Problem Set 3

Phys 715

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1 Sunlight

We want to find the energy density per volume for blackbody radiation for given wavelength λ and temperature T.

(a) $\rho(T, \lambda)$

We can start with the expression for U in terms of an integral over k:

$$U = 2\frac{V}{(2\pi)^3} 4\pi\hbar c \int_0^\infty dk\, k^3 \left(e^{\beta\hbar c k} - 1\right)^{-1} \tag{1}$$

We want this integral in terms of λ. We use $k = \frac{2\pi}{\lambda}$, and $dk = -\frac{2\pi}{\lambda^2}\, d\lambda$, to rewrite:

$$U = 2\frac{V}{(2\pi)^3} 4\pi\hbar c \int_{k=0}^{k=\infty} dk \left(\frac{2\pi}{\lambda}\right)^3 \left(e^{\frac{\beta\hbar c 2\pi}{\lambda}} - 1\right)^{-1} \tag{2}$$

$$U = 2\frac{V}{(2\pi)^3} 4\pi\hbar c \int_{\lambda=\infty}^{\lambda=0} \left(-\frac{2\pi}{\lambda^2}\right) d\lambda \left(\frac{2\pi}{\lambda}\right)^3 \left(e^{\frac{\beta\hbar c 2\pi}{\lambda}} - 1\right)^{-1} \tag{3}$$

$$\frac{U}{V} = \frac{(2\pi)^4}{(\pi)^3} \pi\hbar c \int_{\lambda=\infty}^{\lambda=0} \left(-\frac{1}{\lambda^2}\right) d\lambda \left(\frac{1}{\lambda}\right)^3 \left(e^{\frac{\beta\hbar c 2\pi}{\lambda}} - 1\right)^{-1} \tag{4}$$

$$\frac{U}{V} = \frac{(2\pi)^4}{\pi^2} \hbar c \int_{\lambda=\infty}^{\lambda=0} \left(-\frac{1}{\lambda^2}\right) d\lambda \left(\frac{1}{\lambda}\right)^3 \left(e^{\frac{\beta\hbar c 2\pi}{\lambda}} - 1\right)^{-1} \tag{5}$$

$$\frac{U}{V} = -16\pi^2\hbar c \int_{\lambda=\infty}^{\lambda=0} d\lambda\, \frac{1}{\lambda^5} \left(e^{\frac{\beta\hbar c 2\pi}{\lambda}} - 1\right)^{-1} \tag{6}$$

$$\frac{U}{V} = 16\pi^2\hbar c \int_0^\infty d\lambda\, \frac{1}{\lambda^5} \left(e^{\frac{\beta\hbar c 2\pi}{\lambda}} - 1\right)^{-1} \tag{7}$$

We want the energy density per wavelength, so we can identify ρ with the integrand:

$$\rho(\lambda, \beta) = 16\pi^2\hbar c \frac{1}{\lambda^5} \left(e^{\frac{\beta\hbar c 2\pi}{\lambda}} - 1\right)^{-1} \tag{8}$$

This means

$$\rho(\lambda, T) = \frac{16\pi^2\hbar c}{\lambda^5} \left(e^{\frac{2\pi\hbar c}{k_B T \lambda}} - 1\right)^{-1} \tag{9}$$

(b) Finding λ to maximise ρ

Let's rewrite ρ a bit:

$$\rho(\lambda, T) = \frac{16\pi^2\hbar c}{\lambda^5\left(e^{\frac{2\pi\hbar c}{k_B T\lambda}} - 1\right)} \tag{10}$$

To simplify the math a bit, we can notice that maximising ρ should be equivalent to minimising the denominator. Let's do that:

$$0 = \frac{d}{d\lambda}\left(\lambda^5\left(e^{\frac{2\pi\hbar c}{k_B T\lambda}} - 1\right)\right) \tag{11}$$

$$0 = \lambda^5\frac{d}{d\lambda}\left(e^{\frac{2\pi\hbar c}{k_B T\lambda}} - 1\right) + \left(e^{\frac{2\pi\hbar c}{k_B T\lambda}} - 1\right)\frac{d}{d\lambda}\lambda^5 \tag{12}$$

