

Graduate Stat. Mech

HW #6 - solution

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① Pathria 6.1

$$S = \sum_k S_k = \sum_k \gamma k_B T \ln(1 - \gamma e^{-\beta(\epsilon_k - \mu)}) ; \quad \gamma = \begin{cases} +1, & \text{bosons} \\ -1, & \text{fermions} \end{cases}$$

$$= \sum_k \gamma k_B T \ln(1 - \gamma e^{-\beta(\epsilon_k - \mu)}) \quad \dots \quad (1)$$

now

$$S = - \left(\frac{\partial S}{\partial T} \right)_{V, \mu} = - \sum_k \left[\gamma k_B \ln(1 - \gamma e^{-\beta(\epsilon_k - \mu)}) + \frac{\gamma k_B T \left(\frac{\epsilon_k - \mu}{k_B} \right) \left(\frac{-1}{T^2} \right) e^{-\beta(\epsilon_k - \mu)}}{1 - \gamma e^{-\beta(\epsilon_k - \mu)}} \right]$$

$$= \sum_k \left[\gamma k_B \ln(1 - \gamma e^{-\beta(\epsilon_k - \mu)}) - \frac{k_B \beta (\epsilon_k - \mu) e^{-\beta(\epsilon_k - \mu)}}{1 - \gamma e^{-\beta(\epsilon_k - \mu)}} \right]$$

let $x = e^{-\beta(\epsilon_k - \mu)}$

$$\ln x = -\beta(\epsilon_k - \mu)$$

$$\Rightarrow S = - \sum_k \left[\gamma k_B \ln(1 - \gamma x) + \frac{(k_B \ln x)x}{1 - \gamma x} \right]$$

$$= -k_B \sum_k \frac{\gamma (1 - \gamma x) \ln(1 - \gamma x) + x \ln x}{(1 - \gamma x)} ; \quad \gamma^2 = +1$$

$$= -k_B \sum_k \frac{\gamma \ln(1 - \gamma x) - x \ln(1 - \gamma x) + x \ln x}{(1 - \gamma x)}$$

$$= k_B \sum_k \frac{-\gamma \ln(1 - \gamma x) + x \ln(1 - \gamma x) - x \ln x}{(1 - \gamma x)}$$

$$S = k_B \sum_K \frac{\gamma \ln\left(\frac{1}{1-\gamma x}\right) + x \ln\left(\frac{1-\gamma x}{x}\right)}{(1-\gamma x)}$$

$$= k_B \left[\sum_K \frac{\gamma}{1-\gamma x} \ln\left(\frac{1}{1-\gamma x}\right) + \sum_K \left(\frac{x}{1-\gamma x} \right) \ln\left(\frac{1-\gamma x}{x}\right) \right] - \beta(\epsilon_k - \mu)$$

Now $\bar{n}_e = \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1} = \frac{1}{\frac{1}{x} - \gamma}$; where $x = e$

$$= \frac{x}{1-\gamma x} \Rightarrow \boxed{\frac{1-\gamma x}{x} = \frac{1}{\bar{n}_e}} \Rightarrow \frac{1}{x} - \gamma = \frac{1}{\bar{n}_e}$$

$$\Rightarrow \frac{1}{x} = \frac{1}{\bar{n}_e} + \gamma = \frac{1 + \gamma \bar{n}_e}{\bar{n}_e} \Rightarrow x = \frac{\bar{n}_e}{1 + \gamma \bar{n}_e} \Rightarrow \text{relabel}$$

$$\bar{n}_e \equiv n_e \Rightarrow \boxed{x = \frac{n_e}{1 + \gamma n_e}}$$

now substitute in (2)

$$S = k_B \left[\sum_K \frac{\gamma}{1 - \frac{\gamma n_e}{1 + \gamma n_e}} \ln\left(\frac{1}{1 - \frac{\gamma n_e}{1 + \gamma n_e}}\right) + \sum_K n_e \ln\left(\frac{1}{n_e}\right) \right]$$

$$= k_B \sum_K \left(\gamma \left(1 + \gamma n_e \right) \ln\left(1 + \gamma n_e\right) - n_e \ln n_e \right)$$

