Goal: Derive average fractional occupancy assuming a non-cooperative model.

Given:

$$\langle N \rangle = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln \mathcal{Z}$$

The binding sites of hemoglobin has the following states, if we assume a non-cooperative model:

# Binding Sites	# Configurations	Configuration Notation
0	1	E
1	4	O_1, O_2, O_3, O_4
2	6	$T_1, T_2, T_3, T_4, T_5, T_6$
3	4	H_1, H_2, H_3, H_4
4	1	F

If we assume a non-cooperative model, then we only need to look at the states individually using the grand partition function $\mathcal{Z}$ (split on two lines for readability):

$$\mathcal{Z} = \sum_s e^{-\beta(E(s) - \mu N_s)}$$

$$\mathcal{Z} = e^{-\beta\left(E(\overline{E}) - \mu N_{\overline{E}}\right)} + \sum_{i=1}^{4} e^{-\beta\left(E(\overline{O_i}) - \mu N_{\overline{O_i}}\right)} + \sum_{i=0}^{6} e^{-\beta\left(E(\overline{T_i}) - \mu N_{\overline{T_i}}\right)}$$

$$+ \sum_{i=0}^{4} e^{-\beta\left(E(\overline{H_i}) - \mu N_{\overline{H_i}}\right)} + e^{-\beta\left(E(\overline{F}) - \mu N_{\overline{F}}\right)}$$

However, we know the values of $E(s)$ and N_s.

State	$E(s)$	N_s
E	0	0
O	1	1
T	2	2
H	3	3
F	4	4

This means if we call the energy of the system ε, then State $E(\overline{T}) = 2\varepsilon$, for example. So we can simplify $\mathcal{Z}$ to:

$$\mathcal{Z} = 1 + 4e^{-\beta(\varepsilon - \mu)} + 6e^{-2\beta(\varepsilon - \mu)} + 4e^{-3\beta(\varepsilon - \mu)} + e^{-4\beta(\varepsilon - \mu)}$$

$$\frac{\partial \mathcal{Z}}{\partial \mu} = \beta[4e^{-\beta(\varepsilon - \mu)} + 12e^{-2\beta(\varepsilon - \mu)} + 12e^{-3\beta(\varepsilon - \mu)} + 4e^{-4\beta(\varepsilon - \mu)}]$$

Since we're given that:

$$\langle N \rangle = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln \mathcal{Z} \Rightarrow \langle N \rangle = \frac{1}{\beta} \frac{1}{\mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial \mu}$$

So:

$$\langle N \rangle = \frac{1}{\beta} \frac{\beta[4e^{-\beta(\varepsilon-\mu)} + 12e^{-2\beta(\varepsilon-\mu)} + 12e^{-3\beta(\varepsilon-\mu)} + 4e^{-4\beta(\varepsilon-\mu)}]}{1 + 4e^{-\beta(\varepsilon-\mu)} + 6e^{-2\beta(\varepsilon-\mu)} + 4e^{-3\beta(\varepsilon-\mu)} + e^{-4\beta(\varepsilon-\mu)}}$$

$$\langle N \rangle = \frac{4e^{-\beta(\varepsilon-\mu)} + 12e^{-2\beta(\varepsilon-\mu)} + 12e^{-3\beta(\varepsilon-\mu)} + 4e^{-4\beta(\varepsilon-\mu)}}{1 + 4e^{-\beta(\varepsilon-\mu)} + 6e^{-2\beta(\varepsilon-\mu)} + 4e^{-3\beta(\varepsilon-\mu)} + e^{-4\beta(\varepsilon-\mu)}}$$

Note that this equation only holds for the non-cooperative model for hemoglobin (Assuming $J = 0$).