MAU34406: Statistical Physics II
Homework 3 due 18/04/2022

Ruaidhrí Campion
19333850
JS Theoretical Physics

Exercise 1

$$
\begin{aligned}
N_{\mathrm{F}} &= N_{\mathrm{B}} \\
-\frac{A}{\lambda_T^2}\,\mathrm{Li}_1(-z_{\mathrm{F}}) &= \frac{A}{\lambda_T^2}\,\mathrm{Li}_1(z_{\mathrm{B}}) \\
\implies \ln(1+z_{\mathrm{F}}) &= -\ln(1-z_{\mathrm{B}}) \\
\implies z_{\mathrm{B}} &= \frac{z_{\mathrm{F}}}{1+z_{\mathrm{F}}}
\end{aligned}
$$

$$
\begin{aligned}
z\frac{d}{dz}\,\mathrm{Li}_r(z) &= \mathrm{Li}_{r-1}(z) \\
\implies \frac{d}{dz}\,\mathrm{Li}_2(z) &= \frac{\mathrm{Li}_1(z)}{z} \\
&= -\frac{\ln(1-z)}{z} \\
\implies -\int_0^{-z_{\mathrm{F}}} \frac{d}{dz}\,\mathrm{Li}_2(z)\,dz &= \int_0^{-z_{\mathrm{F}}} \frac{\ln(1-z)}{z}\,dz \\
-\mathrm{Li}_2(-z_{\mathrm{F}}) &= \int_0^{z_{\mathrm{F}}} \frac{\ln(1+u)}{u}\,du && (u=-z)
\end{aligned}
$$

$$
\begin{aligned}
\frac{1}{u} &= \frac{1}{1+u} + \frac{1}{f(u)} \\
\implies (1+u)f(u) &= uf(u) + u(1+u) \\
\implies f(u) &= u(1+u)
\end{aligned}
$$

$$
\begin{aligned}
\implies -\operatorname{Li}_2(-z_{\mathrm{F}}) &= \int_0^{z_{\mathrm{F}}} \frac{\ln(1+u)}{1+u}\,du + \int_0^{z_{\mathrm{F}}} \frac{\ln(1+u)}{u(1+u)}\,du \\
&= \left.\frac{\ln^2(1+u)}{2}\right|_0^{z_{\mathrm{F}}} - \int_0^{z_{\mathrm{F}}} \ln\!\left(\frac{1}{1+u}\right)\frac{1+u}{u}\frac{du}{(1+u)^2} \\
&= \frac{\ln^2(1+z_{\mathrm{F}})}{2} - \int_0^{\frac{z_{\mathrm{F}}}{1+z_{\mathrm{F}}}} \ln(1-v)\,\frac{dv}{v} && (v = \tfrac{u}{1+u}) \\
&= \frac{\ln^2(1+z_{\mathrm{F}})}{2} + \int_0^{z_{\mathrm{B}}} \frac{d}{dv}\operatorname{Li}_2(v)\,dv \\
&= \frac{\ln^2(1+z_{\mathrm{F}})}{2} + \operatorname{Li}_2(z_{\mathrm{B}}) \\
\implies -\frac{AkT}{\lambda_T^2}\operatorname{Li}_2(-z_{\mathrm{F}}) &= \frac{AkT}{\lambda_T^2}\left[\frac{\ln^2(1+z_{\mathrm{F}})}{2} + \operatorname{Li}_2(z_{\mathrm{B}})\right] \\
E_{\mathrm{F}} &= E_{\mathrm{B}} + \left[\frac{A}{\lambda_T^2}\ln(1+z_{\mathrm{F}})\right]^2 \frac{kT}{2A}\lambda_T^2 \\
&= E_{\mathrm{B}} + \frac{N^2kT}{2A}\frac{h^2}{2\pi mkT} \\
&= E_{\mathrm{B}} + \frac{N^2h^2}{4\pi mA} \\
\implies \left(\frac{\partial E_{\mathrm{F}}}{\partial T}\right)_{V,N} &= \left(\frac{\partial E_{\mathrm{B}}}{\partial T}\right)_{V,N} + 0 \\
\implies C_{V,\mathrm{F}} &= C_{V,\mathrm{B}}
\end{aligned}
$$