- for bosons, $\gamma = +1$

$$S = k_B \sum_K \left[\left(1 + n_e \right) \ln\left(1 + n_e\right) - n_e \ln n_e \right] \quad \text{--- (3)}$$

- for fermions, $\gamma = -1$

$$S = k_B \sum_K \left[-(1 - n_e) \ln(1 - n_e) - n_e \ln n_e \right] \quad \text{--- (4)}$$

Alternative method

- for fermions, $P_\varepsilon(n) = \begin{cases} \bar{n}_\varepsilon & ; \text{for } n=1 \\ 1-\bar{n}_\varepsilon & ; \text{for } n=0 \end{cases}$ see equations
6.3.10 and
6.3.11 of

$$\Rightarrow S = -k_B \sum_{\varepsilon} \sum_n P_\varepsilon(n) \ln P_\varepsilon(n)$$

Pathria

Note: $\bar{n}_\varepsilon \equiv n_\varepsilon$

$$= -k_B \sum_{\varepsilon} (1-\bar{n}_\varepsilon) \ln(1-\bar{n}_\varepsilon) + \bar{n}_\varepsilon \ln \bar{n}_\varepsilon ; \text{ same as (4)}$$

$-\beta(\varepsilon_k - \mu)$

- for bosons, $\bar{n}_\varepsilon = \frac{1}{\frac{1}{x}-1} \Rightarrow x = \frac{\bar{n}_\varepsilon}{1+\bar{n}_\varepsilon} ; x=e$

again let $\bar{n}_\varepsilon \rightarrow n_\varepsilon$ (relabel) \Rightarrow

$$x = \frac{n_\varepsilon}{1+n_\varepsilon}$$

$$P_\varepsilon(n) = \frac{x^n}{\sum_n x^n} = \frac{x^n}{\frac{1}{1-x}} = x^n(1-x) ; \text{ where } \sum x^n = \frac{1}{1-x}$$

$$= \left(\frac{n_\varepsilon}{1+n_\varepsilon} \right)^n \left(1 - \frac{n_\varepsilon}{1+n_\varepsilon} \right) = \left(\frac{n_\varepsilon}{1+n_\varepsilon} \right)^n \left(\frac{1}{1+n_\varepsilon} \right)$$

$$= \frac{n_\varepsilon^n}{(1+n_\varepsilon)^{n+1}}$$

$$\text{now } S = -k_B \sum_n P_\varepsilon(n) \ln P_\varepsilon(n)$$

$$= -k_B \sum_n P_\varepsilon(n) \ln \frac{n_\varepsilon^n}{(1+n_\varepsilon)^{n+1}}$$

$$= -k_B \left[\sum_n P_\varepsilon(n) n \ln n_\varepsilon - P_\varepsilon(n) (n+1) \ln (1+n_\varepsilon) \right]$$

$$= -k_B \ln n_\varepsilon \underbrace{\sum_n n P_\varepsilon(n)}_{\langle n_\varepsilon \rangle = \bar{n}_\varepsilon \equiv n_\varepsilon} + k_B \ln (1+n_\varepsilon) \underbrace{\sum_n P_\varepsilon(n) (n_\varepsilon+1)}_{\langle \bar{n}_\varepsilon + 1 \rangle \equiv n_\varepsilon + 1}$$

$$S = -k_B \bar{n}_\varepsilon \ln \bar{n}_\varepsilon + k_B (\bar{n}_\varepsilon + 1) \ln (\bar{n}_\varepsilon + 1)$$

same as (3)

$$(2) \sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \quad \text{geometric series} \quad \dots (1)$$

a) taking the first derivative of (1), gives

$$\sum_{n=1}^{\infty} n x^{n-1} = \frac{1}{(1-x)^2} \quad \dots (2) ; \text{ here } n \text{ can not start from zero}$$

$$\sum_{n=0}^{\infty} (n+1) x^n = \frac{1}{(1-x)^2} \Rightarrow \underbrace{\sum_0^{\infty} n x^n + \sum_0^{\infty} x^n}_{\frac{1}{1-x}} = \frac{1}{(1-x)^2}$$

$$\Rightarrow \sum_{n=0}^{\infty} n x^n + \frac{1}{1-x} = \frac{1}{(1-x)^2}$$

$$\Rightarrow \sum_{n=0}^{\infty} n x^n = \frac{1}{(1-x)^2} - \frac{1}{1-x} = \frac{1}{1-x} \left[\frac{1}{1-x} - 1 \right] = \frac{x}{(1-x)^2}$$

