PHY452 Problem Set 3

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Problem 1

(a) The Hamiltonian of the gas is given by $\mathcal{H} = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m} - \gamma B S_i^z \right]$ where the $\{\mathbf{q}_i, \mathbf{p}_i\}$ coordinates are treated classically and confined to a volume V, but the $S_i^z = -1, 0, 1$ is quantized spin-1. The partition function $\mathcal{Z}(T, N, V, B)$ is then given by a continuous component which must be integrated over, and a discrete component involving a sum over the spins. By definition

$$\mathcal{Z} = \sum_{\{\mu\}} e^{-\beta \mathcal{H}(\mu)} \tag{1.1}$$

$$= \frac{1}{h^3 N!} \int \prod_{i=1}^{N} d^3 q_i d^3 p_i \, e^{-\beta \sum_k \frac{p_k^2}{2m}} \cdot \sum_{\{\mu\}} e^{\beta \gamma B \sum_k S_k^z} \tag{1.2}$$

$$= \mathcal{Z}_{\text{KE}} \cdot \mathcal{Z}_{\text{SPINS}} \tag{1.3}$$

Since the partition functions of the microstates regarding momentum and spin are seperable, we can compute them individually. The partition function obtained from the kinetic energy portion of the Hamiltonian is found by integration:

$$\mathcal{Z}_{\text{KE}} = \frac{1}{h^3 N!} \int \prod_{i=1}^{N} d^3 q_i d^3 p_i \, e^{-\beta \sum_k \frac{p_k^2}{2m}} \tag{1.4}$$

$$= \frac{1}{h^3} \frac{V^N}{N!} \int \prod_{i=1}^{N} d^3 p_i e^{-\beta \sum_k \frac{p_k^2}{2m}} \tag{1.5}$$

$$= \frac{1}{h^3} \frac{V^N}{N!} \left[\int dp \, e^{-\beta \frac{p^2}{2m}} \right]^{3N} \tag{1.6}$$

$$= \frac{V^N}{h^3 N!} \left[\sqrt{\frac{2\pi m}{\beta}} \right]^{3N} \tag{1.7}$$

where (1.6) came from the fact that we performed the same three-dimensional integral N times, giving $3N$ Gaussians. The parition functions for the spins is slightly easier to compute, as we just sum over the possibilities of spins for all N particles:

$$\mathcal{Z}_{\text{SPINS}} = \sum_{\{\mu\}} e^{\beta \gamma B \sum_k S_k^z} \tag{1.8}$$

$$= \left(\sum_{S_i^z = -1,0,1} e^{\beta \gamma B S_i^z} \right)^N \tag{1.9}$$

$$= \left(1 + e^{\beta \gamma B} + e^{-\beta \gamma B} \right)^N \tag{1.10}$$

$$= \left(1 + 2\cosh(\beta B \gamma) \right)^N . \tag{1.11}$$

$$= (\mathcal{Z}_{\text{SINGLE}})^N \tag{1.12}$$

According to (1.3), the total partition function is then the product of (1.7) and (1.11), hence

$$\mathcal{Z}(T,N,V,B) = \frac{V^N}{N!}\left[\frac{\sqrt{2\pi mkT}}{h}\right]^{3N}\left[1+2\cosh\left(\frac{B\gamma}{kT}\right)\right]^N. \tag{1.13}$$

(**b**) We can now examine the individual probabilities of finding a particle in a specific spin state. The joint probability is given by measuring the probability of finding some particle with spin S^z at a position q and momentum p, which is just $\mathbb{P}(\mu) = \dfrac{e^{-\beta\mathcal{H}(\mu)}}{\mathcal{Z}}$ measured out of the N particles. For a specific particle, however, the probabilities are unconditional, hence measuring the spin of one particle in the absence of spin-spin interactions is that of the angular component of the Hamiltonian out of the single spin partition function:

$$\mathbb{P}(S^z) = \frac{e^{\beta B\gamma S^z}}{\mathcal{Z}_{\text{SINGLE}}} = \frac{e^{\beta B\gamma S^z}}{1+2\cosh(\beta B\gamma)}. \tag{1.14}$$

