Statistical Mechanics - Exam

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PROBLEM 1

Part (a)

The energy for a given configuration of spins is

$$E = J\sum_{i<j} s_i s_j - h\sum_i s_i$$

There is a single state with all spins up, four states with a single spin down, six states with two spins down, four states with a single spin up, and one state with all spins down. The energies and degeneracies of the states are

State	Degeneracy	Energy
↑↑↑↑	1	$6J-4h$
↓↑↑↑	4	$-2h$
↓↓↑↑	6	$-2J$
↓↓↓↑	4	$2h$
↓↓↓↓	1	$6J+4h$

The partition function is

$$Z = \sum_i e^{-\beta E_i} = \sum_{states} e^{-\beta J\sum_{i<j} s_i s_j + \beta h\sum_i s_i} = e^{-\beta(6J-4h)} + 4e^{-\beta(-2h)} + 6e^{-\beta(-2J)} + 4e^{-\beta(2h)} + e^{-\beta(6J+4h)}$$

$$= 2e^{-6\beta J}\cosh(4\beta h) + 8\cosh(2\beta h) + 6e^{2\beta J}$$

Part (b)

Note: Most of the calculations in parts (b), (c), (d) were performed with Mathematica. The notebook is attached after problem 2.

The free energy is

$$F = -T\ln Z = -T\ln\left[2e^{-6\beta J}\cosh(4\beta h) + 8\cosh(2\beta h) + 6e^{2\beta J}\right]$$

This doesn't seem to have any nicer expression.

The entropy is

$$S = -\frac{\partial F}{\partial T} = \ln Z + \frac{T}{Z}\frac{\partial Z}{\partial T} = \ln Z + \frac{6J\left(-2e^{\frac{4(h+2J)}{T}} + e^{\frac{8h}{T}} + 1\right) - 4h\left(e^{\frac{8h}{T}} + 2e^{\frac{6(h+J)}{T}} - 2e^{\frac{2(h+3J)}{T}} - 1\right)}{T\left(e^{\frac{8h}{T}} + 4e^{\frac{6(h+J)}{T}} + 6e^{\frac{4(h+2J)}{T}} + 4e^{\frac{2(h+3J)}{T}} + 1\right)}$$

Part (c)

The energy E is

$$E = -\frac{\partial \ln Z}{\partial \beta} = \frac{6J\left(e^{8\beta h} - 2e^{4\beta(h+2J)} + 1\right) - 4h\left(e^{8\beta h} + 2e^{6\beta(h+J)} - 2e^{2\beta(h+3J)} - 1\right)}{e^{8\beta h} + 4e^{6\beta(h+J)} + 6e^{4\beta(h+2J)} + 4e^{2\beta(h+3J)} + 1}$$

As a check on some of our previous results, we can see that our expressions for S, F, and E satisfy $S = \frac{E-F}{T}$.

The heat capacity with $h = 0$ is

$$C = \frac{\partial E}{\partial T} = -\beta^2 \frac{\partial E}{\partial \beta} = \frac{12\beta^2 J^2 \left(-2e^{2\beta J} + e^{4\beta J} + 3\right)}{(\sinh(\beta J) + \sinh(3\beta J) + 2\cosh(3\beta J))^2}$$

As $\beta \to 0$, this goes to zero as

$$C \sim 6J^2\beta^2$$

As $\beta \to \infty$, our expression for C does not have a good expansion, but the limit still exists, and

$$\lim_{\beta \to \infty} C = 0$$

Part (d)

The magnetization is

$$M = \left\langle \sum_i s_i \right\rangle = \frac{T}{Z}\frac{\partial Z}{\partial h} = \frac{4\left(2e^{\frac{6(h+J)}{T}} - 2e^{\frac{2(h+3J)}{T}} + e^{\frac{8h}{T}} - 1\right)}{4e^{\frac{6(h+J)}{T}} + 6e^{\frac{4(h+2J)}{T}} + 4e^{\frac{2(h+3J)}{T}} + e^{\frac{8h}{T}} + 1}$$

