Solution to Problem 1

1 a
$N = 3$

$$\begin{aligned}
Z &= \sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1}\sum_{\sigma_3=\pm1} e^{\beta J(\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_1)+\beta h(\sigma_1+\sigma_2+\sigma_3)} \\
&= \underbrace{e^{3\beta(J+h)}}_{\sigma_1=1,\sigma_2=1,\sigma_3=1} + \underbrace{e^{\beta(-J+h)}}_{\sigma_1=1,\sigma_2=1,\sigma_3=-1} + \underbrace{e^{\beta(-J+h)}}_{\sigma_1=1,\sigma_2=-1,\sigma_3=1} + \underbrace{e^{\beta(-J-h)}}_{\sigma_1=1,\sigma_2=-1,\sigma_3=-1} \\
&+ \underbrace{e^{\beta(-J+h)}}_{\sigma_1=-1,\sigma_2=1,\sigma_3=1} + \underbrace{e^{\beta(-J-h)}}_{\sigma_1=-1,\sigma_2=1,\sigma_3=-1} + \underbrace{e^{\beta(-J-h)}}_{\sigma_1=-1,\sigma_2=-1,\sigma_3=1} + \underbrace{e^{3\beta(J-h)}}_{\sigma_1=-1,\sigma_2=-1,\sigma_3=-1} \\
&= e^{3\beta(J+h)} + 3\ e^{\beta(-J+h)} + 3\ e^{\beta(-J-h)} + e^{3\beta(J-h)}
\end{aligned}$$

Even though the exam did not ask for this, let us also check that the above result for Z agrees with the general formula $Z = \lambda_+^N + \lambda_-^N$, for $N = 3$.

$$\begin{aligned}
Z &= \lambda_+^3 + \lambda_-^3 \\
&= e^{3K}\left[\left(\cosh(\omega) + \sqrt{\sinh^2(\omega) + e^{-4K}}\right)^3 + \left(\cosh(\omega) - \sqrt{\sinh^2(\omega) + e^{-4K}}\right)^3\right] \\
&= 2e^{3K}\left[\cosh^3(\omega) + 3\cosh(\omega)\left(\sinh^2(\omega) + e^{-4K}\right)\right] \\
&= 6e^{-K}\cosh(\omega) + 2e^{3K}\left(4\cosh^3(\omega) - 3\cosh(\omega)\right).
\end{aligned}$$

Here, we have used $\cosh^2(\omega) - \sinh^2(\omega) = 1$ to eliminate $\sinh^2(\omega)$ in favor of $\cosh^2(\omega)$. Using $\cosh(\omega) = (e^\omega + e^{-\omega})/2$, we find $4\cosh^3(\omega) - 3\cosh(\omega) = (e^{3\omega} + e^{-3\omega})/2$. Hence, we get

$$\begin{aligned}
Z &= 3e^{-K}\left(e^\omega + e^{-\omega}\right) + e^{3K}\left(e^{3\omega} + e^{-3\omega}\right) \\
&= e^{3(K+\omega)} + e^{3(K-\omega)} + 3e^{-(K-\omega)} + 3e^{-(K+\omega)}.
\end{aligned}$$

This is the same as what we found by direct enumeration of the partition function for $N = 3$, setting $K = \beta J$ and $\omega = \beta h$.

1 b
In general, we have

$$\begin{aligned}
M &= \langle\sum_{i=1}^N \sigma_i\rangle \\
&= \frac{1}{Z}\sum_{\{\sigma_i\}}\sum_{i=1}^N \sigma_i\ e^{-\beta H} \\
&= \frac{\partial}{\partial\beta h}\ln(Z).
\end{aligned}$$

When $N \to \infty$, we have $Z = \lambda_+^N\left(1 + (\lambda_-/\lambda_+)^N\right) \approx \lambda_+^N$, thus

$$M = N\frac{\partial \ln\lambda_+}{\partial\beta h}$$

$$
\begin{aligned}
&= N\frac{1}{\lambda_+}\frac{\partial\lambda_+}{\partial\omega} \\
&= N\frac{1}{e^K\left[\cosh(\omega)+\sqrt{\sinh^2(\omega)+e^{-4K}}\right]}e^K\left[\sinh(\omega)+\frac{2\sinh(\omega)\cosh(\omega)}{2\sqrt{\sinh^2(\omega)+e^{-4K}}}\right] \\
&= \frac{N\sinh(\omega)}{\sqrt{\sinh^2(\omega)+e^{-4K}}} = N\ \frac{\Gamma}{\sqrt{1+\Gamma^2}}.
\end{aligned}
$$

where $\Gamma \equiv \sinh(\omega)\ e^{2K} = \frac{1}{2}\left(e^{\omega+2K} - e^{-(\omega-2K)}\right)$.

m is the uniform magnetization. Increasing the uniform magnetic field h increases the alignment of the spins (along h), such that for fixed T, J, m increases with h.

