1. First problem:

   (a) $\langle(\delta E)^2\rangle = \langle E^2\rangle - \langle E\rangle^2$. We already know that $\langle E^2\rangle = \dfrac{1}{Q^2}\dfrac{\partial^2 Q}{\partial\beta^2}$ and $\langle E\rangle = \dfrac{-1}{Q}\dfrac{\partial Q}{\partial\beta}$.
   Thus, $\langle(\delta E)^2\rangle = \dfrac{1}{Q^2}\dfrac{\partial^2 Q}{\partial\beta^2} - \dfrac{1}{Q^2}\Big(\dfrac{\partial Q}{\partial\beta}\Big)^2$.
   Now just for kicks, let's take the second derivative of $\ln Q$ with respect to $-\beta$. We have

$$\begin{aligned}
\frac{\partial^2 \ln Q}{\partial\beta^2} &= \frac{\partial}{\partial\beta}\Big(\frac{1}{Q}\frac{\partial Q}{\partial\beta}\Big) \\
&= \frac{-1}{Q^2}\Big(\frac{\partial Q}{\partial\beta}\Big)^2 + \frac{1}{Q}\frac{\partial^2 Q}{\partial\beta^2} \text{ (using product rule and chain rule)} \\
&= -\langle E\rangle^2 + \langle E^2\rangle \\
\frac{\partial^2 \ln Q}{\partial\beta^2} &= \langle(\delta E)^2\rangle
\end{aligned}$$

   So we proved it! Also note that $-\dfrac{\partial\langle E\rangle}{\partial\beta} = \dfrac{\partial^2 \ln Q}{\partial\beta^2}$ because $\langle E\rangle = \dfrac{\partial \ln Q}{\partial\beta}$. Thus, $\langle(\delta E)^2\rangle = -\dfrac{\partial\langle E\rangle}{\partial\beta}$.

   (b) $q = \sum_{n=0}^{\infty} e^{-\beta E_n} = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+1/2)} = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega/2}e^{-\beta\hbar\omega n} = e^{-\beta\hbar\omega/2}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}$.
   This is just the sum of a geometric series with a pre-factor ahead of it. Using this fact, we find that

$$q = \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}} = \frac{1}{e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}}$$

   (c) Now this big Q is just a product of the individual q's because the oscillators are independent. Thus, we can find that

$$\begin{aligned}
Q(\beta, N, V) &= \sum_{n_1, n_2, ..=0}^{\infty} \exp\Big[-\beta\sum_{\alpha}(\frac{1}{2}+n_\alpha)\hbar\omega_\alpha\Big] \\
&= \Big(\sum_{n_1=0}^{\infty} e^{-\beta\hbar\omega(n_1+1/2)}\Big)\Big(\sum_{n_2=0}^{\infty} e^{-\beta\hbar\omega(n_2+1/2)}\Big)...\Big(\sum_{n_{DN}=0}^{\infty} e^{-\beta\hbar\omega(n_{DN}+1/2)}\Big) \\
&= \prod_{\alpha=1}^{DN}\Big(\sum_{n} e^{-\beta\hbar\omega_\alpha(n+1/2)}\Big) = \prod_{\alpha=1}^{DN} q(\alpha) \\
&= \prod_{\alpha=1}^{DN} \frac{1}{e^{\beta\hbar\omega_\alpha/2} - e^{-\beta\hbar\omega_\alpha/2}}
\end{aligned}$$

   Notice that this is a product of partition functions. When you take the log of this, the product turns into a sum, giving

$$\ln Q = -\sum_{\alpha=0}^{DN} \ln\left(e^{\beta\hbar\omega_\alpha/2} - e^{-\beta\hbar\omega_\alpha/2}\right)$$

(d) $\langle E\rangle = \dfrac{-\partial \ln Q}{\partial \beta}$. Using this and the answer to part(c), we can find

$$\langle E\rangle = \sum_{\alpha=0}^{DN} \frac{\hbar\omega_\alpha}{2} \frac{e^{\beta\hbar\omega_\alpha/2} + e^{-\beta\hbar\omega_\alpha/2}}{e^{\beta\hbar\omega_\alpha/2} - e^{-\beta\hbar\omega_\alpha/2}}$$

