1) Since the # of particles is variable, we will work in grand canonical ensemble

1/2

$$\mathcal{Q} = \sum_{N_b=1}^{N} z^{N_b} Q_{N_b} \qquad z = e^{\beta\mu}$$

Now we need to evaluate Q_{N_b}

$$Q_{N_b} = \sum_{\varepsilon} a(\varepsilon)\, e^{-\beta\varepsilon} \qquad a(\varepsilon) = \text{degeneracy}$$

the Hamiltonian is

$$H = -\varepsilon \sum_{i=1}^{N} \sigma_i - \varepsilon' \sum_{\langle i,j\rangle} \sigma_i \sigma_j \quad \leftarrow \text{nearest neighbors} \qquad \sigma_i = 0, 1$$

interaction term is difficult, so use mean-field approximation

$$\sigma_j \simeq \langle \sigma_j \rangle = \theta = \frac{N_b}{N}$$

$$H \simeq -\varepsilon \sum_i \sigma_i - \varepsilon' \frac{q\theta}{2} \sum \sigma_i \qquad q = \text{coordination \#} = 4$$

$$= -\left(\varepsilon + \frac{\varepsilon' q}{2}\right) \sum \sigma_i = -\left(\varepsilon + \frac{\varepsilon' q\theta}{2}\right) N_b = E(N_b)$$

in MF approx, all states w/ N_b are equivalent so degeneracy factor is $a(N_b) = \binom{N}{N_b} = \frac{N!}{N_b!\,(N-N_b)!}$

putting it together

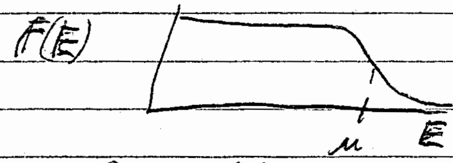
$$\mathcal{Q} = \sum_{N_b} z^{N_b} \binom{N}{N_b} e^{+\beta N_b\left(\varepsilon + \frac{\theta\varepsilon' q}{2}\right)}$$

$$= \left(1 + z e^{\beta\left(\varepsilon + \frac{\varepsilon' q}{2}\theta\right)}\right)^N$$

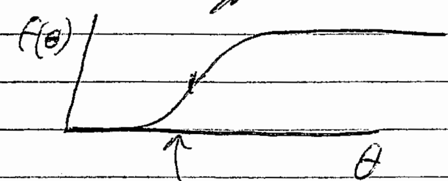
$$\langle N_b \rangle = z \frac{\partial \ln \mathcal{Q}}{\partial z} = \frac{N z e^{\beta(\varepsilon + \varepsilon' q\theta/2)}}{1 + z e^{\beta(\varepsilon + \varepsilon' q\theta/2)}}$$

$$\theta = \frac{\langle N_b \rangle}{N} = \frac{1}{z^{-1} e^{-\beta(\varepsilon + \varepsilon' q\theta/2)} + 1} \quad \#$$

The ~~left~~ right side of this equation is just a Fermi occupation function.



but energy $\propto -\theta$ so:

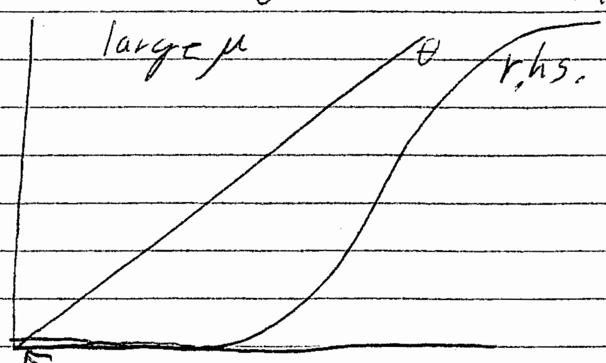


midpoint given by $\mu = -\left(\varepsilon + \frac{\varepsilon' q \theta}{2}\right)$

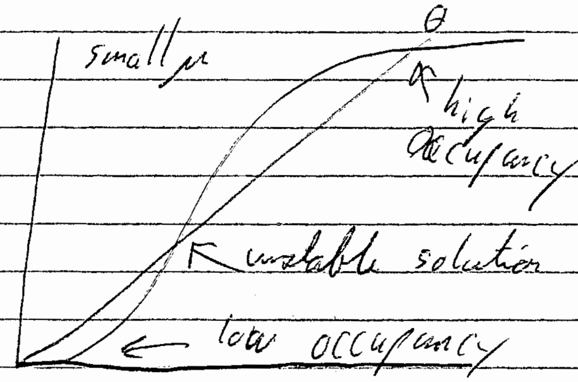
$$\theta = \frac{-2}{\varepsilon' q}(\mu + \varepsilon)$$