b) taking the second derivative of (1), gives

$$\sum_{n=2}^{\infty} n(n-1) x^{n-2} = \frac{2}{(1-x)^3} ; \quad n \text{ starts from 2}$$

$$\sum_{n=0}^{\infty} (n+2)(n+1) x^n = \frac{2}{(1-x)^3} \Rightarrow \sum_{n=0}^{\infty} (n^2 + 3n + 2) x^n = \frac{2}{(1-x)^3}$$

$$\Rightarrow \sum_{n=0}^{\infty} n^2 x^n + 3 \sum_{n=0}^{\infty} n x^n + 2 \sum_{n=0}^{\infty} x^n = \frac{2}{(1-x)^3}$$

$$\sum_{n=0}^{\infty} n^2 x^n + \frac{3x}{(1-x)^2} + \frac{2}{1-x} = \frac{2}{(1-x)^3}$$

$$\begin{aligned} \sum_{n=0}^{\infty} n^2 x^n &= \frac{2}{(1-x)^3} - \frac{3x}{(1-x)^2} - \frac{2}{(1-x)} \\ &= \frac{1}{(1-x)^3} \left[2 - 3x(1-x) - 2(1-x)^2 \right] \end{aligned}$$

$$= \frac{1}{(1-x)^3} [x + x^2] = \frac{x(x+1)}{(1-x)^3} \quad Q.E.D$$

③ Pahria 6.2

$$P_{\varepsilon}(n) = \begin{cases} \frac{\bar{n}_{\varepsilon}^n}{(\bar{n}_{\varepsilon} + 1)^{n+1}} & ; \text{ B.E} \\ \bar{n}_{\varepsilon} ; n=1 \\ 1 - \bar{n}_{\varepsilon} ; n=0 \end{cases} ; \text{ F.D}$$

$$\frac{\bar{n}_{\varepsilon}}{n!} e^{-\bar{n}_{\varepsilon}} ; \text{ M.B}$$

- B.E

$$P_{\varepsilon}(n) = \frac{\bar{n}_{\varepsilon}^n}{(\bar{n}_{\varepsilon} + 1)^{n+1}} ; \text{ let } r = \frac{\bar{n}_{\varepsilon}}{\bar{n}_{\varepsilon} + 1}$$

$$\Rightarrow P_{\varepsilon}(n) = \frac{r^n}{(1-r)^2} / 1/(1-r)^{n+1}$$

$$= (1-r) r^n$$

$$\Rightarrow \frac{1}{r} - 1 = \frac{1}{\bar{n}_{\varepsilon}}$$

$$\Rightarrow \frac{1-r}{r} = \frac{1}{\bar{n}_{\varepsilon}}$$

$$\langle n_{\varepsilon} \rangle = \sum_n n_{\varepsilon} P_{\varepsilon}(n) ; \text{ here } n_{\varepsilon} = n$$

where n_{ε} : # of bosons in state with energy ε

$$\Rightarrow \bar{n}_{\varepsilon} = \frac{r}{1-r} \dots (1)$$

$$\text{and } \bar{n}_{\varepsilon} + 1 = \frac{1}{1-r}$$

$P_{\varepsilon}(n)$: probability of state ε to have n bosons

$$\langle n_{\varepsilon} \rangle = \sum_n n_{\varepsilon} P_{\varepsilon}(n) ; \quad n_{\varepsilon} = n$$

$$= \sum_{n=0}^{\infty} n P_{\varepsilon}(n) = (1-r) \underbrace{\sum_{n=0}^{\infty} n r^n}_{\frac{r}{(1-r)^2}} = (1-r) \frac{r}{(1-r)^2} = \frac{r}{1-r} \dots (2)$$

$$\text{and } \langle n_e^2 \rangle = \sum_n n_e^2 P_e(n) ; \quad n_e = n$$

$$= \sum_n n^2 P_e(n) ; \quad P_e(n) = (1-r)^r n$$

$$= (1-r) \underbrace{\sum_{n=0}^{\infty} n^2 r^n}_{\frac{r(r+1)}{(1-r)^3}} = (1-r) \frac{r(r+1)}{(1-r)^3} = \frac{r(r+1)}{(1-r)^2}$$