For fixed h, the system behaves differently for $J > 0$ and $J < 0$ as T is varied.

<u>$J > 0$, T decreases</u>
$J > 0$ promotes ferromagnetic ordering, i.e. all spins align in the same direction (up or down), i.e. uniform magnetization. As T decreases, the spins order more and more, and m increases with decreasing T.

<u>$J < 0$, T decreases</u>
It will suffice to consider the case $h > 0$. $J < 0$ promotes antiferromagnetic ordering, i.e. neighboring spins align in opposite direction. On the other hand, the uniform magnetic field promotes spins ordering parallel. Hence, there is a competition between J and h in terms of spin-ordering. We must distinguish between two cases, namely the case where J dominates h, and the opposite case where h dominates J. When $J \gg h$, and T decreases, the spins order antiferromagnetically, and m decreases with decreasing T. When $h \gg J$, and T decreases, the spins order ferromagnetically, and m increases with decreasing T. From the low-T limit of the expression for $m = M/N$, we see that the changes in behavior of m at low T is determined by the behavior of $e^{\omega-2|K|} - e^{-(\omega+2|K|)} \approx e^{\omega-2|K|}$. When $\omega - 2|K|$ changes sign from positive value to a negative value, Γ changes from a very large value to a very small value, such that m changes from 1 to a very small value.

1 c
The model is an Ising spin-model defined on a ring with ferromagnetic nearest-neighbor ($J_1 > 0$) and ferromagnetic next-nearest-neighbor ($J_2 > 0$) spin-interactions. Introducing $\tau_i = \sigma_i\sigma_{i+1}$, we have

$$
\begin{aligned}
H &= -\sum_{i=1}^{N}\left[J_1\ \sigma_i\sigma_{i+1} + J_2\ \sigma_i\sigma_{i+2}\right] \\
&= -\sum_{i=1}^{N}\left[J_2\ \tau_i\tau_{i+1} + J_1\ \tau_i\right].
\end{aligned}
$$

Here we have used that $\tau_i\tau_{i+1} = \sigma_i\underbrace{\sigma_{i+1}\sigma_{i+1}}_{=1}\sigma_{i+2} = \sigma_i\sigma_{i+2}$. This model is exactly the same as the one we studied above, if we make the substitutions $h \to J_1, J_1 \to J_2$, i.e. $K = \beta J_2, \omega = \beta J_1$. We may therefore take over directly the results for the partition function $Z = e^{-\beta G}$. The Gibbs energy is then given by, in the limit $N \to \infty$

$$
\begin{aligned}
G &= -Nk_BT\ln\lambda_+ \\
&= -Nk_BT\left[K + \ln\left(\cosh(\omega)+\sqrt{\sinh^2(\omega)+e^{-4K}}\right)\right].
\end{aligned}
$$

Let us now look at low temperatures $\beta J_1 \gg 1, \beta J_2 \gg 1$. We then have $\cosh(\omega) + \sqrt{\sinh^2(\omega) + e^{-4K}} \approx e^{\omega}$, and hence $\ln\left(\cosh(\omega) + \sqrt{\sinh^2(\omega) + e^{-4K}}\right) \approx \omega$. From this, we find that

$$\begin{aligned} G &\approx -Nk_BT\left(K+\omega\right) \\ &= -N\left(J_1+J_2\right). \end{aligned}$$

This is nothing but the ground state energy H when all spins are completely ordered (either up or down). On general grounds, we have $G = U - hM - TS$. In this case, $h = 0$, so that $G = U - TS$. In the low-temperature limit, the entropy-term TS is negligible, so that G is dominated by $U = \langle H \rangle$. When all spins are ordered, $\sigma_i\sigma_{i+1} = 1$, $\sigma_i\sigma_{i+2} = 1$. Hence, we see from inspection directly from the expression for H that $H = -N(J_1 + J_2)$, which is the low-temperature limit of G.