Solve occupancy condition graphically

$$\theta = \frac{1}{e^{-\beta\left(\varepsilon + \varepsilon' \frac{q\theta}{2} + \mu\right)} + 1}$$



one solution: low occupancy



3 solutions

2) $F = E - TS$

$$S = k_B \ln \frac{N!}{N_A!\, N_B!}$$

$$= k_B \Big[\underbrace{N}_{N_A+N_B} \ln N - \cancel{N} - N_A \ln N_A + \cancel{N_A} - N_B \ln N_B + \cancel{N_B} \Big]$$

$$= k_B \Big[-N_A \ln \frac{N_A}{N} - N_B \ln \frac{N_B}{N} \Big]$$

To compute the energy, first consider the q sites surrounding each A particle. On average $\frac{N_A}{N} q$ will be A particles and $\frac{N_B}{N} q$ will be B's.

So the interaction energy per A particle is

double counting

$$\frac{1}{2} q \left(\varepsilon_{11} \frac{N_A}{N} + \varepsilon_{12} \frac{N_B}{N} \right)$$

similarly, around each B site the interaction energy is

$$\frac{1}{2} q \left(\varepsilon_{12} \frac{N_A}{N} + \varepsilon_{22} \frac{N_B}{N} \right)$$

So the total free energy is

$$F = \frac{N_A}{2} q \left(\varepsilon_{11} \frac{N_A}{N} + \varepsilon_{12} \frac{N_B}{N} \right) + \frac{N_B}{2} q \left(\varepsilon_{12} \frac{N_A}{N} + \varepsilon_{22} \frac{N_B}{N} \right) + k_B T \left(N_A \ln \frac{N_A}{N} + N_B \ln \frac{N_B}{N} \right)$$

$$= \frac{q}{2} \left(\frac{N_A^2}{N_A+N_B} \varepsilon_{11} + \frac{N_B^2}{N_A+N_B} \varepsilon_{22} + 2 \frac{N_A N_B \varepsilon_{12}}{N_A+N_B} \right) + k_B T \left(-N_A \ln\left(1+\frac{N_B}{N_A}\right) - N_B \ln\left(1 + \frac{N_A}{N_B}\right) \right)$$

$$\mu_A = \left(\frac{\partial F}{\partial N_A}\right)_{N_B} = \frac{q}{2} \left[\varepsilon_{11} \frac{2N_A(N_A+N_B) - N_A^2}{(N_A+N_B)^2} + 2\varepsilon_{12} \frac{(N_A+N_B)N_B - N_A N_B}{(N_A+N_B)^2} - \frac{N_B^2 \varepsilon_{22}}{(N_A+N_B)^2} \right]$$

$$+ k_B T \left[-\ln\left(1 + \frac{N_B}{N_A}\right) \cancel{- N_A \frac{-\frac{N_B}{N_A^2}}{1+\frac{N_B}{N_A}} - N_B \frac{1/N_B}{1+\frac{N_A}{N_B}}} \right]$$

$$= \frac{q}{2} \left[\varepsilon_{11} \frac{N_A^2 + 2N_A N_B}{(N_A+N_B)^2} - \varepsilon_{22} \frac{N_B^2}{(N_A+N_B)^2} + 2\varepsilon_{12} \frac{N_B^2}{(N_A+N_B)^2} \right] + kT \ln \frac{N_A}{N_A+N_B}$$

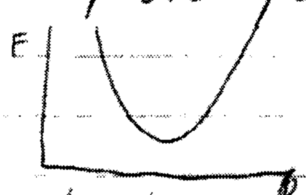
$$\mu_B = \left(\frac{\partial F}{\partial N_B}\right)_{N_A} = \frac{q}{2} \left[\varepsilon_{22} \frac{N_B^2 + 2N_A N_B}{(N_A+N_B)^2} - \varepsilon_{11} \frac{N_A^2}{(N_A+N_B)^2} + 2\varepsilon_{12} \frac{N_A^2}{(N_A+N_B)^2} \right] + kT \ln \frac{N_B}{N_A+N_B}$$