Continuing on, pausing only to admire symmetry,

$$-\lambda^5\frac{d}{d\lambda}\left(e^{\frac{2\pi\hbar c}{k_B T\lambda}} - 1\right) = \left(e^{\frac{2\pi\hbar c}{k_B T\lambda}} - 1\right)\frac{d}{d\lambda}\lambda^5 \tag{13}$$

$$-\lambda^5 e^{\frac{2\pi\hbar c}{k_B T\lambda}}\left(-\frac{2\pi\hbar c}{k_B T\lambda^2}\right) = \left(e^{\frac{2\pi\hbar c}{k_B T\lambda}} - 1\right)\left(5\lambda^4\right) \tag{14}$$

$$\frac{2\pi\hbar c}{k_B T}\lambda^3 e^{\frac{2\pi\hbar c}{k_B T\lambda}} = \left(e^{\frac{2\pi\hbar c}{k_B T\lambda}} - 1\right)\left(5\lambda^4\right) \tag{15}$$

Defining $y = \frac{2\pi\hbar c}{k_B T}$:

$$y e^{\frac{y}{\lambda}} = 5\lambda\left(e^{\frac{y}{\lambda}} - 1\right) \tag{16}$$

$$\frac{y}{\lambda} = 5\left(1 - e^{-\frac{y}{\lambda}}\right) \tag{17}$$

I solved this for $\frac{y}{\lambda}$ in Mathematica, giving us two solutions. There's the pathological solution where $\frac{y}{\lambda} = 0$ This corresponds to λ going to infinity. Looking back at (9), we may find ourselves more interested in the other solution, which we get to be $\frac{y}{\lambda} \approx 4.966$. We can solve this for $\lambda_{\max}$ for a given temperature:

$$\frac{y}{\lambda_{\max}} = 4.966 \tag{18}$$

$$\lambda_{\max} = \frac{y}{4.966} \tag{19}$$

$$\lambda_{\max} = \frac{2\pi\hbar c}{4.966 k_B T} \tag{20}$$

(c) Solar temperature from λ_{max}

We're given here that λ_{max} for sunlight is 480 nm, and we want to find the temperature of the radiation-emitting surface of the sun. We can solve (20) for T:

$$T = \frac{2\pi\hbar c}{4.966 k_B \lambda_{max}} \tag{21}$$

I unnecessarily used Mathematica to solve for T, giving $T = 6036\,\mathrm{K}$, which seems to be around the number I get when searching around.

(d) Differences between real spectrum and blackbody

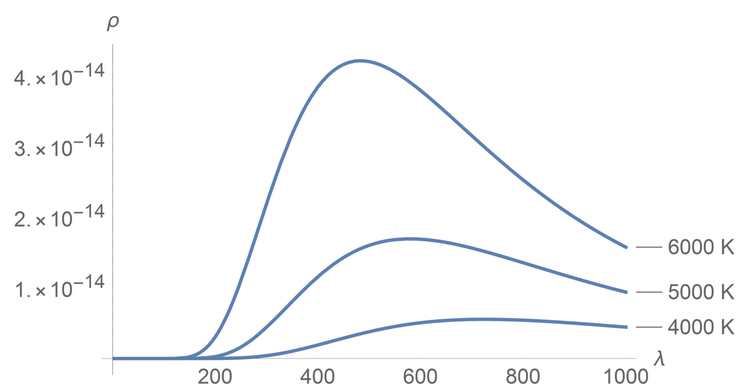

Figure 1: Spectra for 4000 K, 5000 K and 6000 K

The mention of the surface of the sun is important for the earlier part, as different layers of the sun are at different temperatures. Some brief searching suggests that the photosphere ranges from 4000 K to 6000 K. Figure 1 shows some spectra for this temperature range. The sum of these spectra (depending on the total power at each temperature for the overall scale) may probably look different than the spectrum from just one temperature.

