u}$$

$$= +\frac{1}{\beta} \int_\infty^0 du \left[\frac{u}{\beta A}\right]^{-3/n} e^{-u} = -\frac{1}{\beta}\left[\frac{1}{\beta A}\right]^{-3/n} \underbrace{\int_0^\infty u^{-3/n} e^{-u}}_{\equiv G}$$

flip & get − sign

$$G = \int_0^\infty du\, u^{-3/n} e^{-u} = \int_0^\infty du\, u^{\left(-\frac{3}{n}+1\right)-1} e^{-u}$$

$$= \Gamma\left(1 - 3/n\right)$$

$$\beta P = \rho + \frac{2\pi\rho^2}{3\beta}\left[\beta A\right]^{3/n} \Gamma\left(1 - 3/n\right)$$

b) If $n = 1$ or 3, $\Gamma(1 - 3/n) = \infty$

so the pressure is predicted to be infinite

If $n = 2$, $\Gamma(1 - 3/n) = -2\sqrt{\pi}$

pressure decreases relative to ideal

unphysical for repulsive potential so prob means approximations not ok here

For $n > 3$, pressure increases b/c $\Gamma(1 - 3/n) > 0$