2 (cont) Now we need to establish where the phase transition occurs.
First we write the free energy in terms of the density of A particles

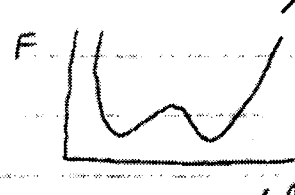
$$\phi = \frac{N_A}{N} = \frac{N_A}{N_A + N_B}$$

$$\frac{F}{N} = \frac{q}{2}\left(\epsilon_{11}\phi^2 + \epsilon_{22}(1-\phi)^2 + 2\epsilon_{12}\phi(1-\phi)\right) + kT\left(\phi\ln\phi + (1-\phi)\ln(1-\phi)\right)$$

to have phase separation we need to have multiple minima in $F(\phi)$



single phase system



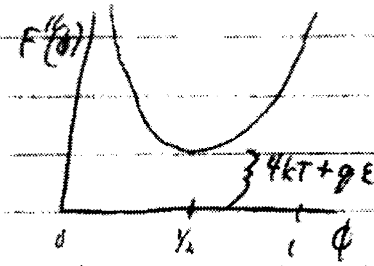
phase separated system

In order to have multiple minima, there must be some range of ϕ for which $\frac{\partial^2 F}{\partial \phi^2} < 0$ (negative curvature) so we compute F''

$$\frac{\partial F/N}{\partial \phi} = \frac{q}{2}\left(2\epsilon_{11}\phi - 2\epsilon_{22}(1-\phi) + 2\epsilon_{12}(1-2\phi)\right) + kT\left[\ln\phi + \frac{\phi}{\phi} - \ln(1-\phi) + \cancel{\frac{1}{1-\phi}(1-\phi)}\right]$$

$$\frac{\partial^2 F/N}{\partial \phi^2} = \frac{q}{2}\left(\underbrace{2\epsilon_{11} + 2\epsilon_{22} - 4\epsilon_{12}}_{2\epsilon}\right) + kT\left[\frac{1}{\phi} + \frac{1}{1-\phi}\right]$$

$$= q\epsilon + kT\left(\frac{1}{\phi} + \frac{1}{1-\phi}\right) \quad \text{so} \rightarrow$$



we want to look at the minimum of F'' to see when it first crosses 0

minimize F'' $\quad \frac{\partial^3 F/N}{\partial \phi^3} = 0 = kT\left(\frac{-1}{\phi^2} + \frac{1}{(1-\phi)^2}\right)$

$$\cancel{\phi^2} = 1 - 2\phi + \cancel{\phi^2} \qquad \phi = \frac{1}{2}$$

must be negative

so the condition for phase separation is

$$\left(\frac{\partial^2 F/N}{\partial \phi^2}\right)\Bigg|_{\phi = 1/2} = 0 = q\epsilon + kT(2+2) \rightarrow T_c = \frac{q|\epsilon|}{4k_B}$$

factor of 2 error?

12.20 p 1/3

$\Psi = -hm + q + rm^2 + sm^4 + um^6$

for spontaneous magnetization we are interested in $h=0$ so

$$\Psi' = 2rm + 4sm^3 + 6um^5$$
$$= 2m(r + 2sm^2 + 3um^4)$$

there are 5 solutions to $\Psi'=0$ these are:

$$m=0 \qquad m^2 = \frac{-2s \pm \sqrt{4s^2 - 4(3u)r}}{6u} = \frac{-s \pm \sqrt{s^2-3ur}}{3u}$$

a) $r>0$, $s > -(3ur)^{1/2}$

if $|s| < \sqrt{3ur}$ the argument of the square root is negative giving a complex solution

if $s > \sqrt{3ur}$ m^2 is always negative because $\sqrt{s^2-3ur} < s$

therefore $m=0$ is only solution (out of 5) that is real

b,c,d) define $s = -\sqrt{nur}$ where $3<n<4$ (part b)
$n=4$ (part c)
$n>4$ (part d)

the nonzero solutions of $\Psi'=0$ become

$$m_\pm^2 = \frac{-s \pm \sqrt{s^2-3ur}}{3u} = \frac{\sqrt{nur} \pm \sqrt{(n-3)ur}}{3u}$$
$$= \frac{1}{3}\sqrt{\frac{r}{u}}\left(\sqrt{n} \pm \sqrt{n-3}\right)$$

