Phys 427 - HW3

1) DNA, N links, $E = \begin{cases} 0 & \text{if closed} \\ E_0 & \text{if open} \end{cases}$

a) know $Z = \sum_{n=1}^{N} \exp(-E_n/k_BT)$ looks like $\sum_{n=1}^{N} a r^n = \left(\frac{1-r^{N+1}}{1-r}\right) a$

for Z, $a=1$, $r=e$, $E_n = E_0 n \Rightarrow$ $\boxed{Z = \frac{1-\exp(-(N+1)E_0/(k_BT))}{1-\exp(-E_0/(k_BT))}}$

b) in limit $E_0 \gg k_BT$, $E_0/k_BT \to \infty$

$$\lim_{E_0/k_BT \to \infty} Z = \frac{1-\exp(-(N+1)\infty)}{1-\exp(-\infty)} = \frac{1-0}{1-0} = 1$$

if $Z=1$, only 1 possible state, which only occurs when no breaks occur. Since no breaks occur, k_BT is not enough to overcome E_0.

$\boxed{\therefore \langle \text{open links} \rangle = 0}$

more rigorously, $\langle E \rangle = -\partial_\beta \ln(Z) = -\partial_\beta \ln(1) = -\partial_\beta(0) = 0$

$\Rightarrow \langle E \rangle = 0$, mean energy being 0 means

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2) $C_V = (\partial\langle E\rangle/\partial T)_V$

a) use $Z(T)$ to show $C_V = \sigma_E^2/(kT^2)$

not writing bounds for Σ_i, all $\Sigma = \sum_{i=1}^{\infty}$

find $\langle E\rangle$, $\langle E\rangle = -\partial_\beta \ln Z = -\partial_\beta\left[\ln\left(\sum_{i=1}^{\infty} \exp(-\epsilon_i\beta)\right)\right]$

$$= -\frac{1}{\Sigma \exp(-\epsilon_i\beta)} \cdot \Sigma -\exp(-\epsilon_i\beta)\epsilon_i = \underline{\frac{\Sigma \epsilon_i \exp(-\epsilon_i\beta)}{\Sigma \exp(-\epsilon_i\beta)} = \langle E\rangle}$$

now take $\partial/\partial T$ of $\langle E\rangle \Rightarrow \frac{\partial\langle E\rangle}{\partial T} = \frac{\partial\langle E\rangle}{\partial\beta}\frac{\partial\beta}{\partial T}$

$$\Rightarrow \frac{\partial\langle E\rangle}{\partial\beta} = \frac{\partial}{\partial\beta}\left(\frac{\Sigma \epsilon_i \exp(-\epsilon_i\beta)}{\Sigma \exp(-\epsilon_i\beta)}\right)$$, use quotient rule $\frac{\partial}{\partial x}\left(\frac{f}{g}\right) = \frac{gf' - fg'}{g^2}$

$$= \frac{[\Sigma \exp(-\epsilon_i\beta)][\Sigma \epsilon_i \exp(-\epsilon_i\beta)\Sigma(-1)\epsilon_i] - [\Sigma \epsilon_i \exp(-\epsilon_i\beta)][\Sigma \exp(-\epsilon_i\beta)\Sigma(-1)\epsilon_i]}{[\Sigma \exp(-\epsilon_i\beta)]^2}$$

$$= -\frac{\Sigma \epsilon_i \exp(-\epsilon_i\beta)\epsilon_i}{\Sigma \exp(-\epsilon_i\beta)} + \frac{[\Sigma \epsilon_i \exp(-\epsilon_i\beta)][\Sigma \exp(-\epsilon_i\beta)\epsilon_i]}{[\Sigma \exp(-\epsilon_i\beta)]^2}$$

$$\frac{\partial\langle E\rangle}{\partial\beta} \, {}^{\shortparallel}$$

$$= \left(\frac{\Sigma \epsilon_i \exp(-\epsilon_i\beta)}{\Sigma \exp(-\epsilon_i\beta)}\right)\left(\frac{\Sigma \epsilon_i \exp(-\epsilon_i\beta)}{\Sigma \exp(-\epsilon_i\beta)}\right) - \frac{\Sigma \epsilon_i^2 \exp(-\epsilon_i\beta)}{\Sigma \exp(-\epsilon_i\beta)} = \underline{\langle E\rangle^2 - \langle E^2\rangle = -\sigma_E^2}$$