Thus for a single particle, we find the probabilities of measuring net spin $\pm 1, 0$ to be

$$\mathbb{P}(+1) = \frac{\exp\left\{\frac{B\gamma}{kT}\right\}}{1+2\cosh\left(\frac{B\gamma}{kT}\right)} \tag{1.15}$$

$$\mathbb{P}(0) = \frac{1}{1+2\cosh\left(\frac{B\gamma}{kT}\right)} \tag{1.16}$$

$$\mathbb{P}(-1) = \frac{\exp\left\{-\frac{B\gamma}{kT}\right\}}{1+2\cosh\left(\frac{B\gamma}{kT}\right)} \tag{1.17}$$

(**c**) We now consider the average dipole moment $\langle M\rangle$, where $M = \gamma\sum_{i=1}^{N} S_i^z$. Returning to equation (1.8), we can reduce the partition function fixed to a single microstate $\{\mu\}$, from which we observe that

$$\log \mathcal{Z}_{\text{SPINS}} = \beta\gamma B\sum_{i=1}^{N} S_i^z \tag{1.18}$$

$$\implies \frac{\partial(\log \mathcal{Z}_{\text{SPINS}})}{\partial B} = \beta\gamma\sum_{i=1}^{N} S_i^z \tag{1.19}$$

$$= \beta M$$

and hence, averaged over all microstates by linearity of the derivative, we obtain

$$\langle M\rangle = \frac{1}{\beta}\frac{\partial(\log \mathcal{Z}_{\text{SPINS}})}{\partial B} = \frac{1}{\beta}\frac{1}{\mathcal{Z}_{\text{SPINS}}}\frac{\partial \mathcal{Z}_{\text{SPINS}}}{\partial B}. \tag{1.20}$$

In terms of the spin partition function found in (1.11), we find the average magnetic moment per unit volume to be

$$\frac{\langle M\rangle}{V} = \frac{kT}{V\left(1+2\cosh\left(\frac{B\gamma}{kT}\right)\right)^N}\frac{\partial}{\partial B}\left[1+2\cosh\left(\frac{B\gamma}{kT}\right)\right]^N \tag{1.21}$$

$$= \frac{NkT}{V\left(1+2\cosh\left(\frac{B\gamma}{kT}\right)\right)^N}\cdot\left(1+2\cosh\left(\frac{B\gamma}{kT}\right)\right)^{N-1}\cdot\left(2\sinh\left(\frac{B\gamma}{kT}\right)\right)\cdot\frac{\gamma}{kT} \tag{1.22}$$

$$= \frac{2N\gamma}{V}\frac{\sinh\left(\frac{B\gamma}{kT}\right)}{1+2\cosh\left(\frac{B\gamma}{kT}\right)} \tag{1.23}$$

Intuitively, in the $T\to\infty$ limit, then (1.21) approaches 0, and approaches $\dfrac{2N\gamma}{V}$ in the $T\to 0$ limit (permanent magnet).

(d) The zero field susceptibility is given as $\left.\dfrac{\partial\langle M\rangle}{\partial B}\right|_{B=0}$, which is the measure of magnetization in the absence of the B-field. Taking the derivative of (1.23), we have

$$\left.\frac{\partial\langle M\rangle}{\partial B}\right|_{B=0} = 2N\gamma\,\frac{\partial}{\partial B}\left.\left[\frac{\sinh\left(\frac{B\gamma}{kT}\right)}{1+2\cosh\left(\frac{B\gamma}{kT}\right)}\right]\right|_{B=0} \tag{1.24}$$

$$= 2N\gamma\left.\left[\frac{\cosh\left(\frac{B\gamma}{kT}\right)}{1+2\cosh\left(\frac{B\gamma}{kT}\right)}\frac{\gamma}{kT} - \frac{2\sinh^2\left(\frac{B\gamma}{kT}\right)}{\left[1+2\cosh\left(\frac{B\gamma}{kT}\right)\right]^2}\frac{\gamma}{kT}\right]\right|_{B=0} \tag{1.25}$$

$$= 2N\gamma\left[\frac{1}{1+2}\frac{\gamma}{kT} - (0)\right] \tag{1.26}$$

$$= \frac{2N\gamma^2}{3kT} \tag{1.27}$$

hence the gas is 'more magnetizable' at lower temperatures.