we need to determine which solutions are minima, maxima, & inflection points

$$\Psi'' = 2r + 12sm^2 + 30um^4$$

$$\Psi''(m_\pm) = 2r + 4\overbrace{s}^{-\sqrt{nur}}\sqrt{\frac{r}{u}}\left(\sqrt{n} \pm \sqrt{n-3}\right) + 30u\frac{1}{9}\frac{r}{u}\left(\sqrt{n} \pm \sqrt{n-3}\right)^2$$
$$= 2r - 4r\left(n \pm \sqrt{n(n-3)}\right) + \frac{10r}{3}\left(n \pm 2\sqrt{n(n-3)} + n - 3\right)$$
$$= r\left(2 - 4n \mp 4\sqrt{n(n-3)} + \frac{20n}{3} \pm \frac{20}{3}\sqrt{n(n-3)} - 10\right) = r\left(-8 + \frac{8}{3}n \pm \frac{8}{3}\sqrt{n(n-3)}\right)$$
$$= \frac{8r}{3}\left(n - 3 \pm \sqrt{n(n-3)}\right)$$

12.20 (cont) p 2/3

now define $\eta = n-3$ so η is always ≥ 0.

$$\Psi''(m_\pm) = \frac{8r}{3}\left(\eta \pm \sqrt{(\eta+3)\eta}\right) = \frac{8r}{3}\left(\eta \pm \sqrt{\eta^2+3\eta}\right)$$

clearly $\sqrt{\eta^2+3\eta} > \eta$ for all $\eta > 0$, therefore $\Psi''(m_-) < 0$ maxima

$\Psi''(m_+) > 0$ minima

now we need to compare $\Psi(0)$ to $\Psi(m_+)$

$$\Psi(0) = q$$

$$\Psi(m_+) = q + \overbrace{m_+^2}^{\text{positive}}(r + s m_+^2 + u m_+^4)$$

$$= q + m_+^2\left(r - \underbrace{\sqrt{nur}}_{s}\,\frac{1}{3}\sqrt{\frac{r}{u}}\left[\sqrt{n} + \sqrt{n-3}\right] + \cancel{u}\frac{1}{9}\frac{r}{\cancel{u}}\left[n + 2\sqrt{n(n-3)} + n-3\right]\right)$$

$$= q + r m_+^2\left(1 - \frac{n}{3} - \frac{1}{3}\sqrt{(n-3)n} + \frac{2}{9}n + \frac{2}{9}\sqrt{n(n-3)} - \frac{1}{3}\right)$$

$$= q + r m_+^2\left(\frac{2}{3} - \frac{n}{9} - \frac{1}{9}\sqrt{n(n-3)}\right)$$ substitute $\eta = n-3$ again

$$= q + \underbrace{\frac{r m_+^2}{9}}_{\text{positive}}\left[3 - \left(\eta + \sqrt{\eta^2+3\eta}\right)\right]$$ monotonically increasing function of η

if $\eta = 1$ $(n=4)$

$$\Psi(m_+)\Big|_{\eta=1} = q + \frac{r m_+^2}{9}\left[3 - 1 - \sqrt{4}\right] = q \quad \text{(part c)}$$

so

$\Psi(m_+) > q$ if $\eta < 1$ $(n<4)$ (part b)

$\Psi(m_+) < q$ if $\eta > 1$ $(n>4)$ (part d)

e) $r = 0$, $s < 0$ $\quad \Psi = q + s m^4 + u m^6$

$$\Psi' = 4 s m^3 + 6 u m^5 = 2 m^3 (2s + 3u m^2)$$

$$m = 0 \quad \text{or} \quad m^2 = -\frac{2s}{3u} \rightarrow m = \sqrt{\frac{2|s|}{3u}}$$

at small m the sm^4 term dominates over um^6 term. Since $s<0$ this means that Ψ decreases as $|m|$ increases (for small m) therefore these solutions have free energy below $\Psi(0) = q$