now take $\frac{\partial\beta}{\partial T} = \frac{\partial}{\partial T}\left(\frac{1}{kT}\right) = \frac{-1}{kT^2}$

$$\Rightarrow \frac{\partial\langle E\rangle}{\partial\beta}\frac{\partial\beta}{\partial T} = -\sigma_E^2 \cdot \frac{-1}{kT^2} = \boxed{\frac{\sigma_E^2}{kT^2} = C_V} = \left.\frac{\partial\langle E\rangle}{\partial T}\right|_V = \frac{\partial\langle E\rangle}{\partial\beta}\frac{\partial\beta}{\partial T}$$

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2b) find $\sigma_E / \langle E \rangle$, w/ $\epsilon = p^2/2m$ — know variance decreases as N increases

know $\sigma = \sqrt{\sigma^2} = \sqrt{\frac{\langle E^2 \rangle}{\langle N^2 \rangle} - \frac{\langle E \rangle^2}{\langle N \rangle^2}}$ — $\langle E \rangle, \langle E^2 \rangle$

(2) * We can say $\sum_0^\infty \exp(-\epsilon_i \beta) \approx \int_0^\infty dV_\epsilon \exp(-\epsilon_i \beta)$ as $\epsilon \ll kT$ ∴ very fine spacing in ϵ_i *

* is where the term or assumption is defined

- $\langle E \rangle = \frac{\sum_0^\infty \epsilon_i \exp(-\epsilon_i \beta)}{\langle N \rangle = Z}$, so find each part — $\alpha \equiv \beta/2m$

- $Z = \sum_0^\infty \exp(-\epsilon_i \beta) \overset{(2)}{\approx} \int_0^\infty dV_\epsilon \exp(-\epsilon \beta) = \iiint_0^\infty d\vec{V}_p \exp(p^2 \beta/2m)$ (energy V, momentum V)

(6)* convert to (sp) $\Rightarrow \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_0^\infty dV_p \exp(p^2\alpha) = 4\pi \int_0^\infty dV_p \exp(-p^2\alpha)$

*(1) $\boxed{\text{w/ } V = p^3,\ dV = 3p^2}$ $\Rightarrow 12\pi \int_0^\infty dp\, p^2 \exp(-p^2\alpha) = 12\pi \left[-\partial_\alpha \int_0^\infty dp \exp(-p^2\alpha) \right] = 12\pi \left[-\partial_\alpha \left(\frac{1}{2} \sqrt{\pi/\alpha} \right) \right]$

$= 6\pi \left(\frac{1}{2} \frac{\sqrt{\pi}}{\alpha^{3/2}} \right) = Z = 3\pi^{3/2} \alpha^{-3/2}$ *(3)

convert to (sp) (6)

- $\sum_0^\infty \epsilon_i \exp(-\epsilon_i \beta) \overset{(2)}{\approx} \int_0^\infty dV_E\, \epsilon \exp(\epsilon\beta) = \int_0^\infty d\vec{V}_p \frac{p^2}{2m} \exp(-p^2\alpha) = 4\pi \int_0^\infty dV \frac{p^2}{2m} \exp(-p^2\alpha)$

$\overset{(1)}{=} \frac{6\pi}{m} \int_0^\infty dp\, p^4 \exp(-p^2\alpha) = \frac{6\pi}{m} \left[\partial_\alpha^2 \int_0^\infty dp \exp(-p^2\alpha) \right] = \frac{6\pi}{m} \left[\partial_\alpha^2 \left(\frac{1}{2} \sqrt{\frac{\pi}{\alpha}} \right) \right]$ *(4)

$= \frac{3\pi^{3/2}}{m} \left[\frac{1}{2} \cdot \frac{3}{2} \cdot \frac{1}{\alpha^{5/2}} \right] = \frac{9\pi^{3/2}}{4m\alpha^{5/2}} = \sum \epsilon_i \exp(-\epsilon_i\beta)$

