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Midterm II reflection

Exercise 1.1 Magnetic field spin level splitting (*2013 midterm II p1*)

A particle with spin S has $2S+1$ states $-S, -S+1, \cdots S-1, S$. When exposed to a magnetic field, state splitting results in energy $E_m = \hbar m B$. Calculate the partition function, and use this to find the temperature specific magnetization. A "sum the geometric series" hint was given.

Answer for Exercise 1.1

Our partition function is

$$\begin{aligned} Z &= \sum_{m=-S}^{S} e^{-\hbar \beta m B} \\ &= e^{-\hbar \beta S B} \sum_{m=-S}^{S} e^{-\hbar \beta (m+S) B} \\ &= e^{\hbar \beta S B} \sum_{n=0}^{2S} e^{-\hbar \beta n B}. \end{aligned} \tag{1.1}$$

Writing

$$a = e^{-\hbar \beta B}, \tag{1.2}$$

that is

$$\begin{aligned} Z &= a^{-S} \sum_{n=0}^{2S} a^n \\ &= a^{-S} \frac{a^{2S+1} - 1}{a - 1} \\ &= \frac{a^{S+1} - a^{-S}}{a - 1} \\ &= \frac{a^{S+1/2} - a^{-S-1/2}}{a^{1/2} - a^{-1/2}}. \end{aligned} \tag{1.3}$$

Substitution of a gives us

$$\boxed{Z = \frac{\sinh(\hbar\beta B(S+1/2))}{\sinh(\hbar\beta B/2)}.} \tag{1.4}$$

To calculate the magnetization M, I used

$$M = -\left\langle H \right\rangle / B. \tag{1.5}$$

As [1] defines magnetization for a spin system. It was pointed out to me after the test that magnetization was defined differently in class as

$$\mu = \frac{\partial B}{\partial F}. \tag{1.6}$$

These are, up to a sign, identical, at least in this case, since we have β and B traveling together in the partition function.

In terms of the average energy

$$\begin{aligned} M &= -\frac{\left\langle H \right\rangle}{B} \\ &= \frac{1}{B}\frac{\partial}{\partial\beta}\ln Z(\beta B) \\ &= \frac{1}{ZB}\frac{\partial}{\partial\beta}Z(\beta B) \\ &= \frac{1}{Z}\frac{\partial}{\partial(\beta B)}Z(\beta B) \end{aligned} \tag{1.7}$$

Compare this to the in-class definition of magnetization

$$\begin{aligned} \mu &= \frac{\partial F}{\partial B} \\ &= \frac{\partial}{\partial B}\left(-k_{\mathrm{B}} T \ln Z(\beta B)\right) \\ &= -\frac{\partial}{\partial B}\frac{\ln Z(\beta B)}{\beta} \\ &= -\frac{1}{\beta Z}\frac{\partial}{\partial B}Z(\beta B) \\ &= -\frac{1}{Z}\frac{\partial}{\partial(\beta B)}Z(\beta B). \end{aligned} \tag{1.8}$$

Defining the magnetic moment in either of these fashions is really a cheat, because it's done without any connection to physics of the situation. In §3.9 of [2] is a much better seeming approach, where the moment is defined as $M_z = -\left\langle \boldsymbol{\mu} \cdot \mathbf{H} \right\rangle / H$, but this is then shown to have the form eq. (1.8).

Calculating it For this derivative we have

$$\begin{aligned}\frac{\partial}{\partial(\beta B)}\ln Z &= \frac{\partial}{\partial(\beta B)}\ln\frac{\sinh(\hbar\beta B(S+1/2))}{\sinh(\hbar\beta B/2)} \\ &= \frac{\partial}{\partial(\beta B)}\left(\ln\sinh(\hbar\beta B(S+1/2)) - \ln\sinh(\hbar\beta B/2)\right) \\ &= \frac{\hbar}{2}\left((2S+1)\coth(\hbar\beta B(S+1/2)) - \coth(\hbar\beta B/2)\right).\end{aligned} \tag{1.9}$$