Because of their historical importance, we also know that absorption lines are visible in the sun's spectrum. We'd expect these to show up as sharp dips in the spectrum at specific wavelengths, which would be very easily to differentiate from the blackbody spectrum.

Listing 1: Mathematica script

```
(* ::Package:: *)

```

```
BeginPackage["PS3Prob1Script`"]

CurrentDir = DirectoryName[FileNameJoin[{Directory[], $ScriptCommandLine[[1]]}]]
ImageDir = FileNameJoin[{CurrentDir, "images"}]
outFile = OpenWrite[FileNameJoin[{CurrentDir, "prob1ScriptOutput.txt"}]]

Print["All the stuff for problem 1"]

(* Part b *)
sols = NSolve[ x == 5(1 - E^(-x)), x]

Print[StringTemplate["Got solutions: `1`"][x /. sols]]
WriteString[outFile, StringTemplate["Got solutions for part b: `1`\n"][x /. sols]]

(* Part c *)
T[\[Lambda]_] := UnitSimplify[(2 * Pi * Quantity[1, "ReducedPlanckConstant"] * Quantity[1, "SpeedOfLight"]) / (4.966 * Quantity[1, "BoltzmannConstant"] * \[Lambda])]
Print[StringTemplate["Temperature: `1`"][T[ Quantity[480, "Nanometers"]]]]
WriteString[outFile, StringTemplate["Solar temperature for 480 nm: `1`\n"][T[ Quantity[480, "Nanometers"]]]]

(* Part d *)

rho[\[Lambda]_, T_] := (16 * Pi^2 * Quantity[1, "ReducedPlanckConstant"] * Quantity[1, "SpeedOfLight"]) / (\[Lambda]^5 (E^((2 * Pi * Quantity[1, "ReducedPlanckConstant"] * Quantity[1, "SpeedOfLight"])/( Quantity[1, "BoltzmannConstant"] * T * \[Lambda])) - 1))

Print["Plotting spectra..."]
Export[FileNameJoin[{ImageDir, "4000And6000Spectrum.jpg"}],
        Show[
                Plot[rho[Quantity[l, "Nanometers"], Quantity[4000, "Kelvins"]], {l, 1, 1000},  AxesLabel->{\[Lambda], \[Rho]}, PlotLabels->"4000 K"],
                Plot[rho[Quantity[l, "Nanometers"], Quantity[5000, "Kelvins"]], {l, 1, 1000},  AxesLabel->{\[Lambda], \[Rho]}, PlotLabels->"5000 K"],
                Plot[rho[Quantity[l, "Nanometers"], Quantity[6000, "Kelvins"]], {l, 1, 1000},  AxesLabel->{\[Lambda], \[Rho]}, PlotLabels->"6000 K"],
                PlotRange->All, PlotLabels->Automatic
        ],
         ImageResolution -> 1000
```

```
]


EndPackage[]
```

Listing 2: Mathematica output

```
Got solutions for part b: {0., 4.96511}
Solar temperature for 480 nm: 6035.95 kelvins
```

2 Langevin Function

We are for this problem interested in considering a system with N magnetic moments of magnitude μ, where the ith moment is oriented at some angle θ_i from the vertical. Our Hamiltonian has an external field H, but no coupling between moments:

$$\mathcal{H} = -H \sum_{n=1}^{N} \mu \cos\theta_n \tag{22}$$

I'm making a couple assumptions. We're not told that the moments are constrained to rotate within a particular plane, so I'm going to have each moment expressed with polar angle θ, (which assumes the external field is in the z-direction). We want to begin by finding the equilibrium magnetisation M.