Solution to Problem 2

2 a

In this case, the Hamiltonian is given in terms of a sum of single-particle Hamiltonians, and the partition function Z therefore factorizes into a product N single-particle partition functions, as follows

$$\begin{aligned} Z &= \frac{1}{N!h^{3N}} \; Z_1^N \\ Z_1 &= \int d\mathbf{r} \int d\mathbf{p} e^{-\beta \mathbf{p}^2/2m - \beta\alpha r^3} \\ &= \left(\frac{2\pi m}{\beta}\right)^{3/2} \int d\mathbf{r} e^{-\beta\alpha r^3} \\ &= \left(\frac{2\pi m}{\beta}\right)^{3/2} Q_1 \\ Q_1 &= \int d\mathbf{r} e^{-\beta\alpha r^3} \end{aligned}$$

In the Q_1-integral, the integrand is isotropic, and we may perform the angular integrations with ease, leaving us with one radial integral to perform, thus

$$\begin{aligned} Q_1 &= 4\pi \int_0^R dr \; r^2 \; e^{-\beta\alpha r^3} \\ &= \frac{4\pi}{3} \int_0^{R^3} du \;\; e^{-\beta\alpha u} \\ &= \frac{4\pi}{3} \frac{1}{\beta\alpha} \left(1 - e^{-\beta\alpha R^3}\right) \\ &= V \left(\frac{1 - e^{-x}}{x}\right), \end{aligned}$$

where we have introduced $x = 3\alpha\beta V/4\pi$ by substituting $R^3 = 3V/4\pi$. Therefore, we have

$$\begin{aligned} Z &= \frac{1}{N!h^{3N}} \; \left(\frac{2\pi m}{\beta}\right)^{3N/2} \; V^N \; \left(\frac{1 - e^{-x}}{x}\right)^N \\ &= \frac{V^N}{N!\Lambda^{3N}} \left(\frac{1 - e^{-x}}{x}\right)^N, \end{aligned}$$

where we have introduced $\Lambda = h/\sqrt{2\pi m k_B T}$. We note that when $x \ll$, we have $(1 - e^{-x})/x \approx 1$, whence we have

$$Z = \frac{V^N}{N!\Lambda^{3N}}.$$

This is the standard well-known result for the partition function of an ideal gas, where the confining potential αr^3 plays no role. This is easily understood, since when $x \ll 1$, this means that the volume is small, such that the particles are always close to the origin. In this case, the effect of the confining potential is not felt, and the particles exert a pressure on the walls of the container as if the confining potential were not there.

2 b

The internal energy is given by $U = \langle H \rangle = -1/Z\partial Z/\partial\beta = -\partial \ln Z/\partial\beta$. We thus have

$$\begin{aligned}
U &= -\frac{\partial \ln Z}{\partial \beta} \\
&= \frac{3}{2}Nk_BT - N\frac{\partial}{\partial\beta}\ln\left(\frac{1-e^{-x}}{x}\right) \\
&= \frac{3}{2}Nk_BT - N\frac{\partial}{\partial x}\ln\left(\frac{1-e^{-x}}{x}\right)\frac{\partial x}{\partial\beta} \\
&= \frac{3}{2}Nk_BT + N\frac{3\alpha V}{4\pi}\left(\frac{1}{x} - \frac{1}{e^x-1}\right) \\
&= \langle\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}\rangle + \langle\sum_{i=1}^{N}\alpha r_i^3\rangle.
\end{aligned}$$

The first term is the average of the kinetic energy of the system (as per the equipartitition principle), while the second term is the average of the potential energy term αr_i^3.

Let us next consider two limiting cases, namely $x \ll 1$ and $x \gg 1$. In the former case, we expect the effect of the confining potential to be negligible, since the particles in any case are close to the origin due to the wall-constrictions of the system.

When $x \ll 1$, we have $1/x - 1/(e^x - 1) \approx 1/2$. Then we obtain

$$\begin{aligned}
U &= \frac{3}{2}Nk_BT + N\frac{3\alpha V}{4\pi}\frac{1}{2} \\
&= \frac{3}{2}Nk_BT\left(1 + \frac{1}{3}x\right) \approx \frac{3}{2}Nk_BT.
\end{aligned}$$

This is in accord with the intuition that for small volumes, the particles are contained close to the origin not by the anharmonic trap, but by the walls, as if the anharmonic trap were not there.

When $x \gg 1$, we have $1/x - 1/(e^x - 1) \approx 1/x$. Then we obtain

$$\begin{aligned}
U &= \frac{3}{2}Nk_BT + N\frac{3\alpha V}{4\pi}\left(\frac{1}{x} - \frac{1}{e^x-1}\right) \\
&\approx \frac{3}{2}Nk_BT + N\frac{3\alpha V}{4\pi}\frac{1}{x} \\
&= \frac{3}{2}Nk_BT + Nk_BT = \frac{5}{2}Nk_BT.
\end{aligned}$$

As before, the term $3Nk_BT/2$ comes from the kinetic energy as per the equipartition principle. The term Nk_BT comes from the average of the potential energy αr^3, which now comes into full play since the walls of the system effectively are moved so far out from the origin that the particles are confined to the system not by the walls but entirely by the confining potential.