The susceptibility is

$$\chi(T) = \frac{\partial M}{\partial h} = \frac{32e^{\frac{4h}{T}}\left(3\left(e^{\frac{4h}{T}} + 1\right)e^{\frac{2(h+7J)}{T}} + 8e^{\frac{4(h+3J)}{T}} + 3\left(e^{\frac{8h}{T}} + 1\right)e^{\frac{8J}{T}} + 2e^{\frac{4h+6J}{T}}\cosh\left(\frac{2h}{T}\right)\left(\cosh\left(\frac{4h}{T}\right) + 4\right) + 2e^{\frac{4h}{T}}\right)}{T\left(4\left(e^{\frac{4h}{T}} + 1\right)e^{\frac{2(h+3J)}{T}} + 6e^{\frac{4(h+2J)}{T}} + e^{\frac{8h}{T}} + 1\right)^2}$$

In the absence of an external field, the spins want to become anti-aligned at low temperature, to minimize energy. The addition of a field can make it more difficult for the spins to adopt their preferred alignment, as there is an additional cost to flipping. However, at zero temperature the magnetization is fixed - the spins no longer have the energy to flip. Therefore, the magnetization does not depend on the field, and $\chi = \frac{\partial M}{\partial h} = 0$.

Indeed, calculating the limit with Mathematica shows that $\chi(0) = 0$.

PROBLEM 2

Part (a)

The energy for a single particle is

$$\varepsilon = \frac{\vec{p}^2}{2m} + \frac{k}{2}\vec{r}^2$$

For general temperature, the expression for N is

$$N = 2\int \frac{d^3p d^3x}{(2\pi\hbar)^3} \frac{1}{e^{\frac{\vec{p}^2}{2mT} + \frac{k}{2T}\vec{r}^2 - \frac{\mu}{T}} + 1} = \frac{2(4\pi)^2}{(2\pi\hbar)^3} \int_0^\infty dp \int_0^\infty dr \frac{p^2 r^2}{e^{\frac{p^2}{2mT} + \frac{kr^2}{2T} - \frac{\mu}{T}} + 1}$$

The factor of 2 in the initial expression comes from the spin degeneracy. Either of these integrals can be evaluated in terms of the Polylogarithm, so integrating over r, we find

$$N = -\frac{4}{\pi\hbar^3}\sqrt{\frac{\pi}{2}}\left(\frac{T}{k}\right)^{3/2} \int_0^\infty dp\, p^2 Li_{3/2}\left(-e^{-\frac{p^2}{2mT} + \frac{\mu}{T}}\right)$$

$$= -\frac{4}{\pi\hbar^3}\sqrt{\frac{\pi}{2}}\left(\frac{T}{k}\right)^{3/2} \sum_{j=1}^{\infty} \frac{(-1)^j}{j^{3/2}} e^{\frac{\mu j}{T}} \int_0^\infty dp\, p^2 e^{-\frac{p^2 j}{2mT}} = -\frac{2T^3 m^{3/2}}{\hbar^3 k^{3/2}} Li_3\left(-e^{\frac{\mu}{T}}\right)$$

The Fermi energy is the chemical potential at $T = 0$, so we will need to take the limit as $T \to 0$. Fortunately, there is a known expression[1] for the limit of $Li_s(z)$:

$$\lim_{x\to\infty} Li_s\left(-e^x\right) = -\frac{x^s}{\Gamma(s+1)}$$

so our expression for N becomes

$$-\frac{2m^{3/2}}{\hbar^3 k^{3/2}} \lim_{T\to 0} T^3 Li_3\left(-e^{\frac{\mu}{T}}\right) = \frac{2m^{3/2}}{\hbar^3 k^{3/2}} \frac{T^3}{\Gamma(4) T^3} \mu^3(T=0)$$

The Fermi energy is then

$$\varepsilon_F = \hbar\sqrt{\frac{k}{m}}(3N)^{1/3}$$

Part (b)

The density of states is simple to find from our expression for ε_F:

$$g(\varepsilon) = \frac{\partial N}{\partial \varepsilon} = \frac{\varepsilon^2 m^{3/2}}{\hbar^3 k^{3/2}}$$

Part (c)