(e) For the canonical ensemble, $P_\nu = \dfrac{e^{-\beta E_\nu}}{Q}$. Thus, $\ln P_\nu = -\beta E_\nu - \ln Q$. Let's plug all this into the expression for S.

$$\begin{aligned}
S &= -k_B \sum_\nu \frac{1}{Q}(-\beta E_\nu e^{-\beta E_\nu} - \ln Q e^{-\beta E_\nu}) \\
&= k_B \sum_\nu \beta E_\nu \frac{e^{-\beta E_\nu}}{Q} + k_B \ln Q \sum_\nu \frac{e^{-\beta E_\nu}}{Q} \\
&= k_B\beta\langle E\rangle + k_B \ln Q \text{ (because Q} = \sum_\nu e^{-\beta E_\nu}) \\
&= \frac{\langle E\rangle}{T} + k_B \ln Q \\
TS &= \langle E\rangle + k_B T \ln Q \\
\implies -k_B T \ln Q &= \langle E\rangle - TS \equiv A \\
A &= -k_B T \ln Q
\end{aligned}$$

Thus, we can obtain the Helmholtz free energy from the partition function.

(f) We know that $g(\omega)d\omega = \delta(\omega - \omega_0)d\omega$. To get A using this and Q, we compute $A = -k_B T \int_0^\infty Q(\omega)g(\omega)d\omega$, where $Q(\omega)$ is our answer from (c). Let's do this integral!

$$\begin{aligned}
A &= -k_B T \int_0^\infty d\omega \delta(\omega - \omega_0) \sum_\alpha - \ln\left(e^{\beta\hbar\omega_\alpha/2} - e^{-\beta\hbar\omega_\alpha/2}\right) \\
&= k_B T \ln\left(e^{\beta\hbar\omega_0/2} - e^{-\beta\hbar\omega_0/2}\right)
\end{aligned}$$

We can do this since the δ function just picks out the frequency ω_0.

2. Second problem:

(a) Now the expression for P_ν changes because we're looking at the grand canonical partition function. We have $P_\nu = \dfrac{e^{-\beta E_\nu + \beta\mu N_\nu}}{Z}$. Same as in question 1, let's take the log of this expression. Then, $\ln P_\nu = -\beta E_\nu + \beta\mu N_\nu - \ln Z$. Plugging into the Gibb's entropy, we find that

$$\begin{aligned} S &= -k_B \sum_\nu \frac{-\beta E_\nu e^{-\beta E_\nu + \beta\mu N_\nu}}{Z} + \frac{\beta\mu N_\nu e^{-\beta E_\nu + \beta\mu N_\nu}}{Z} + \frac{-\ln Z e^{-\beta E_\nu + \beta\mu N_\nu}}{Z} \\ S &= k_B\beta\langle E\rangle - k_B\beta\mu\langle N\rangle + k_B \ln Z \text{ (using that } Z = \sum_\nu e^{-\beta E_\nu + \beta\mu N_\nu}) \end{aligned}$$

(b) $E = TS - pV + \mu N$ and $\Phi \equiv E - TS + \mu N \implies \Phi = -pV$.

(c) Let's manipulate S some more from (a).

$$\begin{aligned} S &= k_B\beta\langle E\rangle - k_B\beta\mu\langle N\rangle + k_B \ln Z \\ S &= \frac{\langle E\rangle}{T} - \frac{\mu\langle N\rangle}{T} + k_B \ln Z \\ TS &= \langle E\rangle - \mu\langle N\rangle + k_B T \ln Z \\ \implies -k_B T\ln Z &= \langle E\rangle - \mu\langle N\rangle - TS \\ \text{or } k_B T \ln Z &= -\Phi \end{aligned}$$

Additionally, this also means $k_B T \ln Z = pV$ or $\ln Z = \beta pV$!