(a) Finding the magnetisation

I think we can start by trying to minimise the free energy. We can use $A = -k_{\mathrm{B}}T \ln Q$. To find Q:

$$Q = \underbrace{\int \cdots \int}_{N} d\Omega_1 \cdots d\Omega_N \, e^{-\beta\mathcal{H}} \tag{23}$$

$$Q = \underbrace{\int \cdots \int}_{N} d\Omega_1 \cdots d\Omega_N \, e^{\beta H \sum_{n=1}^{N} \mu\cos\theta_n} \tag{24}$$

$$Q = \underbrace{\int \cdots \int}_{N} d\Omega_1 \cdots d\Omega_N \prod_{n=1}^{N} e^{\beta H \mu \cos\theta_n} \tag{25}$$

All the integrals are independent of one another, because of the lack of coupling. Additionally, each integral is the same. Thus,

$$Q = \left(\int d\Omega \, e^{\beta H \mu \cos\theta} \right)^N \tag{26}$$

$$= \left(\int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) \, e^{\beta H \mu \cos\theta} \right)^N \tag{27}$$

This becomes

$$Q = \left(2\pi \int_{-1}^{1} d(\cos\theta) \, e^{\beta H \mu \cos\theta} \right)^N \tag{28}$$

$$Q = \left(2\pi \frac{1}{\beta H \mu} \, e^{\beta H \mu \cos\theta} \Big|_{-1}^{1} \right)^N \tag{29}$$

$$Q = \left(2\pi \frac{1}{\beta H \mu} \left(e^{\beta H \mu} - e^{-\beta H \mu} \right) \right)^N \tag{30}$$

$$Q = \left(\frac{2\pi}{\beta H \mu} \right)^N \left(e^{\beta H \mu} - e^{-\beta H \mu} \right)^N \tag{31}$$

$$= \left(\frac{2\pi}{\beta H \mu} \right)^N (2 \sinh(\beta H \mu))^N \tag{32}$$

To find the average magnetisation, we want to compute

$$\langle M \rangle = \frac{1}{Q} \underbrace{\int \cdots \int}_{N} d\Omega_1 \cdots d\Omega_N \sum_{i=1}^{N} \mu \cos\theta_i e^{-\beta \mathcal{H}(\cos\theta)} \tag{33}$$

For each θ_i, we have $N-1$ copies of the integral we already did for Q with no $\cos\theta_i$ in the integrand, and so we can write this as

$$\langle M \rangle = \frac{1}{Q} \left(\frac{2\pi}{\beta H \mu} \right)^{N-1} (2 \sinh(\beta H \mu))^{N-1} \sum_{i=1}^{N} \int d\Omega_i \, \mu \cos\theta_i e^{-\beta \mathcal{H}_i} \tag{34}$$

There are N identical integrals being summed together, and we can cancel out the terms in Q. Here, $\mathcal{H}_i$ represents the contribution to the Hamiltonian of the ith atom. Every other part of the Hamiltonian has been integrated over.

$$\langle M \rangle = \frac{1}{\frac{2\pi}{\beta H \mu} 2 \sinh(\beta H \mu)} N \int d\Omega_i \, \mu \cos\theta_i e^{-\beta \mathcal{H}_i} \tag{35}$$

$$\frac{M}{N} = \frac{\int d\Omega_i \, \mu \cos\theta_i e^{-\beta \mathcal{H}_i}}{\frac{2\pi}{\beta H \mu} 2 \sinh(\beta H \mu)} \tag{36}$$

We've dropped the average brackets on M. Let's integrate:

$$\frac{M}{N} = \frac{\int d\phi\, d\theta \sin\theta \mu \cos\theta e^{H\beta\mu\cos\theta}}{\frac{2\pi}{\beta H\mu} 2\sinh(\beta H\mu)} \tag{37}$$

$$= 2\pi\mu \frac{\int_{-1}^{1} d(\cos\theta) \cos\theta e^{H\beta\mu\cos\theta}}{\frac{2\pi}{\beta H\mu} 2\sinh(\beta H\mu)} \tag{38}$$

$$= \frac{2\pi\mu}{H\mu} \frac{\frac{d}{d\beta} \int_{-1}^{1} d(\cos\theta)\, e^{H\beta\mu\cos\theta}}{\frac{2\pi}{\beta H\mu} 2\sinh(\beta H\mu)} \tag{39}$$

