Exercise 10

1. a) In the zero temperature limit we have minimum energy in the system $E = -J(N-1)$. Here all the spins are parallel meaning all the terms $s_i s_{i+1} = 1 \Rightarrow s_i = \pm 1$ for all $i \Rightarrow$ there are 2 states $\Rightarrow S = k_B \ln(2)$.

High T limit $T \to \infty$; All the spins move freely so $\langle s_i \rangle = 0$ and $\langle E \rangle = 0$. Possible states are now $2^N \Rightarrow S = k_B \ln(2^N)$

b) PF. $$Z_N = \sum_{s_1=\pm 1} \dots \sum_{s_N=\pm 1} e^{\beta J \sum_{i=1}^{N-1} s_i s_{i+1}} = \sum_{s_1=\pm 1} \dots \sum_{s_{N-1}=\pm 1} e^{\beta J \sum_{i=1}^{N-2} s_i s_{i+1}} \sum_{s_N=\pm 1} e^{\beta J s_{N-1} s_N}$$

$$= \sum_{s_1=\pm 1} \dots \sum_{s_{N-1}=\pm 1} \underbrace{\left(e^{-\beta J s_{N-1}} + e^{\beta J s_{N-1}}\right)}_{= e^{-\beta J} + e^{\beta J} \text{ for both } s_{N-1} = \pm 1} e^{\beta J \sum_{i=1}^{N-2} s_i s_{i+1}}$$

$$= \left(e^{-\beta J} + e^{\beta J}\right) Z_{N-1}$$

$$\Rightarrow Z_N = \left(e^{-\beta J} + e^{\beta J}\right)^{N-2} Z_2$$

$$Z_2 = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} e^{\beta J (s_1 s_2)} = \sum_{s_1=\pm 1} e^{-\beta J s_1} + e^{\beta J s_1} = 2\left(e^{-\beta J} + e^{\beta J}\right)$$

$$\Rightarrow Z_N = 2\left(e^{-\beta J} + e^{\beta J}\right)^{N-1}.$$

c) $$F = -k_B T \ln(Z)$$

$$= -k_B T \left[\ln(2) + (N-1)\ln\big(\underbrace{e^{-\beta J} + e^{\beta J}}_{2\cosh(\beta J)}\big)\right]$$

$$= -k_B T \left[\ln(2) + (N-1)\ln(2) + (N-1)\ln\left(\cosh\left(\frac{J}{k_B T}\right)\right)\right]$$

$$= -k_B T \left[N \ln(2) + (N-1)\ln\left(\cosh\left(\frac{J}{k_B T}\right)\right)\right].$$

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$$\langle E\rangle = -\frac{\partial \ln Z}{\partial \beta} = -\frac{\partial}{\partial \beta}\left((N-1)\ln(\cosh(\beta J))\right)$$
$$= -(N-1)\frac{1}{\cosh(\beta J)}\sinh(\beta J)\, J = \underline{\underline{(1-N) J \tanh(\beta J)}}.$$

$$S = -\left(\frac{\partial F}{\partial T}\right)_{V,N} = \frac{\partial}{\partial T}\left\{ k_B T\left[N\ln(2) + (N-1)\ln\left(\cosh\left(\frac{J}{k_B T}\right)\right)\right]\right\}$$
$$= k_B\left[N\ln(2) + (N-1)\ln\left(\cosh\left(\frac{J}{k_B T}\right)\right)\right] + k_B T (N-1)\frac{1}{\cosh\left(\frac{J}{k_B T}\right)}\sinh\left(\frac{J}{k_B T}\right)\left(-\frac{J}{k_B T^2}\right)$$
$$= \underline{\underline{N k_B \ln(2) + (N-1) k_B \ln\left(\cosh\left(\frac{J}{k_B T}\right)\right) - \frac{J}{T}(N-1)\tanh\left(\frac{J}{k_B T}\right)}}.$$

Limits; $\underline{T\to 0}$; $\langle E\rangle \simeq \underline{\underline{(1-N)J = -J(N-1)}}$.