Since $T \ll \varepsilon_F$, we can use the usual result for $\mu(T)$ from Sommerfeld expansion with $\mu \sim \varepsilon_F$:

$$\mu \approx \varepsilon_F - \frac{\pi^2 T^2}{6}\left(\frac{1}{g(\mu)}\frac{dg(\mu)}{d\mu}\right)\Big|_{\mu=\varepsilon_F} = \varepsilon_F - \frac{\pi^2 T^2}{6}\left(\frac{2g}{\varepsilon_F g}\right) = \varepsilon_F - \frac{\pi^2 T^2}{3\varepsilon_F}$$

Part (d)

The heat capacity is given by

$$C = \frac{\partial E}{\partial T}$$

and can again be approximated using the Sommerfeld expansion, as was done in class:

$$C = \frac{\pi^2 T}{3} g(\varepsilon_F) = \frac{T\pi^2\varepsilon^2 m^{3/2}}{2\hbar^3 k^{3/2}}$$

[1] D. Wood, "The Computation of Polylogarithms", *https://www.cs.kent.ac.uk/pubs/1992/110/content.pdf*

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(*===================================

          PROBLEM 1

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ClearAll[Z, Z1, J, h, T, β]
(*Partition Functions*)
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$$Z[T\_] := e^{-6\,J/T}\left(e^{4\,h/T} + e^{-4\,h/T}\right) + 4\left(e^{2\,h/T} + e^{-2\,h/T}\right) + 6\,e^{2\,J/T};$$
$$Z1[\beta\_] := e^{-6\,J\,\beta}\left(e^{4\,h\,\beta} + e^{-4\,h\,\beta}\right) + 4\left(e^{2\,h\,\beta} + e^{-2\,h\,\beta}\right) + 6\,e^{2\,J\,\beta};$$

```
(*Free Energy*)
FullSimplify[-T Log[Z[T]]]
```

Out[•]= $-T\,\mathrm{Log}\left[6\,e^{\frac{2J}{T}} + 8\,\mathrm{Cosh}\left[\frac{2\,h}{T}\right] + 2\,e^{-\frac{6J}{T}}\,\mathrm{Cosh}\left[\frac{4\,h}{T}\right]\right]$

In[•]:= (*Entropy - ln(Z)*)

$$\mathrm{FullSimplify}\left[\mathrm{Expand}\left[\frac{T}{Z[T]}\,D[Z[T],\,T]\right]\right]$$

Out[•]= $\left(-4\left(-1+e^{\frac{4h}{T}}\right)\left(1+e^{\frac{4h}{T}}+2\,e^{\frac{2(h+3J)}{T}}\right)h + 6\left(1+e^{\frac{8h}{T}}-2\,e^{\frac{4(h+2J)}{T}}\right)J\right)\Big/\left(\left(1+e^{\frac{8h}{T}}+6\,e^{\frac{4(h+2J)}{T}}+4\,e^{\frac{2(h+3J)}{T}}\left(1+e^{\frac{4h}{T}}\right)\right)T\right)$

In[•]:= (*Energy*)