(d) The average energy is $\langle E\rangle = \sum_\nu E_\nu P_\nu$. Plugging in for P_ν, we get $\langle E\rangle = \sum_\nu E_\nu \dfrac{e^{-\beta E_\nu + \beta\mu N_\nu}}{Z}$.
Note that

$$\begin{aligned} -\Big(\frac{\partial \ln Z}{\partial\beta}\Big)_{\mu,V} &= -\frac{1}{Z}\sum_\nu (-E_\nu + \mu N_\nu) e^{-\beta E_\nu + \beta\mu N_\nu} \\ &= \langle E\rangle - \mu\langle N\rangle \\ \implies \langle E\rangle &= \mu\langle N\rangle - \Big(\frac{\partial \ln Z}{\partial\beta}\Big)_{\mu,V} \end{aligned}$$

This looks more complicated than before because we're working in the grand canonical ensemble where μ, V, β are held constant and this is not the natural set of variables to yield a clean expression for $\langle E\rangle$.

(e) Similar to E, we can write $\langle N\rangle = \sum_\nu N_\nu P_\nu = \sum_\nu N_\nu \dfrac{e^{-\beta E_\nu + \beta\mu N_\nu}}{Z}$. We can take the derivative of $\ln Z$ with respect to μ to get a similar expression.

$$\Big(\frac{\partial \ln Z}{\partial\mu}\Big)_{\beta,V} = \frac{1}{Z}\sum_\nu \beta N_\nu e^{-\beta E_\nu + \beta\mu N_\nu} = \beta\langle N\rangle$$

Thus, $\langle N\rangle = \dfrac{1}{\beta}\Big(\dfrac{\partial \ln Z}{\partial\mu}\Big)_{\beta,V} = \Big(\dfrac{\partial \ln Z}{\partial\beta\mu}\Big)_{\beta,V}$. Here, we can pull the β into the derivative as it is constant, and can either be inside or outside.

(f) We take derivatives with respect to the conjugate field that causes a variable to fluctuate in any ensemble. E is controlled by the "field" $-\beta$ and N is controlled by the "field" $\beta\mu$. Taking the derivatives of the log of the partition function with respect to these fields gives the average of the fluctuating quantity. This is a useful pattern to note – you should be able to identify the correct field for a variable in order to take the correct derivative for any old partition function.

(g) As we did for $\langle(\delta E)^2\rangle$ in question 1, we can do a similar manipulation in the grand canonical ensemble for $\langle(\delta N)^2\rangle$.

$\langle(\delta N)^2\rangle = \langle N^2\rangle - \langle N\rangle^2$. We can again infer that $\langle N^2\rangle = \frac{1}{Z^2}\frac{\partial^2 Z}{\partial(\beta\mu)^2}$ and $\langle N\rangle = \frac{1}{Z}\frac{\partial Z}{\partial\beta\mu}$. Thus, $\langle(\delta N)^2\rangle = \frac{1}{Z^2}\frac{\partial^2 Z}{\partial(\beta\mu)^2} - \frac{1}{Z^2}\Big(\frac{\partial Z}{\partial\beta\mu}\Big)^2$.

Back to the log derivatives...

$$\begin{aligned}
\frac{\partial^2 \ln Z}{\partial(\beta\mu)^2} &= \frac{\partial}{\partial\beta\mu}\Big(\frac{1}{Z}\frac{\partial Z}{\partial\beta\mu}\Big) \\
&= \frac{-1}{Z^2}\Big(\frac{\partial Z}{\partial\beta\mu}\Big)^2 + \frac{1}{Z}\frac{\partial^2 Z}{\partial(\beta\mu)^2} \text{ (using product rule and chain rule)} \\
&= -\langle N\rangle^2 + \langle N^2\rangle \\
\frac{\partial^2 \ln Z}{\partial(\beta\mu)^2} &= \langle(\delta N)^2\rangle
\end{aligned}$$

Thus, this is the appropriate derivative to find $\langle(\delta N)^2\rangle$. Note again that we took the second derivative with respect to the "field" $\beta\mu$!

Also, $\frac{\partial\langle N\rangle}{\partial\beta\mu} = \frac{\partial^2 \ln Z}{\partial(\beta\mu)^2}$ because $\langle N\rangle = \frac{\partial \ln N}{\partial\beta\mu}$. Thus, $\langle(\delta N)^2\rangle = \frac{\partial\langle N\rangle}{\partial\beta\mu}$.