Solution to Problem 1 on midterm. The easiest way to do this problem is recognizing the correspondence with a non-interacting Ising model in an external field (hw1, prob1). If we define an occupation variable $n_i \in \{0, 1\}$ for each site i, the excluded volume potential implies this variable only has two variables, just like an Ising spin. The chemical potential acts like the external field, since $\sum_i n_i = N$.

$$\Xi(\mu, M, \beta) = \sum_{N=0}^{\infty} \frac{1}{N!} e^{\mu\beta N} \sum_{\Gamma_N} e^{-\beta E(\Gamma_N)} \tag{1}$$

With the excluded volume potential, $e^{-\beta E(\Gamma_N)} \in \{0, 1\}$, so then $\sum_{\Gamma_N} e^{-\beta E(\Gamma_N)}$ is the number of allowed states with N particles on M sites. The key is writing this sum over states of N particles as a sum over occupation variables for each site. This is possible if we include a factor of $N!$ for the number of ways N particles can be arranged on N sites. For each choice of occupation variables $n_1 \ldots n_M$ such that $\sum_i^M n_i = N$, there are $N!$ configurations of particles that give this "spin" configuration. Then the sum over Γ_N can be replaced by a sum over occupation variables n_i for $j = 1 \ldots M$ such that $\sum_i n_i = N$. The additional sum over all N implies a free summation over the occupation variables,

$$\sum_{N=0}^{\infty} \sum_{\Gamma_N} \leftrightarrow \sum_{n_1=0,1} \sum_{n_2=0,1} \cdots \sum_{n_M=0,1} \tag{2}$$

again an example of the mathematical convenience of the grand canonical ensemble.

$$\Xi(\mu, M, \beta) = \prod_{i=1}^{M} \sum_{n_i=0,1} e^{\beta\mu \sum_i n_i} = \left(1 + e^{\beta\mu}\right)^M \tag{3}$$

The ensemble average of densities can be calculated as averages over the occupation variables n_i, so $\langle \rho(\mathbf{x}) \rangle = \langle n_i \rangle$ where i denotes the site $\mathbf{x}$ and $\langle \rho(\mathbf{x})\rho(\mathbf{x}') \rangle = \langle n_i n_j \rangle$. As the mathematics is entirely equivalent to the previous homework problem, I quote the results:

$$\langle \rho(\mathbf{x}) \rangle = \frac{e^{\beta\mu}}{1 + e^{\beta\mu}} \tag{4}$$

$$\langle \rho(\mathbf{x})\rho(\mathbf{x}') \rangle = \left(\frac{e^{\beta\mu}}{1 + e^{\beta\mu}} \right)^2 \tag{5}$$

The key physical insight here is the density is uncorrelated on different sites, or the average of a product of two densities is the product of the averages of single site densities.

There is an alternative method for solving this problem which involves combinatorics. We have

$$\sum_{\Gamma_N} e^{-\beta E(\Gamma_N)} = \frac{M!}{(M-N)!} \tag{6}$$

since the sum over all states with N particles is the number of ways of putting N distinguishable particles on M sites, or the number of ways of picking N ordered sites from M sites. Another way of thinking about this result is that there are M sites for the first particle, $M-1$ sites for the second, and so on, until there are $M-N+1$ sites for the last particle. Then

$$\begin{aligned}
&\Xi(\mu, M, \beta)\\
&= \sum_{N=0}^{M} \frac{M!}{(M-N)!N!} e^{\mu\beta N} = \sum_{N=0}^{M} \frac{M!}{(M-N)!N!} e^{\mu\beta N} 1^{(M-N)} = \left(1+e^{\beta\mu}\right)^M
\end{aligned}$$

by the binomial theorem. To calculate the average of a density operator,

$$\langle \rho(\mathbf{x}) \rangle = \frac{1}{\Xi} \sum_{N=0}^{\infty} \sum_{\Gamma_N} \left(\sum_{i=1}^{N} \delta(\mathbf{x}, \mathbf{r}_i) \right) \frac{1}{N!} e^{\beta\mu N} H(\Gamma_N) \tag{7}$$

note that this quantity is non-zero only if there is a particle at site $\mathbf{x}$, and the N terms in the sum over i are the same since any particle could occupy the site $\mathbf{x}$. With the $\delta(\mathbf{x}, \mathbf{r}_1)$ restriction, the sum over Γ_N is the number of ways of putting $N-1$ particles on $M-1$ sites. Then

$$\begin{aligned}
&\langle \rho(\mathbf{x}) \rangle\\
&= \frac{1}{(1+e^{\beta\mu})^M} \sum_{N=0}^{M-1} \frac{1}{N!} \frac{(M-1)!}{(M-N)!} N e^{\beta\mu(N-1)} e^{\beta\mu}\\
&= \frac{1}{(1+e^{\beta\mu})^M} \sum_{N=0}^{M-1} \frac{(M-1)!}{(M-N)!(N-1)!} e^{\beta\mu(N-1)} e^{\beta\mu}\\
&= \frac{e^{\beta\mu}(1+e^{\beta\mu})^{M-1}}{(1+e^{\beta\mu})^M} = \frac{e^{\beta\mu}}{1+e^{\beta\mu}}
\end{aligned}$$

We can use similar ideas to calculate $\langle \rho(\mathbf{x}) \rho(\mathbf{x}') \rangle$ and obtain the result stated previously.