$$
\begin{aligned}
E_{\mathrm{F}}(N,0) &= E_{\mathrm{F}}(N,0) \\
E_{\mathrm{B}}(N,0) + \frac{N^2h^2}{4\pi mA} &= \int_0^{\epsilon_{\mathrm{F}}} \mathcal{W}(1,\epsilon)\epsilon\,d\epsilon \\
0 + \frac{N^2h^2}{4\pi mA} &= \int_0^{\epsilon_{\mathrm{F}}} \frac{2\pi mA}{h^2}\epsilon\,d\epsilon \\
\frac{N^2h^2}{4\pi mA} &= \frac{\pi mA\epsilon_{\mathrm{F}}^2}{h^2} \\
\implies N &= \frac{2\pi mA\epsilon_{\mathrm{F}}}{h^2}
\end{aligned}
$$

$$
\begin{aligned}
E_{\mathrm{F}}(N,0) &= \frac{\pi mA\epsilon_{\mathrm{F}}^2}{h^2} \\
&= \frac{1}{2}\frac{2\pi mA\epsilon_{\mathrm{F}}}{h^2}\epsilon_{\mathrm{F}} \\
&= \frac{1}{2}\epsilon_{\mathrm{F}}N
\end{aligned}
$$

Exercise 2

$$
\begin{aligned}
N &= \int_0^{\epsilon_\mathrm{F}} \mathcal{W}(1,\epsilon)\,d\epsilon \\
&= \frac{1}{2(\hbar\omega_0)^3}\int_0^{\epsilon_\mathrm{F}} \epsilon^2\,d\epsilon \\
&= \frac{\epsilon_\mathrm{F}^3}{6(\hbar\omega_0)^3} \\
\implies \epsilon_\mathrm{F} &= \hbar\omega_0(6N)^{\frac{1}{3}}
\end{aligned}
$$

$$
\begin{aligned}
\langle N\rangle &= \int_0^\infty \frac{\mathcal{W}(1,\epsilon)}{\frac{e^{\beta\epsilon}}{z}+1}\,d\epsilon \\
&= \frac{1}{2(\hbar\omega_0)^3}\int_0^\infty \frac{\epsilon^2}{\frac{e^{\beta\epsilon}}{z}+1}\,d\epsilon \\
&= \frac{1}{2(\hbar\omega_0)^3}\frac{1}{\beta^3}\int_0^\infty \frac{u^2}{\frac{e^u}{z}+1}\,du \\
&= -\frac{\Gamma(3)}{2(\beta\hbar\omega_0)^3}\frac{1}{\Gamma(3)}\int_0^\infty \frac{u^{3-1}}{\frac{e^u}{-z}-1}\,du \\
\langle N\rangle &= -\frac{\mathrm{Li}_3(-z)}{(\beta\hbar\omega_0)^3}
\end{aligned}
$$

$$
\begin{aligned}
\langle E\rangle &= \int_0^\infty \frac{\mathcal{W}(1,\epsilon)\epsilon}{\frac{e^{\beta\epsilon}}{z}+1}\,d\epsilon \\
&= \frac{1}{2(\hbar\omega_0)^3}\int_0^\infty \frac{\epsilon^3}{\frac{e^{\beta\epsilon}}{z}+1}\,d\epsilon \\
&= \frac{1}{2(\hbar\omega_0)^3}\frac{1}{\beta^4}\int_0^\infty \frac{u^3}{\frac{e^u}{z}+1}\,du \qquad (u=\beta\epsilon) \\
&= -\frac{\Gamma(4)}{2\beta^4(\hbar\omega_0)^3}\frac{1}{\Gamma(4)}\int_0^\infty \frac{u^{4-1}}{\frac{e^u}{-z}-1}\,du \\
\langle E\rangle &= -\frac{3\,\mathrm{Li}_4(-z)}{\beta^4(\hbar\omega_0)^3}
\end{aligned}
$$