$$= \frac{2\pi\mu}{H\mu} \frac{\frac{d}{d\beta} \frac{1}{H\beta\mu} \left(e^{H\beta\mu} - e^{-H\beta\mu}\right)}{\frac{2\pi}{\beta H\mu} 2\sinh(\beta H\mu)} \tag{40}$$

$$= \frac{2\pi\beta H\mu}{H^2\mu} \frac{\frac{d}{d\beta} \frac{1}{\beta} \sinh(\beta H\mu)}{2\pi \sinh(\beta H\mu)} \tag{41}$$

$$= \frac{\beta}{H} \frac{\frac{-1}{\beta^2} \sinh(\beta H\mu) + \frac{1}{\beta} H\mu \cosh(\beta H\mu)}{\sinh(\beta H\mu)} \tag{42}$$

$$= \frac{1}{H} \frac{H\mu \cosh(\beta H\mu) - \frac{1}{\beta} \sinh(\beta H\mu)}{\sinh(\beta H\mu)} \tag{43}$$

$$= \frac{1}{H} \left(H\mu \coth(\beta H\mu) - \frac{1}{\beta} \right) \tag{44}$$

$$M = \mu N \left(\coth(\beta H\mu) - \frac{1}{\beta\mu H} \right) \tag{45}$$

This is what we wanted to show.

(b) Finding the susceptibility

We want to find $\chi = \frac{\partial M}{\partial H}$ for low temperatures. The Taylor series for coth is $\coth(x) \approx \frac{1}{x} + \frac{x}{3}$. Plugging this in, we find

$$M \approx \mu N \left(\frac{1}{\beta H\mu} + \frac{\beta H\mu}{3} - \frac{1}{\beta H\mu} \right) \tag{46}$$

$$M \approx \frac{\mu N \beta H\mu}{3} \tag{47}$$

$$M \approx \frac{\mu^2 N \beta H}{3} \tag{48}$$

This gives us $\chi \approx \frac{\mu^2 N\beta}{3}$.

(c) Finding the Curie's law coefficient)

Rewriting β, we get

$$\chi = \frac{\mu^2 N}{3k_\mathrm{B}T}, \tag{49}$$

which satisfies Curie's law for $C = \frac{\mu^2 N}{3k_\mathrm{B}}$

3 Molecules as Harmonic Oscillators

We're given a Hamiltonian

$$\mathcal{H} = \frac{1}{2m}\sum_{n=1}^{N}\left(p_n^2 + {p'}_n^2\right) + \frac{K}{2}\sum_{n=1}^{N}\left|r_n - {r'}_n\right|^2 \tag{50}$$

We want to first find the partition function:

$$Q = \underbrace{\int \cdots \int}_{4N} d^3\{p_i\}\, d^3\{{p'}_i\}\, d^3\{r_i\}\, d^3\{{r'}_i\}\, e^{-\beta\mathcal{H}} \tag{51}$$

This is N identical integrals, one for each particle:

$$Q = \left(\iiiint d^3p\, d^3p'\, d^3r\, d^3r'\, e^{-\beta\left(\frac{1}{2m}\left(p_n^2+{p'}_n^2\right)+\frac{K}{2}|r_n-{r'}_n|^2\right)}\right)^N \tag{52}$$

It separates:

$$Q = \left(\left(\int d^3p\, e^{-\frac{\beta}{2m}p^2}\right)^2 \int d^3r_i\, d^3{r'}_i\, e^{-\beta\frac{K}{2}|r_n-{r'}_n|^2}\right)^N \tag{53}$$

To evaluate this, let's start with the p integrals, going right away to spherical coordinates:

$$\int d^3p\, e^{-\frac{\beta}{2m}p^2} = 4\pi\int_0^\infty dp\, p^2 e^{-\frac{\beta}{2m}p^2} \tag{54}$$

$$= 4\pi(-2m)\frac{d}{d\beta}\int_0^\infty dp\, e^{-\frac{\beta}{2m}p^2} \tag{55}$$