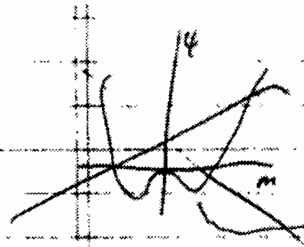
12.20 (cont) 3/3

f) Again, for small m, rm^2 term dominates over $m^4 + m^6$ terms therefore minimum must be displaced from $m=0$

$$m_\pm^2 = \frac{-s \pm \sqrt{s^2-3ur}}{3u} = 0 \text{ or } -2s$$

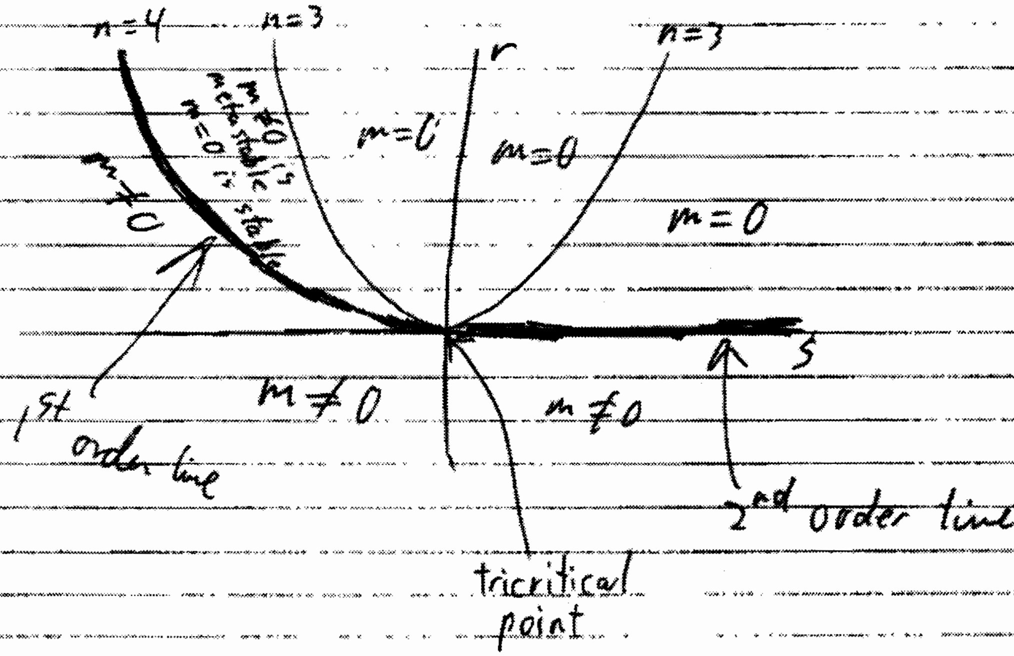
for $r \to 0$

if $s>0$ this solution is imaginary



g) from part e) if $r=0$ solutions are

$m=0$ $\quad m^2 = \frac{-2s}{3u}$ if $s>0$ this gives imaginary solution



4) 1/2 a) $X_N = \cancel{\#} x(N\tau) = \sum_{i=1}^{N} x_i$

$$X_N^2 = \sum_{i,j} x_i x_j = \sum_i x_i^2 + \sum_{i \neq j} x_i \cdot x_j$$

$$\langle X_N^2 \rangle = N \langle x_i^2 \rangle + (N^2 - N) \langle x_i \rangle^2$$

$$\langle x_i \rangle = \int x P(x)\, d^3x = \frac{1}{(2\pi)^{3/2} b^3} \int \underbrace{x}_{odd} \underbrace{e^{-x^2/2b^2}}_{even} d^3x = 0$$

$$\langle x_i^2 \rangle = \int x^2 P(x)\, d^3x = \frac{1}{(2\pi)^{3/2} b^3} \int x^2 e^{-x^2 a}\, d^3x \qquad a = \frac{1}{2b^2}$$

$$= \frac{1}{(2\pi)^{3/2} b^3} \left(-\frac{\partial}{\partial a}\right) \int e^{-x^2 a}\, d^3x = \frac{1}{(2\pi)^{3/2} b^3} \left(\frac{-\partial}{\partial a}\right) \frac{\pi^{3/2}}{a^{3/2}}$$

$$= \frac{1}{(2\cancel{\pi})^{3/2} b^3} \left(\frac{3}{2}\right) \frac{\cancel{\pi}^{3/2}}{a^{5/2}} = \frac{3}{\cancel{2}} \frac{1}{\cancel{2^{3/2}} b^3} 2^{5/2} b^5 = 3b^2$$