2 c

From $F = U - TS$ and $TdS = dU + pdV$ we have $dF = -SdT - pdV$, which means that $p = -\left(\partial F/\partial V\right)_T$. Since $F = -k_BT\ln Z$, we have

$$\begin{aligned}
p &= k_BT\left(\frac{\partial \ln Z}{\partial V}\right)_T \\
&= \frac{Nk_BT}{V} + Nk_BT\left(-\frac{1}{x} + \frac{1}{e^x-1}\right)\underbrace{\frac{\partial x}{\partial V}}_{=x/V}
\end{aligned}$$

$$= \frac{Nk_BT}{V}\,\frac{x}{e^x - 1}$$

When $x \ll 1$, we have $x/(e^x - 1) \approx 1$. Therefore, in this case we have $pV = Nk_BT$, the standard form for the ideal gas equation of state. Again, the effect of the anharmonic trap-potential is seen to vanish for small volumes.

When $x \gg 1$, we have

$$\begin{aligned} p &= \frac{Nk_BT}{V}\,x\,e^{-x} \\ &= \frac{3N\alpha}{4\pi}\,e^{-\frac{3\alpha\beta V}{4\pi}}. \end{aligned}$$

In this case, the pressure is seen to vanish exponentially with the volume as the volume increases for $x \gg 1$. The effect of the confining anharmonic potential is felt strongly, the particles are confined to the center of the system by this potential, and are therefore almost unable to reach the walls of the container. They therefore exert a far smaller pressure on the walls of the container than they do in the absence of a confining trap-potential.

Solution to Problem 3

3 a
We have

$$\begin{aligned}\langle N\rangle &= \frac{\partial \ln Z_g}{\partial \beta\mu} \\ &= -\sum_{\mathbf{k}} \frac{-e^{-\beta(\varepsilon_{\mathbf{k}}-\mu)}}{1-e^{-\beta(\varepsilon_{\mathbf{k}}-\mu)}} \\ &= \sum_{\mathbf{k}} \frac{1}{e^{\beta(\varepsilon_{\mathbf{k}}-\mu)}-1} = \sum_{\mathbf{k}} n_{\mathbf{k}}.\end{aligned}$$

Furthermore, we have $U = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}\, n_{\mathbf{k}}$, which immediately gives

$$U = \sum_{\mathbf{k}} \frac{\varepsilon_{\mathbf{k}}}{e^{\beta(\varepsilon_{\mathbf{k}}-\mu)}-1}.$$

3 b
Introducing the density of states $g(e)$ and the fugacity $z = e^{\beta\mu}$, we have

$$\begin{aligned}\langle N\rangle &= \int d\varepsilon\, \frac{g(\varepsilon)}{e^{\beta\varepsilon}z^{-1}-1} \\ &= \int d\varepsilon\, \frac{zg(\varepsilon)}{e^{\beta\varepsilon}-z} \\ &= \int d\varepsilon\, \frac{zg(\varepsilon)e^{-\beta\varepsilon}}{1-ze^{-\beta\varepsilon}} \\ &= \int d\varepsilon\; g(\varepsilon)\sum_{l=1}^{\infty} z^l\, e^{-\beta\varepsilon l}.\end{aligned}$$

In a similar way, we obtain the expression for U, which differs from that of $\langle N\rangle$ only by a factor ε under the integral, thus we have

$$U = \int d\varepsilon\; \varepsilon\; g(\varepsilon)\sum_{l=1}^{\infty} z^l\, e^{-\beta\varepsilon l}.$$

We have the expression for $g(e) = VK_d e^{d-1}$, $e\; g(e) = VK_d e^d$, with $K_d = (1/2\pi\hbar c)^d(2\pi^{d/2}/\Gamma(d/2))$. Both for $\langle N\rangle$ and U we therefore must compute sums and integrals of the form

$$\begin{aligned}I &= VK_d \int_0^{\infty} d\varepsilon\; \varepsilon^{\nu} \sum_{l=1}^{\infty} z^l\, e^{-\beta\varepsilon l} \\ &= VK_d \sum_{l=1}^{\infty} z^l \int_0^{\infty} d\varepsilon\; \varepsilon^{\nu}\, e^{-\beta\varepsilon l} \\ &= VK_d\Gamma(\nu+1)\sum_{l=1}^{\infty} \frac{z^l}{(\beta l)^{\nu+1}}.\end{aligned}$$