$$S = C + (N-1)\left[k_B \ln\left(\frac{1}{2}\left(e^{-\frac{J}{k_B T}} + e^{\frac{J}{k_B T}}\right)\right) - \frac{J}{T}\frac{e^{\frac{J}{k_B T}} - e^{-\frac{J}{k_B T}}}{e^{J/k_B T} + e^{-J/k_B T}}\right]$$

Neglect $e^{-\frac{J}{k_B T}}$ term.

$$S \simeq C + (N-1)\left[k_B \ln\left(\frac{1}{2}e^{J/k_B T}\right) - \frac{J}{T}\right] = C + (N-1)\left[k_B\ln\left(\frac{1}{2}\right) + \cancel{k_B}\frac{J}{\cancel{k_B} T} - \frac{J}{T}\right]$$
$$= N k_B \ln(2) + (N-1) k_B \ln(2)$$
$$= \underline{\underline{k_B \ln(2)}}.$$

$\underline{T\to\infty}$; $\langle E\rangle \simeq (1-N)J\cdot 0 = \underline{\underline{0}}$.

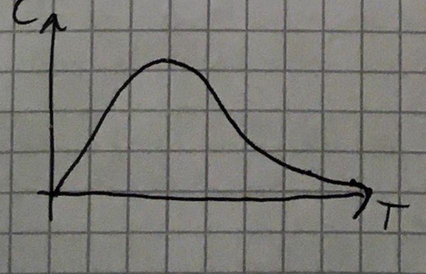
For entropy; ~~neglect~~ $\ln\left(\cosh\left(\frac{J}{k_B T}\right)\right) \underset{T\to\infty}{=} 0$.

$$\lim_{T\to\infty}\frac{\tanh(J/k_B T)}{T} = 0 \Rightarrow S = N k_B \ln 2 = \underline{\underline{k_B \ln(2^N)}}.$$

d) $$C = \frac{\partial\langle E\rangle}{\partial T} = (1-N) J \frac{\partial}{\partial T}\tanh\left(\frac{J}{k_B T}\right) = (1-N) J \frac{1}{\cosh^2\left(\frac{J}{k_B T}\right)}\cdot\left(\frac{-J}{k_B T}\right)$$
$$= (N-1)\frac{J^2}{k_B T}\frac{1}{\cosh^2\left(\frac{J}{k_B T}\right)} = (N-1) J \frac{x}{\cosh^2(x)},\quad x = \frac{J}{k_B T}.$$

$k_B T \ll J \Rightarrow x \gg 1$ $$\lim_{x\to\infty}\frac{x}{\cosh^2(x)} = \lim_{x\to\infty}\frac{1}{2\cosh(x)\sinh(x)} = \lim_{x\to\infty}\frac{1}{2\sinh(x)} = \underline{\underline{0}}.$$

$\Rightarrow C \to 0$ for $x \gg 1$.



2. a) Identical particles

Allowed states.

Bosons; 110 200
101 020
011 002

Fermions: 110 can't have
101 identical states.
011

$$\Rightarrow Z_2^B = \sum_{\text{states}} e^{-\beta \sum_{i=1}^{3} \varepsilon_i}$$

$$= e^{-\beta(\varepsilon_1+\varepsilon_2)} + e^{-\beta(\varepsilon_1+\varepsilon_3)} + e^{-\beta(\varepsilon_2+\varepsilon_3)} + e^{-\beta 2\varepsilon_1} + e^{-\beta 2\varepsilon_2} + e^{-\beta 2\varepsilon_3}.$$

$$Z_2^F = e^{-\beta(\varepsilon_1+\varepsilon_2)} + e^{-\beta(\varepsilon_1+\varepsilon_3)} + e^{-\beta(\varepsilon_2+\varepsilon_3)}.$$

b) Bosons;

$$Z_2^B = \sum_{\substack{i,j \\ \{\text{indistinguishable}\}}}^{N} e^{-\beta(\varepsilon_i+\varepsilon_j)} = \sum_{\substack{i\neq j \\ \{\text{indistinguishable}\}}}^{N} e^{-\beta(\varepsilon_i+\varepsilon_j)} + \sum_{i=1}^{N} e^{-2\beta\varepsilon_i}$$