$$\therefore \langle n_e^2 \rangle - \langle n_e \rangle^2 = \frac{r(r+1)}{(1-r)^2} - \frac{r^2}{(1-r)^2} = \frac{r}{(1-r)^2}$$

$$= \frac{\bar{n}_e}{\bar{n}_e + 1} (\bar{n}_e + 1)^2 = \bar{n}_e (\bar{n}_e + 1)$$

$$= \bar{n}_e^2 + \bar{n}_e$$

$$= \langle n_e \rangle^2 + \langle n_e \rangle \quad \dots (3)$$

- F. D $P_e(n) = \bar{n}_e ; n=1$

$$= 1 - \bar{n}_e ; n=0$$

$$\Rightarrow \langle n_e \rangle = \sum_{n=0}^1 n_e P_e(n) ; \quad n_e = n$$

$$= \sum_{n=0}^1 n P_e(n) = 0 + P_e(n=1) = \bar{n}_e$$

$$\text{and } \langle n_e^2 \rangle = \sum_{n=0}^1 n^2 P_e(n) = 0 + P_e(n=1) = \bar{n}_e$$

$\therefore \boxed{\langle n_e^2 \rangle - \langle n_e \rangle^2 = \bar{n}_e - \bar{n}_e^2 = \langle n_e \rangle - \langle n_e \rangle^2} \quad \dots (4)$

- M.B $P_{\varepsilon}(n) = \frac{\bar{n}_{\varepsilon}^n}{n!} e^{-\bar{n}_{\varepsilon}}$

$$\begin{aligned}
 \langle n_{\varepsilon}(n_{\varepsilon}-1) \rangle &= \sum_n n_{\varepsilon}(n_{\varepsilon}-1) P_{\varepsilon}(n) ; \quad n_{\varepsilon} = \bar{n}_{\varepsilon} \\
 &= \sum_n n(n-1) P_{\varepsilon}(n) = \sum_n n(n-1) \frac{\bar{n}_{\varepsilon}^n}{n!} e^{-\bar{n}_{\varepsilon}} \\
 &= e^{-\bar{n}_{\varepsilon}} \sum n(n-1) \frac{\bar{n}_{\varepsilon}^n}{\cancel{n(n-1)(n-2)!}} = e^{-\bar{n}_{\varepsilon}} \sum_{n=3}^{\infty} \frac{\bar{n}_{\varepsilon}^n}{(n-2)!} \\
 &= e^{-\bar{n}_{\varepsilon}} \sum_{n=0}^{\infty} \frac{\bar{n}_{\varepsilon}^{n+3}}{(n+1)!} = e^{-\bar{n}_{\varepsilon}} \bar{n}_{\varepsilon}^2 \sum_{n=0}^{\infty} \frac{\bar{n}_{\varepsilon}^{n+1}}{(n+1)!} \underbrace{e^{+\bar{n}_{\varepsilon}}}_{\bar{n}_{\varepsilon}}
 \end{aligned}$$

$$\therefore \langle n_{\varepsilon}(n_{\varepsilon}-1) \rangle = \langle n_{\varepsilon}^2 - n_{\varepsilon} \rangle = \langle n_{\varepsilon}^2 \rangle - \langle n_{\varepsilon} \rangle$$

$$\langle n_{\varepsilon} \rangle^2 = \langle n_{\varepsilon}^2 \rangle - \langle n_{\varepsilon} \rangle$$

$$\Rightarrow \boxed{\langle n_{\varepsilon}^2 \rangle - \langle n_{\varepsilon} \rangle^2 = \langle n_{\varepsilon} \rangle} \quad (5)$$