Problem 2

(**a**) Before attacking this problem, we begin by showing that $\langle x^2\rangle = a,\ \langle x^4\rangle = 3a^2$, and $\langle x^6\rangle = 15a^3$, where

$$\langle\varphi(x)\rangle \equiv \frac{\int dx\,\varphi(x)e^{-\frac{x^2}{2a}}}{\int dx\,e^{-\frac{x^2}{2a}}} = \frac{\int dx\,\varphi(x)e^{\frac{-x^2}{2a}}}{\sqrt{2\pi a}} \tag{2.1}$$

where all integrals are over $\mathbb{R}$. I chose to take a different approach to this problem, where instead of just showing you that I can take derivatives, I will prove by induction that

$$\langle x^{2n}\rangle = a^n\prod_{j=0}^{n-1}(2j+1) \tag{2.2}$$

for $n > 0$ natural numbers.

Proof: We begin by showing that this is true for a base case. Fix $n = 1$ so we show that

$$\langle x^2\rangle = a \tag{2.3}$$

from (2.2). This is obtained by observing that, under the Feynman integration technique in derivating with respect to a, we have

$$\frac{\partial}{\partial a}\int dx\,e^{-\frac{x^2}{2a}} = \int dx\,e^{-\frac{x^2}{2a}}\left(-\frac{x^2}{2}\right)\left(-\frac{1}{a^2}\right) \tag{2.4}$$

$$= \frac{1}{2a^2}\int x^2e^{-\frac{x^2}{2a}} \tag{2.5}$$

$$= \frac{\partial}{\partial a}\sqrt{2\pi a} = \frac{1}{2}\sqrt{\frac{2\pi}{a}} \tag{2.6}$$

$$\implies \int dx\,x^2e^{-\frac{x^2}{2a}} = \sqrt{2\pi a}\,a \tag{2.7}$$

$$\implies \langle x^2\rangle = a = \prod_{j=0}^{0}(2j+1)a^{(1)}. \tag{2.8}$$

One may observe that we invoke the $n = 0$ case to obtain the $n = 1$ case by derivating, and this is true for the general induction. We assume the hypothesis that

$$\langle x^{2n}\rangle = a^n\prod_{j=0}^{n-1}(2j+1) \tag{2.9}$$

is true for a fixed $n \in \mathbb{N}\setminus\{0\}$, and we show that this implies that the $n+1$ case is also true. We have that, from (2.1) and (2.2),

$$\sqrt{2\pi a}\,\langle x^{2n}\rangle = \int dx\,x^{2n}e^{-\frac{x^2}{2a}} = \sqrt{2\pi a}\,a^n\prod_{j=0}^{n-1}(2j+1). \tag{2.10}$$

Taking the derivative with respect to a on both sides, we find

$$\frac{\partial}{\partial a}\int dx\,x^{2n}e^{-\frac{x^2}{2a}} = \frac{1}{2a^2}\int dx\,x^{2n}x^2e^{-\frac{x^2}{2a}} \tag{2.11}$$

$$= \frac{1}{2a^2} \int dx\, x^{2(n+1)} e^{-\frac{x^2}{2a}} \tag{2.12}$$

and

$$\frac{\partial}{\partial a} \sqrt{2\pi} a^{n+\frac{1}{2}} \prod_{j=0}^{n-1} (2j+1) = \sqrt{2\pi} \left(n + \frac{1}{2} \right) a^{n-\frac{1}{2}} \prod_{j=0}^{n-1} (2j+1). \tag{2.13}$$