so $\langle X_N^2 \rangle = N(3b^2) + (N^2 - N)0^2 = 3Nb^2$

b) $$P_N(R) = \langle \delta(R - \Sigma x_i) \rangle = \left[\frac{1}{(2\pi)^{3/2} b^3}\right]^N \int \delta(R - \Sigma x_i) \prod_i e^{-x_i^2/2b^2} d^3x_i$$

write delta function as fourier series $\delta(x) = \frac{1}{(2\pi)^3} \int e^{ikx} d^3x$

$$P_N(R) = \left[\frac{1}{(2\pi)^{3/2} b^3}\right]^N \int e^{ik(R - \Sigma x_i)} \prod_i e^{-x_i^2/2b^2} d^3x_i \frac{d^3k}{(2\pi)^3}$$

$$= \left[\frac{1}{(2\pi)^{3/2} b^3}\right]^N \int e^{ikR} \left[\int e^{-x_i^2/2b^2 - ikx_i} d^3x\right]^N \frac{d^3k}{(2\pi)^3}$$

do x integrals first

$$\int e^{-\frac{1}{2b^2}(x_i^2 + 2ikb^2 x_i)} d^3x$$

complete the square $\quad x^2 + 2ikb^2 x = (x^2 + 2ikb^2 x - k^2 b^4) + k^2 b^4$

$$= (x + ikb^2)^2 + k^2 b^4$$

$$\int e^{-\frac{1}{2b^2}(x + ikb^2)^2 - \frac{k^2 b^2}{2}} d^3x = e^{-k^2 b^2/2} \left(\sqrt{2\pi b^2}\right)^3$$

2/2

$$P_N(R) = \cancel{\left[\frac{1}{(2\pi)^{3/2} b^3}\right]^N} \int e^{ikR} e^{-Nk^2b^2/2} \cancel{\left(\sqrt{2\pi b^2}\right)^{3N}} \frac{d^3k}{(2\pi)^3}$$

$$= \int e^{-\frac{N}{2}\left(k^2b^2 - \frac{2ikR}{N}\right)} d^3k \frac{1}{(2\pi)^3}$$

complete square: $k^2b^2 - \frac{2ikR}{N} = \left(kb - i\frac{R}{Nb}\right)^2 + \frac{R^2}{N^2b^2} = k^2b^2 - \frac{2ikR}{N} - \frac{R^2}{N^2b^2} + \frac{R^2}{N^2b^2}$

$$P_N(R) = \int e^{-\frac{N}{2}\left(kb - \frac{iR}{Nb}\right)^2 - \frac{R^2}{2Nb^2}} \frac{d^3k}{(2\pi)^3}$$

$$= e^{-R^2/2Nb^2} \frac{(2\pi)^{3/2}}{(Nb^2)^{3/2}} \frac{1}{(2\pi)^3}$$

$$= \frac{1}{(2\pi)^{3/2}(Nb^2)^{3/2}} e^{-R^2/2Nb^2}$$

$N' = N\lambda \rightarrow N = N'\lambda$

$$= \frac{1}{(2\pi)^{3/2}(N'\lambda b^2)^{3/2}} e^{-R^2/2N'\lambda b^2}$$

$b' = b\lambda^{1/2} \rightarrow b'^2 = b^2\lambda$

$$= \frac{1}{(2\pi)^{3/2}(b'^2N')^{3/2}} e^{-R^2/2(N'b'^2)} = P_{N',b'}(R)$$

15.8 $v(t) = v(0)\, e^{-t/\tau} + e^{-t/\tau}\int_0^t e^{u/\tau} A(u)\, du$

define $F(t)$ such that $\frac{dF}{dt} = e^{t/\tau} A(t)$
then we have

$$v(t) = v(0)\, e^{-t/\tau} + e^{-t/\tau}\left(F(t) - F(0)\right)$$

integrate by parts

$$x(t) = \int_0^t v(t')\,dt' = -\tau v(0)\, e^{-t'/\tau}\Big|_0^t + \int_0^t e^{-t'/\tau}\left(F(t') - F(0)\right) dt'$$

$$x(t) = \tau v(0)\left(1 - e^{-t/\tau}\right) + \left(F(t) - F(0)\right)\left(-\tau e^{-t/\tau}\right) + \tau \int A(t')\,dt'$$