This gives us

$$\begin{aligned}\mu &= -\frac{1}{Z}\frac{\hbar}{2}\left((2S+1)\coth(\hbar\beta B(S+1/2)) - \coth(\hbar\beta B/2)\right) \\ &= -\frac{\sinh(\hbar\beta B/2)}{\sinh(\hbar\beta B(S+1/2))}\frac{\hbar}{2}\left((2S+1)\coth(\hbar\beta B(S+1/2)) - \coth(\hbar\beta B/2)\right)\end{aligned} \tag{1.10}$$

After some simplification (done offline in notes/phy452/mathematica/midtermTwoQ1FinalSimplificationMu. we get

$$\boxed{\mu = \hbar\frac{(s+1)\sinh(\hbar\beta Bs) - s\sinh(\hbar\beta B(s+1))}{\cosh(\hbar\beta B(2s+1)) - 1}.} \tag{1.11}$$

I got something like this on the midterm, but recall doing it somehow much differently.

Exercise 1.2 Perturbation of classical harmonic oscillator (*2013 midterm II p2*)

Consider a single particle perturbation of a classical simple harmonic oscillator Hamiltonian

$$H = \frac{1}{2}m\omega^2\left(x^2+y^2\right) + \frac{1}{2m}\left(p_x^2+p_y^2\right) + ax^4 + by^6 \tag{1.12}$$

Calculate the canonical partition function, mean energy and specific heat of this system.

a. This problem can be attempted in two ways, the first of which was how I did it on the midterm, differentiating under the integral sign, leaving the integrals in exact form, but not evaluated explicitly in any way.

b. By Taylor expanding around $c = 0$ and $d = 0$ with those as the variables in the Taylor expansion (as now done in the Pathria 3.29 problem), we can form a solution in short order. Given my low midterm mark, it seems very likely that this was what was expected.

Answer for Exercise 1.2

The canonical partition function is

$$\begin{aligned}Z &= \int dxdydp_xdp_ye^{-\beta H} \\ &= \int dxe^{-\beta\left(\frac{1}{2}m\omega^2x^2+ax^4\right)}\int dye^{-\beta\left(\frac{1}{2}m\omega^2y^2+by^6\right)}\int dp_xdp_ye^{-\beta p_x^2/2m}e^{-\beta p_y^2/2m}.\end{aligned} \tag{1.13}$$

With

$$u = \sqrt{\frac{\beta}{2m}} p_x \tag{1.14a}$$

$$v = \sqrt{\frac{\beta}{2m}} p_y, \tag{1.14b}$$

the momentum integrals are

$$\int dp_x dp_y e^{-\beta p_x^2/2m} e^{-\beta p_y^2/2m} = \frac{2m}{\beta} \int du du e^{-u^2-v^2} = \frac{m}{\beta} 2\pi \int 2r dr e^{-r^2} = \frac{2\pi m}{\beta}. \tag{1.15}$$

Writing

$$f(x) = \frac{1}{2} m\omega^2 x^2 + ax^4 \tag{1.16a}$$

$$g(x) = \frac{1}{2} m\omega^2 y^2 + by^6, \tag{1.16b}$$

we have

$$\boxed{Z = \frac{2\pi m}{\beta} \int dx e^{-\beta f(x)} \int dy e^{-\beta g(y)}.} \tag{1.17}$$

Part a. Attempt 1: differentiation under the integral sign The mean energy is

$$\begin{aligned}
\langle H \rangle &= \frac{\int H e^{-\beta H}}{\int e^{-\beta H}} \\
&= -\frac{\partial}{\partial \beta} \ln \int e^{-\beta H} \\
&= \frac{\partial}{\partial \beta} \left(\ln \beta - \ln \int dx e^{-\beta f(x)} - \ln \int dy e^{-\beta g(y)} \right) \\
&= \frac{1}{\beta} + \frac{\int dx f(x) e^{-\beta f(x)}}{\int dx e^{-\beta f(x)}} + \frac{\int dy g(y) e^{-\beta g(y)}}{\int dy e^{-\beta g(y)}}.
\end{aligned} \tag{1.18}$$