*(5) $= \langle E \rangle$

$\Rightarrow \langle E \rangle = \frac{9\pi^{3/2}}{4m\alpha^{5/2}} \cdot \frac{\alpha^{3/2}}{3\pi^{3/2}} = \frac{3}{4m\alpha} = \frac{3}{2} kT$ ✓

- next need $\langle E^2 \rangle = \frac{\sum_0^\infty \epsilon_i^2 \exp(-\epsilon_i \beta)}{\langle N \rangle = Z}$, need numerator

- $\sum_0^\infty \epsilon_i^2 \exp(-\epsilon_i\beta) \overset{(2)}{\approx} \int_0^\infty dV_E\, \epsilon^2 \exp(-\epsilon_i\beta) = \int_0^\infty d\vec{V}_p \frac{p^4}{4m^2} \exp(-p^2\beta) \overset{(6)}{=} \frac{\pi}{m^2} \int_0^\infty dV\, p^4 \exp(-p^2\alpha)$

$\overset{(1)}{=} \frac{3\pi}{m^2} \int_0^\infty dp\, p^6 \exp(-p^2\alpha) = \frac{3\pi}{m^2} \left[-\partial_\alpha^3 \int_0^\infty dp \exp(-p^2\alpha) \right] = \frac{3\pi}{m^2} \left[-\partial_\alpha^3 \left(\frac{1}{2} \frac{\sqrt{\pi}}{\sqrt{\alpha}} \right) \right]$

$= \frac{3\pi^{3/2}}{2m^2} \left[\frac{1}{2} \cdot \frac{3}{2} \cdot \frac{5}{2} \cdot \alpha^{-7/2} \right] = \frac{45\pi^{3/2}}{16m^2} \alpha^{-7/2} = \sum \epsilon_i^2 \exp(-\epsilon_i \beta)$ (7)

(7)/(3)

$\Rightarrow \langle E^2 \rangle = \frac{45\pi^{3/2}}{16m^2\alpha^{7/2}} \cdot \frac{\alpha^{3/2}}{3\pi^{3/2}} = \frac{15}{16m^2\alpha^2} = \langle E^2 \rangle$ (8)

know $\langle N \rangle = \sqrt{N}$ & $\langle N^2 \rangle = N \Rightarrow \ldots$

↑ fluctuations → ↖ know from monte carlo error

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2b) cont

$$\sigma^2 = \left[\frac{\langle E^2\rangle}{\langle N^2\rangle} - \left(\frac{\langle E\rangle}{\langle N\rangle}\right)^2\right] = \left[\frac{15}{16m^2\alpha^2 N} - \left(\frac{1}{\sqrt{N}}\right)^2\left(\frac{3}{4m\alpha}\right)^2\right] = \left[\frac{15}{16m^2\alpha^2 N} - \frac{9}{16m^2\alpha^2 N}\right]$$

$$\sigma^2 = \frac{6}{16m^2\alpha^2 N} \Rightarrow \sigma = \sqrt{\sigma^2} = \sqrt{\frac{6}{16m^2\alpha^2 N}} = \sqrt{\frac{3}{8m^2N}\cdot\frac{(2m)^2}{\beta^2 N}} = \sqrt{\frac{3}{2}\frac{\beta^2T^2}{N}}$$

$$\sigma = \beta T\sqrt{\frac{3}{2N}}$$

$$\Rightarrow \frac{\sigma}{\langle E\rangle} = \beta T\sqrt{\frac{3}{2N}}\cdot\frac{2}{3\beta T} = \boxed{\sqrt{\frac{2}{3N}} = \frac{\sigma}{\langle E\rangle}}$$

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3) N 3D ~~particles~~. $E \approx |p|c$, $p = \hbar k$. show $U = 3NkT$

know $E \approx |p|c = |k|\hbar c$ for 1 particle w/ $|k| = \sqrt{k_x^2 + k_y^2 + k_z^2}$

know $U = \langle E \rangle = -\partial_\beta \ln Z$, so find Z

$E \ll kT$, so fine spacing $\to \infty$; volume in k-space

$$\underline{Z} = \sum_{i=0}^{\infty} \exp(-E_i \beta) \approx \int_0^{\infty} dE \exp(-E\beta) = \iiint_{0\,0\,0}^{\infty\,\infty\,\infty} dV_k \exp(-E\beta)$$