$$
\begin{aligned}
\langle N\rangle &= N \\
\int_0^\infty \frac{\mathcal{W}(1,\epsilon)}{e^{\beta\epsilon}z^{-1}+1}\,d\epsilon &= \frac{\epsilon_\mathrm{F}^3}{6(\hbar\omega_0)^3} \\
\frac{1}{2(\hbar\omega_0)^3}\int_0^\infty \frac{\epsilon^2}{e^{\beta\epsilon-\beta\mu}+1}\,d\epsilon &= \frac{(kT_\mathrm{F})^3}{6(\hbar\omega_0)^3} \\
\implies \frac{3}{(kT_\mathrm{F})^3}\frac{1}{\beta^3}\int_0^\infty \frac{x^2}{e^{x-\beta\mu}+1}\,dx &= 1 \\
3\left(\frac{T}{T_\mathrm{F}}\right)^3\int_0^\infty \frac{x^2}{e^{x-\beta\mu}+1}\,dx &= 1
\end{aligned}
$$

Exercise 3

In class, when we considered the Hamiltonian

$$\mathcal{H} = -J\sum_{i=1}^{N-1} s_i s_{i+1} - H\sum_{i=1}^{N} s_i,$$

we found that the expected value $\langle s_i\rangle$ of the spin took the form

$$\langle s_i\rangle = \frac{\mathrm{Tr}\big(\sigma_z\mathcal{T}^N\big)}{\mathrm{Tr}(\mathcal{T}^N)},$$

where the transfer matrix $\mathcal{T}$ and Pauli matrix σ_z are given by

$$\mathcal{T} = \begin{pmatrix} e^{\beta J+\beta H} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J-\beta H}\end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1\end{pmatrix}.$$

Setting $H = 0$, we can find the eigenvalues and eigenvectors of $\mathcal{T}$ to construct an orthogonal matrix $\mathcal{O}$ that diagonalises $\mathcal{T}$.

$$\begin{aligned}
0 &= \det(\mathcal{T} - \lambda I) \\
&= \begin{vmatrix} e^{\beta J} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} - \lambda \end{vmatrix} \\
&= \left(e^{\beta J} - \lambda\right)^2 - e^{-2\beta J} \\
&= \lambda^2 - 2e^{\beta J}\lambda + \left(e^{2\beta J} - e^{-2\beta J}\right) \\
\implies \lambda_\pm &= \frac{2e^{\beta J} \pm \sqrt{4e^{2\beta J} - 4\left(e^{2\beta J} - e^{-2\beta J}\right)}}{2} \\
&= e^{\beta J} \pm e^{-\beta J}
\end{aligned}$$

$$\begin{aligned}
(\mathcal{T} - \lambda_+ I)\mathbf{x} &= \mathbf{0} \\
\begin{pmatrix} -e^{-\beta J} & e^{-\beta J} \\ e^{-\beta J} & -e^{-\beta J} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} &= \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\
\implies x_1 &= x_2 \\
\implies \mathbf{x}_+ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}
\end{aligned}
\qquad
\begin{aligned}
(\mathcal{T} - \lambda_- I)\mathbf{x} &= \mathbf{0} \\
\begin{pmatrix} e^{-\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{-\beta J} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} &= \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\
\implies x_1 &= -x_2 \\
\implies \mathbf{x}_- &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}
\end{aligned}$$

$$\implies \mathcal{O} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \mathcal{O}^{\mathrm{T}} = \mathcal{O}^{-1}$$

$$\begin{aligned}
\mathcal{T}_{\text{diag}} &= \mathcal{O}^{\mathrm{T}} \mathcal{T} \mathcal{O} \\
\implies \mathcal{T} &= \mathcal{O} \mathcal{T}_{\text{diag}} \mathcal{O} \\
\implies \sigma_z \mathcal{T}^N &= \sigma_z \left(\mathcal{O} \mathcal{T}_{\text{diag}} \mathcal{O}\right)^N \\
&= \sigma_z \mathcal{O} \mathcal{T}_{\text{diag}} \mathcal{O} \mathcal{O} \mathcal{T}_{\text{diag}} \mathcal{O} \ldots \mathcal{O} \mathcal{T}_{\text{diag}} \mathcal{O} \\
&= \sigma_z \mathcal{O} \mathcal{T}_{\text{diag}}^N \mathcal{O} \\
&= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\
&= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \lambda_+^N & \lambda_+^N \\ \lambda_-^N & -\lambda_-^N \end{pmatrix} \\
&= \frac{1}{2} \begin{pmatrix} \lambda_+^N + \lambda_-^N & \lambda_+^N - \lambda_-^N \\ -\lambda_+^N + \lambda_-^N & -\lambda_+^N - \lambda_-^N \end{pmatrix}
\end{aligned}$$