Equating (2.12) and (2.13) imply that

$$\frac{1}{2a^2} \int dx\, x^{2(n+1)} e^{-\frac{x^2}{2a}} = \sqrt{2\pi} \left(n + \frac{1}{2} \right) a^{n-\frac{1}{2}} \prod_{j=0}^{n-1} (2j+1) \tag{2.14}$$

and thus

$$\int dx\, x^{2(n+1)} e^{-\frac{x^2}{2a}} = \sqrt{2\pi}\, 2 \left(n + \frac{1}{2} \right) a^{n-\frac{1}{2}+2} \prod_{j=0}^{n-1} (2j+1) \tag{2.15}$$

However, distributing the '2' into the brackets and bringing out the $\sqrt{a}$, we find that

$$\int dx\, x^{2(n+1)} e^{-\frac{x^2}{2a}} = \sqrt{2\pi a}\, a^{n+1} \prod_{j=0}^{n-1} (2j+1)(2n+1) \tag{2.16}$$

$$= \sqrt{2\pi a}\, a^{n+1} \prod_{j=0}^{(n+1)-1} (2j+1) \tag{2.17}$$

hence dividing out the $\sqrt{2\pi a}$ implies that

$$\langle x^{2(n+1)} \rangle = a^{n+1} \prod_{j=0}^{(n+1)-1} (2j+1) \tag{2.18}$$

thus $n \implies n+1$. Since this is true for the base case, it must be true for all natural numbers $n > 0$, and we prove that

$$\langle x^{2n} \rangle = a^n \prod_{j=0}^{n-1} (2j+1) \tag{2.19}$$

as desired. ■

This implies that

$$\langle x^2 \rangle = a \qquad (n = 1) \tag{2.20}$$

$$\langle x^4 \rangle = (1)(3)a^2 = 3a^2 \qquad (n = 2) \tag{2.21}$$

$$\langle x^6 \rangle = (5)(3)(1)a^3 = 15a^3 \qquad (n = 3) \tag{2.22}$$

$$\vdots \qquad\qquad \vdots$$

(**b**) We define the Hamiltonian as $\mathcal{H} = \mathcal{H}_0 - V$, where $\mathcal{H}_0 = \dfrac{p^2}{2m} + cq^2$ and $V = gq^3 + fq^4$ is a perturbation. The Hamiltonian is defined in a continuous space, thus determining the partition function involves integration in one-dimensional phase space in p and q. First considering the unperturbed partition, we have

$$\mathcal{Z}_0 = \frac{1}{h}\int dpdq\, e^{-\beta\frac{p^2}{2m}}e^{-\beta cq^2}. \tag{2.23}$$

We employ the general Gaussian formula over infinitely-bounded integration, $\displaystyle\int dx\, e^{-\frac{x^2}{a}} = \sqrt{\pi a}$, thus by seperability in (2.23) obtaining

$$\mathcal{Z}_0 = \frac{1}{h}\cdot\sqrt{\frac{2m\pi}{\beta}}\cdot\sqrt{\frac{\pi}{\beta c}} \tag{2.24}$$

$$= \frac{1}{h}\frac{\pi}{\beta}\sqrt{\frac{2m}{c}}. \tag{2.25}$$

If we were to now consider the addition of the perturbation $V(q)$, we find the partition function to be

$$\mathcal{Z} = \frac{1}{h}\int dpdq\, e^{-\beta\frac{p^2}{2m}}e^{-\beta cq^2}e^{\beta V} \tag{2.26}$$

$$= \frac{1}{h}\cdot\sqrt{\frac{2m\pi}{\beta}}\int dq\, e^{\beta V}e^{-\beta cq^2} \tag{2.27}$$

$$= \frac{1}{h}\cdot\sqrt{\frac{2m\pi}{\beta}}\cdot\sqrt{\frac{\pi}{\beta c}}\left[\int dq\, e^{-\beta cq^2}\right]^{-1}\cdot\int dq\, e^{\beta V}e^{-\beta cq^2} \tag{2.28}$$

$$= \mathcal{Z}_0\langle e^{\beta V}\rangle_0 \tag{2.29}$$

in accordance (2.1), where $\langle e^{\beta V}\rangle_0$ is the averaged taken with respect to the canonical distribution under $\mathcal{H}_0$.