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FullSimplify[-D[Log[Z1[β]], β]]
```

Out[•]= $\left(-4\left(-1+e^{4h\beta}\right)\left(1+e^{4h\beta}+2\,e^{2(h+3J)\beta}\right)h + 6\left(1+e^{8h\beta}-2\,e^{4(h+2J)\beta}\right)J\right)\Big/\left(1+e^{8h\beta}+4\,e^{6(h+J)\beta}+6\,e^{4(h+2J)\beta}+4\,e^{2(h+3J)\beta}\right)$

In[•]:= (*Heat Capacity with h=0*)

$$\mathrm{FullSimplify}\left[-\beta^2\,D[-D[\mathrm{Log}[Z1[\beta]],\,\beta],\,\beta]\ /.\ h\to 0\right]$$

Out[•]= $\left(12\left(3-2\,e^{2J\beta}+e^{4J\beta}\right)J^2\,\beta^2\right)\Big/\left(2\,\mathrm{Cosh}[3\,J\,\beta]+\mathrm{Sinh}[J\,\beta]+\mathrm{Sinh}[3\,J\,\beta]\right)^2$

In[•]:= (*Heat Capacity - High T*)

Normal @

$$\mathrm{Series}\left[\left(12\left(3-2\,e^{2J\beta}+e^{4J\beta}\right)J^2\,\beta^2\right)\Big/\left(2\,\mathrm{Cosh}[3\,J\,\beta]+\mathrm{Sinh}[J\,\beta]+\mathrm{Sinh}[3\,J\,\beta]\right)^2,\ \{\beta,\,0,\,2\}\right]$$

Out[•]= $6\,J^2\,\beta^2$

In[•]:=
```
(*Heat Capacity - Low T*)
Assuming[J > 0,
 Limit[(12 (3 - 2 e^(2 J β) + e^(4 J β)) J^2 β^2) / (2 Cosh[3 J β] + Sinh[J β] + Sinh[3 J β])^2, β → ∞]]
```

Out[•]= 0

In[•]:=
```
(*Magnetization*)
ExpandDenominator[ExpandNumerator[FullSimplify[T/Z[T] D[Z[T], h]]]]
```

Out[•]= $\left(-4+8\,e^{\frac{4h}{T}+\frac{2(h+3J)}{T}}+4\,e^{\frac{8h}{T}}-8\,e^{\frac{2(h+3J)}{T}}\right)\Big/\left(1+4\,e^{\frac{4h}{T}+\frac{2(h+3J)}{T}}+e^{\frac{8h}{T}}+6\,e^{\frac{4(h+2J)}{T}}+4\,e^{\frac{2(h+3J)}{T}}\right)$

In[•]:=
```
(*Susceptibility*)
FullSimplify[D[T/Z[T] D[Z[T], h], h]]
```

Out[•]= $\left(32\,e^{\frac{4h}{T}}\left(2\,e^{\frac{4h}{T}}+8\,e^{\frac{4(h+3J)}{T}}+3\,e^{\frac{2(h+7J)}{T}}\left(1+e^{\frac{4h}{T}}\right)+3\,e^{\frac{8J}{T}}\left(1+e^{\frac{8h}{T}}\right)+2\,e^{\frac{4h+6J}{T}}\,\mathrm{Cosh}\left[\frac{2h}{T}\right]\left(4+\mathrm{Cosh}\left[\frac{4h}{T}\right]\right)\right)\right)\Big/\left(\left(1+e^{\frac{8h}{T}}+6\,e^{\frac{4(h+2J)}{T}}+4\,e^{\frac{2(h+3J)}{T}}\left(1+e^{\frac{4h}{T}}\right)\right)^2 T\right)$

In[•]:=
```
(*Susceptibility as T→0*)
Assuming[{J > 0, h > 0, h < J},
 Limit[(32 e^(4 h/T) (2 e^(4 h/T) + 8 e^(4 (h+3 J)/T) + 3 e^(2 (h+7 J)/T) (1 + e^(4 h/T)) + 3 e^(8 J/T) (1 + e^(8 h/T)) + 2 e^((4 h+6 J)/T) Cosh[2 h/T]
      (4 + Cosh[4 h/T]))) / ((1 + e^(8 h/T) + 6 e^(4 (h+2 J)/T) + 4 e^(2 (h+3 J)/T) (1 + e^(4 h/T)))^2 T), T → 0]]
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Out[•]= 0

```
(*I'm not sure why Mathematica includes
 conditions on the relationship between h and J.
  Even when they don't hold, the limit is still zero,
as shown by the other limts*)
Assuming[{J > 0, h > 0, h > J},
 Limit[(32 e^(4 h/T) (2 e^(4 h/T) + 8 e^(4 (h+3 J)/T) + 3 e^(2 (h+7 J)/T) (1 + e^(4 h/T)) + 3 e^(8 J/T) (1 + e^(8 h/T)) + 2 e^((4 h+6 J)/T) Cosh[2 h/T]