$u = F(t) - F(0)$ $\quad v = -\tau e^{-t/\tau}$
$du = e^{t/\tau} A(t)\,dt$ $\quad dv = e^{-t/\tau}\,dt'$

$$x(t) = \tau v(0)\left(1 - e^{-t/\tau}\right) - \tau e^{-t/\tau}\int_0^t e^{t'/\tau} A(t') + \tau \int_0^t A(t')\,dt'$$

$$= \tau v(0)\left(1 - e^{-t/\tau}\right) + \tau \int_0^t A(t')\left(1 - e^{(t'-t)/\tau}\right) dt' \quad \checkmark$$

$$\langle x^2 \rangle = \tau^2 v^2(0)\left(1 - e^{-t/\tau}\right)^2 + 2\tau^2 v(0)\left(1 - e^{-t/\tau}\right)\int_0^t \cancel{\langle A(t')\rangle}^{\,0}\left(1 - e^{(t'-t)/\tau}\right) dt'$$

$$+ \tau^2 \int_0^t \int_0^t \langle A(t') A(t'') \rangle \left(1 - e^{(t'-t)/\tau} - e^{(t''-t)/\tau} + e^{(t'+t''-2t)/\tau}\right) dt'\, dt''$$

change variables

$\xi = \frac{1}{2}(t' + t'')$
$s = t' - t''$
$t' = \xi + \frac{1}{2} s \qquad t'' = \xi - \frac{1}{2} s$

$$\langle A(t') A(t'') \rangle \equiv K(s)$$

$$\langle x^2 \rangle = \tau^2 v^2(0)\left(1 - e^{-t/\tau}\right)^2 + \tau^2 \underbrace{\iint K(s)\left(1 - e^{-t/\tau}\left[e^{(\xi + \frac{1}{2}s)/\tau} + e^{(\xi - \frac{1}{2}s)/\tau}\right] + e^{(2\xi - 2t)/\tau}\right) d\xi\, ds}_{\text{take this integral one term at time}}$$

15.8 cont

$$\iint K(s)\, d\xi\, ds = \overset{\xi \text{ integral}}{t}\int K(s)\, ds = \frac{6kT}{M\tau}\, t$$

$$\iint K(s)\, e^{-t/\tau}\left[e^{(\xi+\frac{1}{2}s)/\tau} + e^{(\xi-\frac{1}{2}s)/\tau}\right] d\xi\, ds$$

$$= e^{-t/\tau}\int e^{\xi/\tau}\, d\xi \int \left(e^{s/2\tau} + e^{-s/2\tau}\right) K(s)\, ds$$

$$= e^{-t/\tau}\, \tau\, e^{\xi/\tau}\Big|_0^t \int \left(2 + O(s^2)\right) K(s)\, ds$$

drop $K(s) \neq 0$ only when s is small

$$= e^{-t/\tau}\, \tau \left(e^{t/\tau} - 1\right)\frac{12kT}{M\tau} = \cancel{\tau}\left(1 - e^{-t/\tau}\right)\frac{12kT}{M\cancel{\tau}}$$

$$\iint K(s)\, e^{(2\xi-2t)/\tau}\, d\xi\, ds = e^{-2t/\tau}\int e^{2\xi/\tau}\, d\xi \int K(s)\, ds$$

$$= e^{-2t/\tau}\,\frac{\tau}{2}\left(e^{2t/\tau} - 1\right)\frac{6kT}{M\cancel{\tau}} = \frac{3kT}{M}\left(1 - e^{-2t/\tau}\right)$$

so

$$\langle x^2 \rangle = \tau^2 v^2(0)\left(1 - e^{-t/\tau}\right)^2 + \frac{6kT}{M}t\tau + \frac{3kT}{M}\tau^2 \underbrace{\left(1 - e^{-2t/\tau} - 4 + 4e^{-t/\tau}\right)}_{-3 + 4e^{-t/\tau} - e^{-2t/\tau}}$$

$$\langle x^2 \rangle = \tau^2 v^2(0)\left(1 - e^{-t/\tau}\right) + \frac{6kT}{M}t\tau - \frac{3kT}{M}\tau^2\left(3 - e^{-t/\tau}\right)\left(1 - e^{-t/\tau}\right) \quad ✓$$