This is a Gaussian integral we can do.

$$\int d^3p\, e^{-\frac{\beta}{2m}p^2} = -8m\pi\frac{d}{d\beta}\sqrt{\frac{m\pi}{2\beta}} \tag{56}$$

$$= 4m\pi\sqrt{\frac{m\pi}{2\beta^3}} \tag{57}$$

Plugging back into (53),

$$Q = \left(\left(4m\pi\sqrt{\frac{m\pi}{2\beta^3}}\right)^2 \int d^3r_i\, d^3r'_i\, e^{-\beta\frac{K}{2}|r_n - r'_n|^2}\right)^N \tag{58}$$

$$= \left(16m^2\pi^2\frac{m\pi}{2\beta^3}\int d^3r_i\, d^3r'_i\, e^{-\beta\frac{K}{2}|r_n - r'_n|^2}\right)^N \tag{59}$$

$$Q = \left(\frac{8m^3\pi^3}{\beta^3}\int d^3r_i\, d^3r'_i\, e^{-\beta\frac{K}{2}|r_n - r'_n|^2}\right)^N \tag{60}$$

I believe the standard trick for the r integrals is to define a $\mathbf{q} = \mathbf{r} - \mathbf{r}'$ and integrate over q:

$$\int d^3r_i\, d^3r'_i\, e^{-\beta\frac{K}{2}|r_n - r'_n|^2} = V\int d^3q\, e^{-\beta\frac{K}{2}q^2} \tag{61}$$

The factor of volume roughly accounts for translation invariance (because each q integral could take place with r and r' shifted by a constant vector, which must be accounted for). I'm not sure how valid that makes this result. If certain molecules could be displaced unrestrictedly far from the solid, I think other things would break. In any case, I'm adding a V. It makes the units work out too.

$$\int d^3r_i\, d^3r'_i\, e^{-\beta\frac{K}{2}|r_n - r'_n|^2} = V\int d^3q\, e^{-\beta\frac{K}{2}q^2} \tag{62}$$

Spherical coordinates:

$$\int d^3r_i\, d^3r'_i\, e^{-\beta\frac{K}{2}|r_n - r'_n|^2} = 4\pi V\int_0^\infty dq\, q^2 e^{-\beta\frac{K}{2}q^2} \tag{63}$$

$$= 4\pi\left(-\frac{2}{K}\right)V\frac{d}{d\beta}\int_0^\infty dq\, e^{-\beta\frac{K}{2}q^2} \tag{64}$$

$$= -\frac{8\pi V}{K}\frac{d}{d\beta}\sqrt{\frac{\pi}{2\beta K}} \tag{65}$$

$$= \frac{4\pi V}{K}\sqrt{\frac{\pi}{2\beta^3 K}} \tag{66}$$

$$\tag{67}$$

Plugging this into (60), we get

$$Q = \left(\frac{8m^3\pi^3}{\beta^3}\frac{4\pi V}{K}\sqrt{\frac{\pi}{2\beta^3 K}}\right)^N \tag{68}$$

We can find the Helmholtz free energy from that:

$$A = -\frac{1}{\beta}\ln Q \tag{69}$$

$$= -\frac{N}{\beta}\ln\left(\frac{8m^3\pi^3}{\beta^3}\frac{4\pi V}{K}\sqrt{\frac{\pi}{2\beta^3 K}}\right) \tag{70}$$