(**c**) Let us now consider the average defined in part (b), $\langle e^{\beta V}\rangle_0$. Since $V(q)$ is a perturbation with respect to $\mathcal{H}_0$, and f and g are small, we can expand the integrand in a Taylor series to simplify the integral:

$$\langle e^{\beta V}\rangle_0 = \sqrt{\frac{\beta c}{\pi}}\int dq\, e^{\beta gq^3}e^{\beta fq^4}e^{-\beta cq^2} \tag{2.30}$$

$$\approx \sqrt{\frac{\beta c}{\pi}}\int dq\, \left[1 + \beta gq^3 + \frac{1}{2}\beta^2g^2q^6 + \dots\right]\left[1 + \beta fq^4 + \frac{1}{2}\beta^2f^2q^8 + \dots\right]e^{-\beta cq^2} \tag{2.31}$$

$$= \sqrt{\frac{\beta c}{\pi}}\int dq\, \left[1 + \beta fq^4 + \frac{1}{2}\beta^2f^2q^8 + \frac{1}{2}\beta^2g^2q^6 + \dots)\right]e^{-\beta cq^2} \tag{2.32}$$

$$= \sqrt{\frac{\beta c}{\pi}}\left[\int dq\, e^{-\beta cq^2} + \beta f\int dq\, q^4e^{-\beta cq^2} + \frac{1}{2}\beta^2f^2\int dq\, q^8e^{-\beta cq^2} + \frac{1}{2}\beta^2g^2\int dq\, q^6e^{-\beta cq^2} + \dots\right] \tag{2.33}$$

$$= \sqrt{\frac{\beta c}{\pi}}\left[\sqrt{\frac{\pi}{\beta c}} + \beta f\frac{3}{4\beta^2c^2}\sqrt{\frac{\pi}{\beta c}} + \frac{1}{2}\beta^2g^2\frac{15}{8\beta^3c^3}\sqrt{\frac{\pi}{\beta c}} + \dots\right] \tag{2.34}$$

$$= 1 + \frac{1}{\beta}\frac{3}{4}\frac{f}{c^2} + \frac{1}{\beta}\frac{15}{16}\frac{g^2}{c^3} + \mathcal{O}(\beta^{-2}) \tag{2.35}$$

$$= 1 + \frac{3}{4\beta}Q(f,g,c) + \mathcal{O}(\beta^{-2}) \tag{2.36}$$

where we have defined $Q(f,g,c) = \frac{f}{c^2} + \frac{3g^2}{4c^3}$, used the fact that $\int dx\, x^{2n} e^{-\frac{x^2}{2a}} = \sqrt{2\pi a}\, a^n \prod_{j=0}^{n-1}(2j+1)$ as proven in (2.19), and that the integral of any odd function ($\sim q^{2k+1}e^{-\beta c q^2}$, $k \in \mathbb{N}$) is zero. In concatenation with (2.29), we then obtain the approximate partition function to be $\mathcal{Z} \approx \mathcal{Z}_0(1+\mathcal{Z}_1)$ where $\mathcal{Z}_1 = \frac{3}{4\beta}Q(f,g,c)$. To find the heat capacity, we begin by finding the energy E given by

$$E = -\frac{\partial(\log \mathcal{Z})}{\partial\beta} \tag{2.37}$$

$$= -\frac{\partial(\log \mathcal{Z}_0 + \log(1+\mathcal{Z}_1))}{\partial\beta} \tag{2.38}$$

$$\approx -\frac{\partial(\log \mathcal{Z}_0 + \mathcal{Z}_1)}{\partial\beta} \tag{2.39}$$

$$= -\frac{1}{\mathcal{Z}_0}\frac{\partial \mathcal{Z}_0}{\partial\beta} - \frac{\partial \mathcal{Z}_1}{\partial\beta} \tag{2.40}$$

where we have also employed the approximation $\log(1+x) \approx x$ for small x, which follows since $\mathcal{Z}_1$ is treated as a perturbation in small f and g. We first observe that

$$\frac{\partial \mathcal{Z}_0}{\partial\beta} = \frac{1}{h}\cdot\frac{\partial}{\partial\beta}\left[\frac{\pi}{\beta}\right]\sqrt{\frac{2m}{c}} \tag{2.41}$$

$$= -\frac{1}{\beta}\mathcal{Z}_0 \tag{2.42}$$

from which, applying the same technique to $\mathcal{Z}_1$ implies

$$\frac{\partial \mathcal{Z}_1}{\partial\beta} = -\frac{1}{\beta}\mathcal{Z}_1. \tag{2.43}$$