Now in general $\langle n_{\varepsilon} \rangle = \frac{1}{e^{(\varepsilon-\mu)/k_B T} - \gamma}$; $\gamma = \begin{cases} +1, & \text{bosons} \\ -1, & \text{Fermions} \\ 0, & \text{M.B} \end{cases}$

$$\Rightarrow \langle n_{\varepsilon} \rangle^{-1} = c \frac{(\varepsilon-\mu)/k_B T}{e^{(\varepsilon-\mu)/k_B T} - \gamma} \Rightarrow \text{diff both sides w.r.t } M$$

$$\Rightarrow -\langle n_{\varepsilon} \rangle^{-2} \left(\frac{\partial \langle n_{\varepsilon} \rangle}{\partial M} \right)_T = -\frac{1}{k_B T} e^{(\varepsilon-\mu)/k_B T} = -\frac{1}{k_B T} [\langle n_{\varepsilon} \rangle^{-1} + \gamma]$$

$$\Rightarrow k_B T \left(\frac{\partial \langle n_{\varepsilon} \rangle}{\partial M} \right)_T = \langle n_{\varepsilon} \rangle + \gamma \langle n_{\varepsilon} \rangle^2 \quad (6)$$

Now using equation 6.3.9 Pathria Page 151

$$\frac{\langle n_e^2 \rangle - \langle n_e \rangle^2}{\langle n_e \rangle^2} = \frac{1}{\langle n_e \rangle} + \gamma ; \quad \begin{matrix} \text{Pathria uses} \\ \rightarrow \alpha \text{ instead of } \gamma \end{matrix}$$

$$\Rightarrow \langle n_e^2 \rangle - \langle n_e \rangle^2 = \langle n_e \rangle + \gamma \langle n_e \rangle^2$$

Substitute this back in equation (6), we

get

$$k_B T \left(\frac{\partial \langle n_e \rangle}{\partial M} \right)_T = \langle n_e \rangle + \gamma \langle n_e \rangle^2$$
$$= \langle n_e^2 \rangle - \langle n_e \rangle^2 \quad (\text{Q.E.D.})$$

(4) Quantum gas in d dimensions with $\varepsilon = c |\vec{k}|^a$;

a) $S_L = \sum_k S_{Lk} = \sum_k \gamma k_B T \ln(1 - \gamma e^{\beta(\mu - \varepsilon_k)}) ; \gamma = \begin{cases} +1, \text{Bos} \\ -1, \text{Fer} \end{cases}$

$$= \frac{\gamma k_B T}{(2\pi)^d} \int d^d k \ln(1 - \gamma e^{\beta(\mu - ck^a)})$$

$$= \gamma k_B T \frac{L^d}{(2\pi)^d} \int C_d k^{d-1} dk \ln(1 - \gamma e^{\beta(\mu - ck^a)})$$

Note that in 3d $d^3 k = u \pi k^2 dk \quad 0 < k < \infty$
 in 2d $d^2 k = k dk' d\theta \quad 0 < \theta < 2\pi$

$$\text{in 1d } dk = R^0 dk$$

$$\text{so in d dimensions } dk^d = C_d k^{d-1} dk$$

$$\text{now } S_L = \gamma k_B T \frac{L^d}{(2\pi)^d} C_d \int_0^\infty k^{d-1} dk \ln(1 - \gamma e^{\beta(\mu - ck^a)})$$

integrate by parts $u = \ln(1 - \gamma e^{\beta(\mu - ck^a)})$, $dv = k^{d-1} dk$
 $du = \frac{a \gamma \beta c k^{a-1} e^{\beta(\mu - ck^a)}}{1 - \gamma e^{\beta(\mu - ck^a)}}$, $v = \frac{k^d}{d}$

$$\Rightarrow S_L = \gamma k_B T \frac{L^d}{(2\pi)^d} C_d \left[\frac{1}{d} k^d \ln(1 - \gamma e^{\beta(\mu - ck^a)}) \right]_0^\infty - \int \frac{a \gamma \beta c k^{d+a-1} e^{\beta(\mu - ck^a)}}{d (1 - \gamma e^{\beta(\mu - ck^a)})} dk$$

$$S_L = - \frac{L^d}{(2\pi)^d} C_d \frac{C}{d} a \int \frac{dk R^{d+a-1} e^{\beta(\mu - ck^a)}}{1 - \gamma e^{\beta(\mu - ck^a)}} --- (1)$$

$$b) U = \sum_k \epsilon_k n_k ; n_k = \frac{1}{e^{\beta(\epsilon_k - \mu)} - \gamma}$$