convert to ~~●~~ to avg over angle $\Rightarrow \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_0^{\infty} dV_k \exp(-k\hbar c\beta)$ ← $\alpha \equiv \hbar c\beta$

$$= 4\pi \int_0^{\infty} dV_k \exp(-k\alpha), \text{ but } V = k^3, \text{ so } dV = 3k^2 dk$$

$$= 4\pi \int_0^{\infty} dk\, 3k^2 \exp(-k\alpha) = 12\pi \left[\partial_\alpha^2 \int_0^{\infty} dk \exp(-k\alpha)\right] = 12\pi \left[\partial_\alpha^2 \left(\frac{-1}{\alpha} \exp(-k\alpha)\Big|_0^{\infty}\right)\right]$$

$$= 12\pi \left[\partial_\alpha^2 \left(\frac{-1}{\alpha}[0-1]\right)\right] = 12\pi \left[\partial_\alpha^2 \left(\frac{1}{\alpha}\right)\right] = 12\pi\left(2\alpha^{-3}\right) = 24\pi\alpha^{-3}$$

$$Z_1 = \frac{24\pi}{\hbar^3 c^3 \beta^3} \Rightarrow Z_{\text{tot}} = Z_1^N = \left(\frac{24\pi}{\hbar^3 c^3 \beta^3}\right)^N$$ now find $U = -\partial_\beta \ln Z$

$$\underline{U} = -\partial_\beta \left(N \ln\left(24\pi / \hbar^3 c^3 \beta^3\right)\right) = -N \partial_\beta \left[\ln(\beta^{-3}) + \text{not fn}(\beta)\right]$$

$$= 3N \partial_\beta \left[\ln(\beta)\right] = 3N\left(\frac{1}{\beta}\right)$$

w/ $\beta = 1/kT$, $\boxed{U = 3NkT}$

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4) $\vec{B} = B\hat{z}$, $2j+1$ states per m, $E_j = -\mu B m_j$. Sys in eq w/ bath @ T

a) for some j, have $m = -j, -j+1 \ldots j$, so $Z = \sum_{m=-j}^{j} \exp(B\mu m\beta)$

$$Z = \exp(B\beta\mu(-j)) + \exp(B\beta\mu(-j+1)) + \ldots + \exp(B\beta\mu(j-1)) + \exp(B\beta\mu(j))$$

$$= \exp(-\beta B\mu j)\left[1 + \exp(B\beta\mu) + \ldots + \exp(2B\beta\mu(j-1)) + \exp(2\beta B\mu j)\right]$$

$$= \exp(-\beta B\mu j) \sum_{n=0}^{2j} \exp(\beta B\mu n) = \exp(-\beta B\mu j) \sum_{n=0}^{2j} \exp(\beta B\mu)^n \leftarrow \text{geo series}$$

$$Z = \text{geometric series} = \exp(-\beta B\mu j)\left[\frac{1 - \exp(-\beta B\mu)^{(2j+1)}}{1 - \exp(\beta B\mu)}\right] \qquad \alpha \equiv \beta B\mu = \frac{\mu B}{kT}$$

$$= \exp(-\alpha j)\left[\frac{1 - \exp(\alpha(2j+1))}{1 - \exp(\alpha)}\right] = \exp(-\alpha j)\left[\frac{1 - \exp(2\alpha j)\exp(\alpha)}{1 - \exp(\alpha)}\right]$$

$$= \frac{\exp(-\alpha j) - \exp(\alpha j + \alpha)}{1 - \exp(\alpha)} \times \frac{\exp(-\alpha/2)}{\exp(-\alpha/2)} = \frac{\exp(-\alpha j - \alpha/2) - \exp(\alpha j + \alpha/2)}{\exp(-\alpha/2) - \exp(\alpha/2)}$$

$$= \frac{-\frac{1}{2}\sinh(\alpha j + \alpha/2)}{-\frac{1}{2}\sinh(\alpha/2)} \Rightarrow \boxed{Z_1(T) = \frac{\sinh(\alpha j + \alpha/2)}{\sinh(\alpha/2)} \quad \text{w/ } \alpha = \mu B\beta}$$

