PHY 410

HW #7 (1)

7.1

For Ar at T = 800K: $n_Q = \left(\frac{M\tau}{2\pi\hbar^2}\right)^{3/2}$

$$n_Q = \left(\frac{M k_B T}{2\pi\hbar^2}\right)^{3/2} = \left(\frac{6.634\times10^{-29}\,\text{kg}\times 1.38\times10^{-23}\,\text{m}^2\text{kg}\,\text{s}^{-2}\text{K}^{-1}\times 300\,\text{K}}{2\pi\cdot(1.054\times10^{-34}\,\text{J}\cdot\text{s})^2}\right)^{3/2}$$

$$n_Q = 7.8\times10^{24}\,(\text{cm}^{-3})$$

$n = 10^{16}\,(\text{cm}^{-3})$

$$\frac{\mu}{\tau} = \log\left(\frac{n}{n_Q}\right) = \log\left(\frac{10^{16}}{7.8\times10^{24}}\right) = -20.476$$

$$\lambda = \exp\left(\frac{\mu}{\tau}\right) = \frac{n}{n_Q} = 0.128\times10^{-8}$$

$n = 10^{18}\,(\text{cm}^{-3})$

$$\lambda = \frac{n}{n_Q} = \frac{10^{18}}{7.8\times10^{24}} = 0.128\times10^{-6}$$

$$\frac{\mu}{\tau} = \log\left(\frac{n}{n_Q}\right) = -15.87$$

$n = 10^{20}$

$$\lambda = \frac{n}{n_Q} = \frac{10^{20}}{7.8\times10^{24}} = 0.128\times10^{-4}$$

$$\frac{\mu}{\tau} = \log\left(\frac{n}{n_Q}\right) = -11.266$$

7.2

$$\tau d\sigma = dU + p dV - \mu dN$$

$$\Rightarrow dU = -p dV + \tau d\sigma + \mu dN$$

$$F = U - \tau\sigma \Rightarrow dF = dU - \tau d\sigma - \sigma d\tau$$

$$\Rightarrow dF = -p dV + \tau d\sigma + \mu dN - \tau d\sigma - \sigma d\tau$$

$$dF = -p dV - \sigma d\tau + \mu dN$$

$$\Rightarrow \boxed{p = -\left(\frac{\partial F}{\partial V}\right)_{\tau, N}}$$

$$\boxed{\sigma = -\left(\frac{\partial F}{\partial \tau}\right)_{V, N}}$$

(+)

$$\left.\begin{aligned} \left(\frac{\partial p}{\partial \tau}\right)_{N,V} &= -\frac{\partial^2 F}{\partial \tau \partial V} \\ \left(\frac{\partial \sigma}{\partial V}\right)_{N,\tau} &= -\frac{\partial^2 F}{\partial V \partial \tau} \end{aligned}\right\} \Rightarrow \left(\frac{\partial p}{\partial \tau}\right)_{N,V} = \left(\frac{\partial \sigma}{\partial V}\right)_{N,\tau}$$

7.3

(a) $$\mathcal{Z}(\mu,\tau) = \sum_{N} \sum_{s(N)} \exp[(N\mu - \varepsilon_{s(N)})/\tau]$$

$N = 0 \rightarrow \varepsilon_{s(0)} = 0$

$N = 1 \rightarrow \varepsilon_{s(1)} = 0, \varepsilon$

$$\Rightarrow \mathcal{Z}(\mu,\tau) = \exp(0) + \exp\left(\frac{\mu - 0}{\tau}\right) + \exp\left(\frac{\mu - \varepsilon}{\tau}\right)$$

$$\boxed{\mathcal{Z}(\mu,\tau) = 1 + \lambda + \lambda \exp\left(-\frac{\varepsilon}{\tau}\right)}$$ here $\lambda = \exp\left(\frac{\mu}{\tau}\right)$

(b) $$\langle N \rangle = \tau \frac{\partial \log \mathcal{Z}}{\partial \mu} = \tau \frac{\partial \log \mathcal{Z}}{\partial \lambda} \frac{\partial \lambda}{\partial \mu}$$

or use $\langle N \rangle = \lambda \frac{\partial \ln \mathcal{Z}}{\partial \lambda}$

$= \lambda \frac{1 + \exp(-\varepsilon/\tau)}{\mathcal{Z}}$

$$\langle N \rangle = \tau \frac{\partial \log \mathcal{Z}}{\partial \lambda} \cdot \frac{\lambda}{\tau} = \lambda \frac{\partial \log \mathcal{Z}}{\partial \lambda}$$

$$\langle N \rangle = \lambda \cdot \frac{1 + \exp\left(-\frac{\varepsilon}{\tau}\right)}{\mathcal{Z}}$$

$$\boxed{\langle N \rangle = \frac{\lambda + \lambda \exp\left(-\frac{\varepsilon}{\tau}\right)}{\mathcal{Z}}}$$

(c) $$\langle N(\varepsilon) \rangle = \frac{N(\varepsilon) \cdot \lambda \exp\left(-\frac{\varepsilon}{\tau}\right)}{\mathcal{Z}} = \boxed{\frac{\lambda \exp\left(-\frac{\varepsilon}{\tau}\right)}{\mathcal{Z}}}$$, here $N(\varepsilon) = 1$

(d)

$$\langle U\rangle = \frac{\sum_{ASN} \varepsilon_s \exp[\beta(N\mu - \varepsilon_s)]}{\mathcal{Z}} = \frac{0 + 0.\lambda + \varepsilon.\lambda e^{-\varepsilon/\tau}}{\mathcal{Z}}$$

$$\boxed{\langle U\rangle = \frac{\varepsilon\lambda \exp(-\varepsilon/\tau)}{\mathcal{Z}}}$$