with $\nu = d-1$ for $\langle N\rangle$, and $\nu = d$ for U. We therefore obtain

$$\begin{aligned}\langle N\rangle &= VK_d\Gamma(d)\sum_{l=1}^{\infty} \frac{z^l}{(\beta l)^d} = V\frac{K_d}{\beta^d}\Gamma(d)\sum_{l=1}^{\infty} l\frac{z^l}{l^{d+1}} \\ U &= VK_d\Gamma(d+1)\sum_{l=1}^{\infty} \frac{z^l}{(\beta l)^{d+1}} = V\frac{K_d}{\beta^d}\frac{d\;\Gamma(d)}{\beta}\sum_{l=1}^{\infty} \frac{z^l}{l^{d+1}}\end{aligned}$$

In the expression for U, we have used that $\Gamma(d+1) = d\,\Gamma(d)$ (given formula on the exam sheet). Comparing with

$$\begin{aligned} \langle N \rangle &= V \sum_{l=1}^{\infty} l\, b_l\, z^l \\ \frac{\beta U}{d} &= V \sum_{l=1}^{\infty} b_l\, z^l \end{aligned}$$

we see that the fugacity coefficients b_l are given by

$$b_l = \frac{K_d}{\beta^d} \frac{\Gamma(d)}{l^{d+1}}.$$

Note that $b_l > 0, \forall l$.
Furthermore, we have that $\beta p V = \ln Z_g$ while $\langle N \rangle = z \partial \ln Z_g / \partial z = V \sum_{l=1}^{\infty} l b_l z^l$. This means that $\beta p V = V \sum_{l=1}^{\infty} b_l z^l = \beta U/d$. Hence, we obtain $U/pV = d$, which is a constant independent of temperature and density. The virial expansion for the internal energy of this non-interacting system (see below) is therefore essentially the same as the virial expansion for the pressure. The physics determining the virial coefficients for the internal energy is therefore precisely the same as the physics determining the virial-coefficients of the pressure.

3 c
In order to proceed with the virial expansion for the internal energy U, let us for convenience introduce the auxiliary quantity $\tilde{u} = \beta U/Vd$ and the density $\rho = \langle N \rangle / V$. We then have

$$\begin{aligned} \rho &= \sum_{l=1}^{\infty} l\, b_l\, z^l = b_1 z + 2 b_2 z^2 + ... \\ \tilde{u} &= \sum_{l=1}^{\infty} b_l\, z^l = b_1 z + b_2 z^2 + ... \end{aligned}$$

from which we find

$$\tilde{u} - \rho = -b_2 z^2 + ... \tag{1}$$

From the fugacity expansion for the density, we have $\rho^2 = b_1^2 z^2 + ...$, so computing to second order in ρ, we have $z^2 = \rho^2 / b_1^2 + ...$ Inserting this into the expression for $\tilde{u} - \rho$, we find

$$\begin{aligned} \tilde{u} &= \rho - \frac{b_2}{b_1^2} \rho^2 + ... \\ U &= V d k_B T \left[\rho - \frac{b_2}{b_1^2} \rho^2 + ... \right] \end{aligned}$$

Thus, we have the virial coefficients

$$\begin{aligned} E_1(T) &= V d k_B T > 0 \\ E_2(T) &= -E_1 \frac{b_2}{b_1^2} = -E_1(T) \frac{1}{2^{d+1}} \frac{\beta^d}{K_d} \frac{1}{\Gamma(d)} < 0. \end{aligned}$$

We have $b_2/b_1^2 \sim \hbar^d$. In the classical limit, $\hbar \to 0$, and hence $E_2(T) \to 0$ in the classical limit. The finiteness of $E_2(T)$ is a pure quantum effect.
To interpret the sign of $E_2(T)$, we note from above that $U/d = pV$. In ideal Bose-systems, the Bose-statistics leads to an overpopulation of occupied single-particle states compared to the classical case. The

result $U = \langle N \rangle d k_B T$ is the classical result for the internal energy of an ultrarelativistic gas. The correction to the classical result is essentially the same as the correction to the pressure, due to the statistical "attraction" between ideal Bose-particles. Attraction between particles leads to reduction in pressure, because particles are pulled towards each other which counteracts their exterting pressure on a wall. The negative sign of E_2 is therefore a manifestation of the quantum physics of Bose-Einstein statistical "attraction", since $U/d = pV$.