The specific heat follows by differentiating once more

$$\begin{aligned}
C_V &= \frac{\partial \langle H \rangle}{\partial T} \\
&= \frac{\partial \beta}{\partial T} \frac{\partial \langle H \rangle}{\partial \beta} \\
&= -\frac{1}{k_B T^2} \frac{\partial \langle H \rangle}{\partial \beta} \\
&= -k_B \beta^2 \frac{\partial \langle H \rangle}{\partial \beta} \\
&= -k_B \beta^2 \left(-\frac{1}{\beta^2} + \frac{\partial}{\partial \beta} \left(\frac{\int dx f(x) e^{-\beta f(x)}}{\int dx e^{-\beta f(x)}} + \frac{\int dy g(y) e^{-\beta g(y)}}{\int dy e^{-\beta g(y)}} \right) \right).
\end{aligned} \tag{1.19}$$

Differentiating the integral terms we have, for example,

$$\frac{\partial}{\partial \beta} \frac{\int dx f(x) e^{-\beta f(x)}}{\int dx e^{-\beta f(x)}} = -\frac{\int dx f^2(x) e^{-\beta f(x)}}{\int dx e^{-\beta f(x)}} + \left(\frac{\int dx f(x) e^{-\beta f(x)}}{\int dx e^{-\beta f(x)}} \right)^2, \tag{1.20}$$

so that the specific heat is

$$\boxed{C_V = k_B \left(1 + \frac{\int dx f^2(x) e^{-\beta f(x)}}{\int dx e^{-\beta f(x)}} - \left(\frac{\int dx f(x) e^{-\beta f(x)}}{\int dx e^{-\beta f(x)}} \right)^2 + \frac{\int dy g^2(y) e^{-\beta g(y)}}{\int dy e^{-\beta g(y)}} - \left(\frac{\int dy g(y) e^{-\beta g(y)}}{\int dy e^{-\beta g(y)}} \right)^2 \right).} \tag{1.21}$$

That's as far as I took this problem. There was a discussion after the midterm with Eric about Taylor expansion of these integrals. That's not something that I tried.

Part b. Attempt 2: Taylor expanding in c and d Performing a two variable Taylor expansion of Z, about $(c, d) = (0, 0)$ we have

$$\begin{aligned} Z &\approx \frac{2\pi m}{\beta} \int dx dy e^{-\beta m \omega^2 x^2/2} e^{-\beta m \omega^2 y^2/2} \left(1 - \beta a x^4 - \beta b y^6 \right) \\ &= \frac{2\pi m}{\beta} \frac{2\pi}{\beta m \omega^2} \left(1 - \beta a \frac{3!!}{(\beta m \omega^2)^2} - \beta b \frac{5!!}{(\beta m \omega^2)^3} \right), \end{aligned} \tag{1.22}$$

or

$$\boxed{Z \approx \frac{(2\pi/\omega)^2}{\beta^2} \left(1 - \frac{3a}{\beta (m\omega^2)^2} - \frac{15b}{\beta^2 (m\omega^2)^3} \right).} \tag{1.23}$$

Now we can calculate the average energy

$$\begin{aligned} \langle H \rangle &= -\frac{\partial}{\partial \beta} \ln Z \\ &= -\frac{\partial}{\partial \beta} \left(-2 \ln \beta + \ln \left(1 - \frac{3a}{\beta (m\omega^2)^2} - \frac{15b}{\beta^2 (m\omega^2)^3} \right) \right) \\ &= \frac{2\beta}{-} \frac{\frac{3a}{\beta^2 (m\omega^2)^2} + \frac{30b}{\beta^3 (m\omega^2)^3}}{1 - \frac{3a}{\beta (m\omega^2)^2} - \frac{15b}{\beta^2 (m\omega^2)^3}}. \end{aligned} \tag{1.24}$$

Dropping the c, d terms of the denominator above, we have

$$\boxed{\langle H \rangle = \frac{2\beta}{-} \frac{3a}{\beta^2 (m\omega^2)^2} - \frac{30b}{\beta^3 (m\omega^2)^3}.} \tag{1.25}$$

The heat capacity follows immediately

$$\boxed{C_V = \frac{1}{k_B} \frac{\partial \langle H \rangle}{\partial T} = 2 - \frac{6 a k_B T}{(m\omega^2)^2} - \frac{90 k_B^2 T^2 b}{(m\omega^2)^3}.} \tag{1.26}$$

Bibliography

[1] C. Kittel and H. Kroemer. *Thermal physics*. WH Freeman, 1980. 1

[2] RK Pathria. *Statistical mechanics*. Butterworth Heinemann, Oxford, UK, 1996. 1