$$= \frac{1}{2}\sum_{i\neq j}^{N} e^{-\beta(\varepsilon_i+\varepsilon_j)} + \sum_{i=1}^{N} e^{-2\beta\varepsilon_i}$$

$$= \sum_{i<j}^{N} e^{-\beta(\varepsilon_i+\varepsilon_j)} + \sum_{i=1}^{N} e^{-2\beta\varepsilon_i}.$$

Fermions; the same but without the two particles in the same state

$$\Rightarrow Z_2^F = \sum_{i<j}^{N} e^{-\beta(\varepsilon_i+\varepsilon_j)}.$$

c)

$$Z(\beta) = \sum_{i=1}^{N} e^{-\beta\varepsilon_i}$$

$$[Z_1(\beta)]^2 = \left(\sum_{i=1}^{N} e^{-\beta\varepsilon_i}\right)^2 = \sum_{i,j}^{N} e^{-\beta(\varepsilon_i+\varepsilon_j)} = \sum_{i=1}^{N} e^{-2\beta\varepsilon_i} + \sum_{i\neq j}^{N} e^{-\beta(\varepsilon_i+\varepsilon_j)}$$

$$\Rightarrow \frac{1}{2}[Z_1(\beta)]^2 = \frac{1}{2}\sum_{i=1}^{N} e^{-2\beta\varepsilon_i} + \frac{1}{2}\sum_{i\neq j}^{N} e^{-\beta(\varepsilon_i+\varepsilon_j)},$$

Comparing to expression for bosons; $Z_2^B = \frac{1}{2}[Z_1(\beta)]^2 + \frac{1}{2}Z_1(2\beta)$,

and for fermions; $Z_2^F = \frac{1}{2}[Z_1(\beta)]^2 - \frac{1}{2}Z_1(2\beta)$.

3. a) $Z_1 = \sum_{\vec{k}} e^{-\beta \varepsilon(\vec{k})}$, $E = \frac{\hbar^2 k^2}{2m}$, $\vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$

$= \sum_{\vec{k}}' e^{-\beta \frac{\hbar^2 \vec{k}^2}{2m}}$ Infinitesimal volume $d\Gamma = \frac{d^3\vec{k}}{\left(\frac{2\pi}{L}\right)^3}$.

$\simeq \frac{V}{(2\pi)^3} \int d^3\vec{k}\, e^{-\beta \frac{\hbar^2 \vec{k}^2}{2m}} = \frac{V}{(2\pi)^3} \left[\int_{-\infty}^{\infty} dk_x\, e^{-\beta \frac{\hbar^2 k_x^2}{2m}} \right]^3$

$= \frac{V}{(2\pi)^3} \left(\frac{\pi 2m}{\beta \hbar^2} \right)^{3/2} = \frac{V \left(\sqrt{2 m k_B T \pi}\right)^3}{(2\pi\hbar)^3} = V \left(\frac{\sqrt{2\pi m k_B T}}{h} \right)^3 = \underline{\underline{\frac{V}{\lambda^3}}}$

$\lambda^3 \sim$ the volume occupied by the wavepacket.

When $V < \lambda^3$ the particle's uncertainty is too big and the approx. fails.

b) From 2c). $Z_2^B = \frac{1}{2} Z_1(\beta)^2 + \frac{1}{2} Z_1(2\beta)$

$= \frac{1}{2} \frac{V^2}{\lambda(\beta)^6} + \frac{1}{2} \frac{V}{\lambda(2\beta)^3} = \frac{1}{2} \frac{V^2}{\lambda^6} + \frac{1}{2} \frac{V}{2^{3/2} \lambda^3}$

$= \frac{1}{2} \frac{V}{\lambda^3} \left(\frac{1}{2^{3/2}} + \frac{V}{\lambda^3} \right)$.