      (4 + Cosh[4 h/T]))) / ((1 + e^(8 h/T) + 6 e^(4 (h+2 J)/T) + 4 e^(2 (h+3 J)/T) (1 + e^(4 h/T)))^2 T), T → 0]]
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Out[•]= ConditionalExpression[0, 2 J < h && 3 J < h && h < 7 J]

In[•]:= Assuming[{J > 0, h > 0, h > J, h < 2 J},

$$\text{Limit}\left[\left(32 e^{\frac{4h}{T}}\left(2 e^{\frac{4h}{T}}+8 e^{\frac{4(h+3J)}{T}}+3 e^{\frac{2(h+7J)}{T}}\left(1+e^{\frac{4h}{T}}\right)+3 e^{\frac{8J}{T}}\left(1+e^{\frac{8h}{T}}\right)+2 e^{\frac{4h+6J}{T}}\text{Cosh}\left[\frac{2h}{T}\right]\left(4+\text{Cosh}\left[\frac{4h}{T}\right]\right)\right)\right)\Big/\left(\left(1+e^{\frac{8h}{T}}+6 e^{\frac{4(h+2J)}{T}}+4 e^{\frac{2(h+3J)}{T}}\left(1+e^{\frac{4h}{T}}\right)\right)^2 T\right), T\to 0\right]\Big]$$

Out[•]= 0

In[•]:= Assuming[{J > 0, h > 0, h > 2 J, h < 3 J},

$$\text{Limit}\left[\left(32 e^{\frac{4h}{T}}\left(2 e^{\frac{4h}{T}}+8 e^{\frac{4(h+3J)}{T}}+3 e^{\frac{2(h+7J)}{T}}\left(1+e^{\frac{4h}{T}}\right)+3 e^{\frac{8J}{T}}\left(1+e^{\frac{8h}{T}}\right)+2 e^{\frac{4h+6J}{T}}\text{Cosh}\left[\frac{2h}{T}\right]\left(4+\text{Cosh}\left[\frac{4h}{T}\right]\right)\right)\right)\Big/\left(\left(1+e^{\frac{8h}{T}}+6 e^{\frac{4(h+2J)}{T}}+4 e^{\frac{2(h+3J)}{T}}\left(1+e^{\frac{4h}{T}}\right)\right)^2 T\right), T\to 0\right]\Big]$$

Out[•]= 0

In[•]:= Assuming[{J > 0, h > 0, h > 7 J},

$$\text{Limit}\left[\left(32 e^{\frac{4h}{T}}\left(2 e^{\frac{4h}{T}}+8 e^{\frac{4(h+3J)}{T}}+3 e^{\frac{2(h+7J)}{T}}\left(1+e^{\frac{4h}{T}}\right)+3 e^{\frac{8J}{T}}\left(1+e^{\frac{8h}{T}}\right)+2 e^{\frac{4h+6J}{T}}\text{Cosh}\left[\frac{2h}{T}\right]\left(4+\text{Cosh}\left[\frac{4h}{T}\right]\right)\right)\right)\Big/\left(\left(1+e^{\frac{8h}{T}}+6 e^{\frac{4(h+2J)}{T}}+4 e^{\frac{2(h+3J)}{T}}\left(1+e^{\frac{4h}{T}}\right)\right)^2 T\right), T\to 0\right]\Big]$$

Out[•]= 0

```
(*Weirdness aside, susceptibility goes to zero as T does, as we expect.*)



(*=============================================

              PROBLEM 2

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$$\text{Integrate}\left[\frac{p^2 r^2}{e^{\frac{p^2}{2mT}+\frac{k r^2}{2T}-\frac{\mu}{T}}+1}, \{r, 0, \infty\}\right]$$

Out[•]= $\text{ConditionalExpression}\left[-\frac{p^2\sqrt{\frac{\pi}{2}}\ \text{PolyLog}\left[\frac{3}{2}, -e^{-\frac{p^2}{2mT}+\frac{\mu}{T}}\right]}{\left(\frac{k}{T}\right)^{3/2}}, \text{Re}\left[\frac{k}{T}\right] > 0\right]$

In[•]:= $\text{Integrate}\left[p^2 e^{-\frac{p^2 j}{2mT}+\frac{\mu j}{T}}, \{p, 0, \infty\}\right]$

Out[•]= $\text{ConditionalExpression}\left[\frac{e^{\frac{j\mu}{T}}\sqrt{\frac{\pi}{2}}}{\left(\frac{j}{mT}\right)^{3/2}}, \text{Re}\left[\frac{j}{mT}\right] > 0\right]$