$$\begin{aligned}
\langle s_i \rangle &= \frac{\mathrm{Tr}\left(\sigma_z \mathcal{T}^N\right)}{\mathrm{Tr}(\mathcal{T}^N)} \\
&= \frac{1}{2} \frac{\lambda_+^N + \lambda_-^N - \lambda_+^N - \lambda_-^N}{\lambda_+^N + \lambda_-^N} \\
&= 0
\end{aligned}$$

Exercise 4

1.

From Exercise 3, we have

$$\langle s_i \rangle = \frac{\mathrm{Tr}(\sigma_z \mathcal{T}^N)}{\mathrm{Tr}(\mathcal{T}^N)}.$$

Using Mathematica we find

$$\lim_{N\to\infty} \langle s_i \rangle = \frac{\left(e^{2\beta H} - 1\right) e^{3\beta J}}{\sqrt{e^{6\beta J} + 4e^{2\beta(H+J)} - 2e^{2\beta(H+3J)} + e^{2\beta(2H+3J)}}},$$
$$\lim_{H\to\infty} \left(\lim_{N\to\infty} \langle s_i \rangle \right) = 1.$$

This indicates that for a strong magnetic field, the spins are all aligned with the magnetic field, as expected.

```
T = {{ⅇ^(β J+β H), ⅇ^(-β J)}, {ⅇ^(-β J), ⅇ^(β J-β H)}};
σ = {{1, 0}, {0, -1}};
s = Tr[σ.MatrixPower[T, N]] / Tr[MatrixPower[T, N]];
Limit[s, N → ∞] // FullSimplify
```

$$\frac{e^{3 J \beta}\left(-1 + e^{2 H \beta}\right)}{\sqrt{e^{6 J \beta} + 4 e^{2 (H+J) \beta} - 2 e^{2 (H+3 J) \beta} + e^{4 H \beta + 6 J \beta}}} \quad \text{if} \quad \textit{condition}$$

```
Limit[(ⅇ^(3 J β) (-1 + ⅇ^(2 H β)))/Sqrt[ⅇ^(6 J β) + 4 ⅇ^(2 (H+J) β) - 2 ⅇ^(2 (H+3 J) β) + ⅇ^(4 H β+6 J β)], H → ∞]
```

$$1 \quad \text{if} \quad \left(e^{3 J \beta} \mid e^{6 J \beta} \mid J\right) \in \mathbb{R} \ \&\& \ \beta > 0$$

2.

Using Mathematica we find

$$
\begin{aligned}
&\lim_{H\to 0} \langle s_i \rangle = 0 \\
\implies &\lim_{J\to\infty} \left(\lim_{H\to 0} \langle s_i \rangle \right) = 0.
\end{aligned}
$$

This contradicts the expected behaviour. If instead we rearrange the limits we result in the expected answer, namely

$$
\begin{aligned}
&\lim_{J\to\infty} \langle s_i \rangle = \frac{e^{2N\beta H} - 1}{e^{2N\beta H} - 1} \\
\implies &\lim_{N\to\infty} \left(\lim_{J\to\infty} \langle s_i \rangle \right) = 1 \\
\implies &\lim_{H\to 0} \left[\lim_{N\to\infty} \left(\lim_{J\to\infty} \langle s_i \rangle \right) \right] = 1.
\end{aligned}
$$

```
Limit[s, H → 0]
```

```
0
```

```
Limit[s, J → ∞]
```

$$\frac{-1 + e^{2 H N \beta}}{1 + e^{2 H N \beta}} \quad \text{if} \quad \textit{condition}$$