$Z_2^F = \frac{1}{2} \frac{V}{\lambda^3} \left(-\frac{1}{2^{3/2}} + \frac{V}{\lambda^3} \right)$

3.c) $F = -k_B T \ln(Z) \Rightarrow F_2^B = -k_B T \ln(Z_2^B) = -k_B T \ln\left[\frac{1}{2}\frac{V^2}{\lambda^6} + \frac{1}{2^{5/2}}\frac{V}{\lambda^3}\right]$

$$P_2^B = -\frac{\partial F_2^B}{\partial V} = k_B T \frac{1}{\frac{1}{2}\frac{V^2}{\lambda^6} + \frac{1}{2^{5/2}}\frac{V}{\lambda^3}} \cdot \left(\frac{V}{\lambda^6} + \frac{1}{2^{5/2}\lambda^3}\right)$$

$$= \frac{2k_B T}{V}\left[\underbrace{\frac{1}{1+\frac{\lambda^3}{2^{3/2}V}}}_{\simeq 1 - \frac{\lambda^3}{2^{3/2}V}} + \underbrace{\frac{1}{2\cdot\left(1+\frac{V2^{3/2}}{\lambda^3}\right)}}_{= \frac{\lambda^3}{2^{5/2}V\left(1+\frac{\lambda^3}{2^{3/2}V}\right)} \simeq \frac{\lambda^3}{2^{5/2}V}\left(1-\frac{\lambda^3}{2^{3/2}V}\right)}\right] \qquad \underline{\frac{\lambda^3}{V} \ll 1}$$

$$\Rightarrow P_2^B = \frac{2k_B T}{V}\left[1 - \frac{\lambda^3}{2^{3/2}V} + \frac{\lambda^3}{2^{5/2}V}\left(1 - \underbrace{\frac{\lambda^3}{2^{3/2}V}}_{\text{neglect}}\right)\right] \simeq \underline{\underline{\frac{2k_B T}{V}\left[1 - \frac{1}{2^{5/2}}\frac{\lambda^3}{V}\right]}}.$$

$$P_2^F = -\frac{\partial F_2^F}{\partial V} = k_B T \frac{1}{\frac{1}{2}\frac{V^2}{\lambda^6} - \frac{V}{2^{5/2}\lambda^3}} \cdot \left(\frac{V}{\lambda^6} - \frac{1}{2^{5/2}\lambda^3}\right) = \frac{2k_B T}{V}\left[\underbrace{\frac{1}{1-\frac{\lambda^3}{2^{3/2}V}}}_{\simeq 1 + \frac{\lambda^3}{2^{3/2}V}} - \underbrace{\frac{1}{2\left(-1+\frac{V2^{3/2}}{\lambda^3}\right)}}_{\simeq \frac{\lambda^3}{2^{5/2}V}\left(1+\frac{\lambda^3}{2^{3/2}V}\right)}\right]$$

$$\Rightarrow P_2^F \simeq \frac{2k_B T}{V}\left[1 + \frac{\lambda^3}{2^{3/2}V} - \frac{\lambda^3}{2^{5/2}V}\left(1 + \underbrace{\frac{\lambda^3}{2^{3/2}V}}_{\text{neglect}}\right)\right]$$

$$= \underline{\underline{\frac{2k_B T}{V}\left[1 + \frac{\lambda^3}{2^{5/2}V}\right]}}.$$

Fermions exert more pressure because they can not stay close to each other (not occupy same state). Pauli exclusion principle.

d) Q.M. correction $\frac{\lambda^3}{2^{5/2}V}$, let's say it is important if

$$\frac{\lambda^3}{2^{5/2}V} \sim 0.1 \Rightarrow \frac{h^3}{(2\pi m k_B T)^{3/2} V \cdot 2^{5/2} \cdot 0.1} = 1 \Rightarrow T = \frac{1}{2\pi m k_B}\frac{1}{(2^{5/2}\cdot 0.1)^{2/3}}\cdot\left(\frac{h}{L}\right)^2$$

$$\Rightarrow T \sim \underline{\underline{1\ nK}}.$$