$$\begin{aligned} U &= \frac{L}{(2\pi)^d} \int_0^\infty \frac{C_d R^{d-1} dR}{e^{\beta(\epsilon_k - \mu)} - \gamma} c k^a = \frac{L}{(2\pi)^d} C_d c \int_0^\infty \frac{R^{a+d-1}}{e^{\beta(\epsilon_k - \mu)} - \gamma} dR \\ &= \frac{L}{(2\pi)^d} C_d c \underbrace{\int_0^\infty \frac{R^{a+d-1}}{1 - \gamma e^{\beta(\mu - ck^a)}} e^{\beta(\mu - ck^a)} dR}_{\text{from (1), } = -\Sigma \frac{(2\pi)^d}{L^d} \frac{d}{C_d c a}} \end{aligned}$$

$$= \frac{L}{(2\pi)^d} C_d c \left(-\Sigma \frac{(2\pi)^d}{L^d} \frac{d}{C_d c a} \right) = -\frac{\Sigma d}{a} = \frac{d}{a} (-\Sigma)$$

$$U = +\frac{d}{a} (PV) \Rightarrow PV = \frac{a}{d} U$$

equation of state expected

check ↓ 3d ↓ with $\epsilon \propto k^2 \Rightarrow PV = \frac{2}{3} U$ as expected
 for classical non interacting gas

$$c) N = \sum_k n_k = \sum_k \frac{1}{e^{\beta(\epsilon_k - \mu)} - \gamma} = \frac{L}{(2\pi)^d} \int_0^\infty \frac{C_d R^{d-1}}{e^{\beta(\epsilon_k - \mu)} - \gamma} dR$$

$$= \frac{L}{(2\pi)^d} C_d \int_0^\infty \frac{R^{d-1} dR}{e^{\beta(ck^a - \mu)} - \gamma} = \frac{L}{(2\pi)^d} C_d \int_0^\infty \frac{R^{d-1} dR}{e^{-\mu z} e^{\beta ck^a} - \gamma}$$

$$N = \frac{L}{(2\pi)^d} C_d \int_0^\infty \frac{R^{d-1} dR}{z^{-1} e^{\beta ck^a} - \gamma} ; \text{ when } z = e^{\beta \mu}$$

--- (2)

In the high T limit
 $\beta M \ll 1 \Rightarrow e^{\beta M} \ll e \text{ or } z^{-1} \gg 1$; where $z = e^{\beta M}$

$$\Rightarrow \text{in eqn (2), } z^{-1} e^{\beta c k^a} \gg \gamma = z^{-1}$$

$$\Rightarrow N = \frac{V}{(2\pi)^d} C_d \approx \int_0^\infty dk k^{d-1} e^{-\beta c k^a} \quad \dots \quad (3)$$

for 3D classical ideal gas $\epsilon = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = ck^a$

$$\Rightarrow c = \frac{\hbar^2}{2m} \text{ and } a = 2$$

$$\Rightarrow N = \frac{V}{(2\pi)^3} C_d \approx \int_0^\infty dk k^2 e^{-\beta c k^2}, \text{ let } \beta c k^2 = x^2$$

$$2\beta c k dk = 2x dx$$

$$k^2 dk = \frac{x^2 dx}{(\beta c)^{3/2}}$$

$$= \frac{V}{(2\pi)^3} C_d \frac{e^{\beta M}}{\sqrt{(\beta c)^{3/2}}} \left[\int_0^\infty dx x^2 e^{-x^2} \right]_{\sqrt{\pi}/4}$$

$$= \frac{V}{8\pi^3} C_d \approx e^{\beta M} \frac{1}{(\beta c)^{3/2}} \frac{\sqrt{\pi}}{4}; C_d = 4\pi, d^3 k = \frac{4\pi}{C_d} h^3 dk$$

$$= \frac{V}{8\pi^3} 4\pi e^{\beta M} \frac{1}{\left(\frac{\hbar^2 c}{k_B T 2m}\right)^{3/2}} \frac{\sqrt{\pi}}{4} = \frac{V}{8\pi^3} \frac{8\pi^3}{h^3} e^{\beta M} \left(\frac{2\pi m k_B T}{\hbar^2 c}\right)^{3/2}$$

$$= \frac{V}{h^3 / (2\pi m k_B T)^{3/2}} e^{\beta M} = \frac{V}{\lambda^3} e^{\beta M} \text{ as expected}$$

from equation 6.10 in our lecture notes