Applying (3.41) and (3.42) into (3.39) yields that

$$E = \frac{1}{\beta}\left(1 + \mathcal{Z}_1\right). \tag{2.44}$$

Taking the derivative a second time yields the heat capacity, since

$$C_V = \left(\frac{dE}{dT}\right)_V, \tag{2.45}$$

thus by un-substituting $\beta = \frac{1}{kT}$, we have that

$$C_V = \frac{d}{dT}\left[kT\left(1 + \frac{3}{4}kTQ\right)\right] + \mathcal{O}(T^2) \tag{2.46}$$

$$= k\left[1+\frac{3}{4}kTQ\right] + kT\left[\frac{3}{4}kQ\right]\mathcal{O}(T^2) \tag{2.47}$$

$$= k + \frac{3}{2}k^2TQ + \mathcal{O}(T^2) \tag{2.48}$$

thus arriving at our result

$$C_V = k + \frac{3}{2}k^2T\left[\frac{f}{c^2} + \frac{5}{4}\frac{g^2}{c^3}\right] + \mathcal{O}(T^2) \tag{2.49}$$

which was obtain by re-substituting in our definition of $Q(f,g,c)$ from earlier.

(d) In the last part, we now determine $\langle q\rangle$, where the average is now taken with respect to the full Hamiltonian $\mathcal{H}$ as given in (b). Thus, by definition, we want to compute

$$\langle q\rangle = \frac{\int dpdq\, qe^{-\beta\mathcal{H}}}{\int dpdq\, e^{-\beta\mathcal{H}}} = \frac{\int dq\, qe^{-\beta cq^2+\beta fq^3+\beta gq^4}}{\int dq\, e^{-\beta cq^2+fq^3+gq^4}} \tag{2.50}$$

which follows since the p-integrals cancel to 1. Luckily for us, the approximation desired for $f, g \ll 1$ has been computed in (2.32) and (2.34) already. This then implies that, in this approximation,

$$\sqrt{\frac{\pi}{\beta c}}\left[1+\frac{3}{4\beta}\frac{f}{c^2}+\frac{15}{16\beta}\frac{g^2}{c^3}+\dots\right]\langle q\rangle \approx \int dq\, q\left[1+\beta gq^3+\frac{1}{2}\beta^2g^2q^6+\beta fq^4+\beta^2gfq^7+\frac{1}{2}\beta^2f^2q^8\dots\right]e^{-\beta cq^2} \tag{2.51}$$

from which the only contributing terms are those of even q, since the integral of any odd function over a symmetric region gives 0. At $\mathcal{O}(\beta^2)$, we have

$$\sqrt{\frac{\pi}{\beta c}}\left[1+\frac{3}{4\beta}\frac{f}{c^2}+\frac{15}{16\beta}\frac{g^2}{c^3}+\dots\right]\langle q\rangle \approx \beta g\int dq\, q^4e^{-\beta cq^2} \tag{2.52}$$

$$= \beta g\cdot 3\sqrt{\frac{\pi}{\beta c}}\left(\frac{1}{4\beta^2c^2}\right) \tag{2.53}$$

$$\implies \langle q\rangle = \frac{3g}{4\beta c^2}\left[1+\frac{3}{4\beta}\frac{f}{c^2}+\frac{15}{16\beta}\frac{g^2}{c^3}+\dots\right]^{-1}. \tag{2.54}$$

Taking the leading approximation in the denominator (other contributions are very small, since $\frac{1}{1+x}\approx 1$ for $x\ll 1$) we obtain the expected value of the position of the particle,

$$\langle q\rangle \approx \frac{3g}{4\beta c^2}. \tag{2.55}$$