b) for N particles, $Z = Z_1^N$ & $M = -U/B = \frac{1}{B}\partial_\beta \ln Z = \frac{N}{B}\partial_\beta \ln Z$

$$\Rightarrow \ln Z = \ln(\sinh(\alpha j + \alpha/2)) - \ln(\sinh(\alpha/2)) \qquad \frac{\partial\alpha}{\partial\beta} = \mu B$$

$$\partial_\beta \ln Z = \frac{\cosh(\alpha j + \alpha/2)}{\sinh(\alpha j + \alpha/2)}(j + 1/2)\frac{\partial\alpha}{\partial\beta} - \frac{\cosh(\alpha/2)}{\sinh(\alpha/2)}(1/2)\frac{\partial\alpha}{\partial\beta}$$

$$M = \frac{N}{B}\left(\coth[(j + \tfrac{1}{2})\alpha](j + 1/2)\mu B - \coth[\alpha/2](1/2)\mu B\right)$$

$$\boxed{M = N\mu\left[(j + \tfrac{1}{2})\coth\left([j+1]\frac{\mu B}{kT}\right) - \frac{1}{2}\coth\left(\frac{\mu B}{2kT}\right)\right]}$$

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4b) cont $M(j=1/2) = N\mu\left[\coth(\alpha) - \frac{1}{2}\coth(\alpha/2)\right]$

w/ $\coth(\alpha/2) = \frac{\sinh\alpha}{\cosh\alpha - 1} = \frac{\sinh^2\alpha}{\sinh\alpha\cosh\alpha - \sinh\alpha}$ ← Wikipedia for identities

& $\coth(\alpha) = \frac{\cosh\alpha}{\sinh\alpha} = \frac{\cosh^2\alpha - \cosh\alpha}{\sinh\alpha\cosh\alpha - \sinh\alpha}$

$\coth(\alpha) - \frac{1}{2}\coth(\alpha/2) = \frac{2\cosh^2\alpha - 2\cosh\alpha - \sinh^2\alpha}{\sinh\alpha(\cosh\alpha - 1)} = \frac{\cosh^2\alpha - 2\cosh\alpha + (\cosh^2\alpha - \sinh^2\alpha)}{\sinh\alpha(\cosh\alpha - 1)}$

$= \frac{\cosh^2\alpha + 1 - 2\cosh\alpha}{\sinh\alpha(\cosh\alpha - 1)} = \frac{2 + \sinh^2(\alpha) - 2\cosh\alpha}{\sinh\alpha(\cosh\alpha - 1)} = \frac{2\operatorname{csch}\alpha + \sinh\alpha - 2\coth\alpha}{\cosh\alpha - 1}$

if α is large, $\cosh\alpha - 1 \approx \cosh\alpha \Rightarrow \frac{\operatorname{csch}\alpha + \sinh\alpha - 2\coth(\alpha)}{\cosh\alpha}$

$= \frac{1}{\sinh\alpha\cosh\alpha} + \tanh\alpha - \frac{2}{\sinh\alpha}$, α large, so $\frac{1}{\sinh\alpha} \approx \frac{1}{\sinh\alpha\cosh\alpha} \approx 0$

$\Rightarrow \therefore M(j=1/2) = N\mu\left[0 + \tanh\alpha + 0\right] = N\mu\tanh\alpha$

w/ $\alpha = \beta\mu B$, have same relation as class: $\boxed{M(j=1/2) = N\mu\tanh(\beta\mu B)}$

c) if $T\to\infty$, $\beta\to 0$ & $\beta\propto\alpha$; so $\lim_{\beta\to 0} M = N\mu\tanh\alpha$

Taylor expand $\tanh\alpha \approx \alpha - \frac{\alpha^3}{3} + \dots$ as $\alpha\to 0$, $\alpha^3 \approx 0$

$M \approx N\mu\alpha = \frac{N\mu\mu B}{kT} = \frac{N\mu^2 B}{kT}$ ← $M \propto 1/T$

w/ $M \propto \frac{1}{T}$, as $T\to\infty$ $\boxed{\text{constant of proportionality} = \frac{N\mu^2 B}{k}}$

$\boxed{\text{However, if we follow convention } M = B\chi = \frac{BC}{T} \text{ w/ } C = \frac{N\mu^2}{k}}$