(e) If includes the possibility that orbital 0 and ε may be occupied each by one particle at the same time. The different allowed states and their corresponding energies are

$N = 0$, $\varepsilon_{s(0)} = 0$

$N = 1$, $\varepsilon_{s(1)} = 0, \varepsilon$

$N = 2$, $\varepsilon_{s(2)} = \varepsilon$

$$\Rightarrow \mathcal{Z} = \exp(0) + \exp\left(\frac{\mu - 0}{\tau}\right) + \exp\left(\frac{\mu - \varepsilon}{\tau}\right) + \exp\left(\frac{2\mu - \varepsilon}{\tau}\right)$$

$$\mathcal{Z} = 1 + \lambda + \lambda\exp\left(-\frac{\varepsilon}{\tau}\right) + \lambda^2\exp(-\varepsilon/\tau)$$

$$\mathcal{Z} = (1+\lambda)\left(1 + \lambda\exp\left(-\frac{\varepsilon}{\tau}\right)\right)$$

7.4

(a) absence of CO:

$$\mathcal{Z}_a = 1 + \exp\left(\frac{\mu_{O_2} - \varepsilon_A}{\tau}\right)$$

$$\mathcal{Z}_a = 1 + \lambda(O_2).\exp\left(-\frac{\varepsilon_A}{\tau}\right)$$

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+ probability a heme site was occupied by 1 O_2

$$P(O_2) = \frac{\lambda(O_2)\exp\left(-\frac{\varepsilon_A}{\tau}\right)}{z_a}$$

+ To 90% of Hb sites are occupied by O_2:

$$P(O_2) = 0{,}9 \Leftrightarrow \frac{\lambda(O_2)\exp\left(-\frac{\varepsilon_A}{\tau}\right)}{1+\lambda(O_2)\exp\left(-\frac{\varepsilon_A}{\tau}\right)} = \frac{9}{10}$$

$$\rightarrow \lambda(O_2)\exp\left(-\frac{\varepsilon_A}{\tau}\right) = 9$$

$$\rightarrow -\frac{\varepsilon_A}{\tau} = \log\left(\frac{9}{\lambda(O_2)}\right)$$

$$\rightarrow \varepsilon_A = -\tau\log\left(\frac{9}{\lambda(O_2)}\right) = -k_BT\log\left(\frac{9}{\lambda(O_2)}\right)$$

$$\rightarrow \varepsilon_A = -1.38\times10^{-23}\times 310\ J\ \log\left(\frac{9}{10^{-5}}\right)$$

$$\varepsilon_A = -5.87\times10^{-20}\ J = \boxed{-0.367\ eV}$$

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b

$$z_b = \underset{N=0}{1} + \underset{N_{O_2}=1,\ N_{CO}=0}{\lambda(O_2)\exp\left(-\frac{\varepsilon_A}{\tau}\right)} + \underset{N_{O_2}=0,\ N_{CO}=1}{\lambda(CO)\exp\left(-\frac{\varepsilon_B}{\tau}\right)}$$

To 10% of Hb sites are occupied by O_2

$$\frac{\lambda(O_2)\exp\left(-\frac{\varepsilon_A}{\tau}\right)}{1+\lambda(O_2)\exp\left(-\frac{\varepsilon_A}{\tau}\right)+\lambda(CO)\exp\left(-\frac{\varepsilon_B}{\tau}\right)} = \frac{1}{10}$$

$$\Rightarrow \quad \frac{9}{10 + \lambda(CO)\exp\left(-\frac{\varepsilon_B}{\tau}\right)} = \frac{1}{10}$$

$$\Rightarrow \quad 90 = 10 + \lambda(CO)\exp\left(-\frac{\varepsilon_B}{\tau}\right)$$

$$\Rightarrow \quad \exp\left(-\frac{\varepsilon_B}{\tau}\right) = \frac{80}{\lambda(CO)} = \frac{80}{10^{-7}} = 8 \times 10^{8}$$

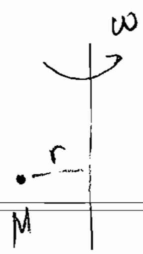
$$-\frac{\varepsilon_B}{\tau} = \log\left(8 \times 10^{8}\right)$$

$$\varepsilon_B = -\tau \log\left(8 \times 10^{8}\right)$$

$$\varepsilon_B = -8.77 \times 10^{-20}\,J = \boxed{-0.548\ eV}$$

$\boxed{7.5}$

$$\mu_{tot} = \mu_{ext} + \mu_{int} = \tau \log\left(\frac{n(r)}{n_Q}\right) + \mu_{ext}$$



$$\vec{F} = -M\omega^2 \vec{r}, \quad U = -\int \vec{F}\, d\vec{r} = \frac{M\omega^2 r^2}{2}$$

$$\Rightarrow \quad \mu_{tot} = \tau \log\left(\frac{n(r)}{n_Q}\right) + \frac{M\omega^2 r^2}{2}$$

(*) In equilibrium μ_{tot} should be independent of r

$$\tau \log\left(\frac{n(r)}{n_Q}\right) + \frac{M\omega^2 r^2}{2} = \tau \log\left(\frac{n(0)}{n_Q}\right)$$

$$\frac{n(r)}{n_Q} \exp\left(\frac{M\omega^2 r^2}{2\tau}\right) = \frac{n(0)}{n_Q}$$

$$\Rightarrow \boxed{n(r) = n(0)\exp\left(-\frac{M\omega^2 r^2}{2\tau}\right)}$$