(b) Specific heat

The specific heat is $C_V = -T\frac{\partial^2 A}{\partial T^2}$. Let's write A in terms of T:

$$A = -Nk_\mathrm{B}T\ln\left(8m^3\pi^3k_\mathrm{B}^3T^3\frac{4\pi V}{K}\sqrt{\frac{\pi k_\mathrm{B}^3T^3}{2K}}\right) \tag{71}$$

$$= -Nk_\mathrm{B}T\ln\left(8m^3\pi^3k_\mathrm{B}^3\frac{4\pi V}{K}\sqrt{\frac{\pi k_\mathrm{B}^3}{2K}}T^3T^{3/2}\right) \tag{72}$$

$$= -Nk_\mathrm{B}T\ln\left(\xi T^{9/2}\right) \tag{73}$$

Differentiating twice:

$$\frac{\partial A}{\partial T} = -Nk_\mathrm{B}\ln\left(\xi T^{9/2}\right) - Nk_\mathrm{B}T\frac{1}{\xi T^{9/2}}\frac{9}{2}T^{7/2} \tag{74}$$

$$\frac{\partial A}{\partial T} = -Nk_\mathrm{B}\ln\left(\xi T^{9/2}\right) - Nk_\mathrm{B}\frac{1}{\xi}\xi\frac{9}{2} \tag{75}$$

and finally

$$C_V = -T\frac{\partial^2 A}{\partial T^2} \tag{76}$$

$$= -T\frac{\partial}{\partial T}\left(-Nk_\mathrm{B}\ln\left(\xi T^{9/2}\right) - Nk_\mathrm{B}\frac{1}{\xi}\xi\frac{9}{2}\right) \tag{77}$$

$$= T\frac{\partial}{\partial T}Nk_\mathrm{B}\ln\left(\xi T^{9/2}\right) \tag{78}$$

$$= Nk_\mathrm{B}T\frac{1}{\xi T^{9/2}}\xi\frac{9}{2}T^{7/2} \tag{79}$$

$$C_V = \frac{9}{2}Nk_\mathrm{B} \tag{80}$$

(c) Mean square separation

We want to find the ensemble average for q^2, as defined earlier. We already established that the position and momentum integrals separate, so they'll cancel, and we only need to do the integral over q:

$$\langle q^2 \rangle = \frac{4\pi V \int_0^\infty dq\, q^2 q^2 e^{-\beta \frac{K}{2} q^2}}{4\pi V \int_0^\infty dq\, q^2 e^{-\beta \frac{K}{2} q^2}} \tag{81}$$

$$= \frac{\frac{d^2}{d\beta^2} \frac{4}{K^2} \int_0^\infty dq\, e^{-\beta \frac{K}{2} q^2}}{\frac{d}{d\beta} \frac{-2}{K} \int_0^\infty dq\, e^{-\beta \frac{K}{2} q^2}} \tag{82}$$

$$= -\frac{2}{K} \frac{\frac{d^2}{d\beta^2} \sqrt{\frac{\pi}{2\beta k}}}{\frac{d}{d\beta} \sqrt{\frac{\pi}{2\beta K}}} \tag{83}$$

$$= -\frac{2}{K} \frac{\frac{d^2}{d\beta^2} \sqrt{\frac{1}{\beta}}}{\frac{d}{d\beta} \sqrt{\frac{1}{\beta}}} \tag{84}$$

$$= -\frac{2}{K} \frac{-\frac{d}{d\beta} \frac{1}{2} \beta^{-3/2}}{-\frac{1}{2} \beta^{-3/2}} \tag{85}$$

$$= -\frac{2}{K} \frac{\frac{d}{d\beta} \beta^{-3/2}}{\beta^{-3/2}} \tag{86}$$

$$= -\frac{2}{K} \frac{-\frac{3}{2} \beta^{-5/2}}{\beta^{-3/2}} \tag{87}$$

$$= \frac{3}{\beta K} \tag{88}$$

This gives us our mean square separation. As we'd expect, for higher temperatures, the molecules are further separated.

4 Phase transition of Ideal Bose System

I think my understanding of this problem was a bit lacking. The lecture notes mention that we should, in order to find C_V above T_c, solve the number equation for $\mu(T)$. The number equation, before any assumptions, looks like

$$n(\mu, T) = \frac{1}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \int_0^\infty \frac{\epsilon^{1/2}\, d\epsilon}{e^{\beta(\epsilon - \mu)} - 1} \tag{89}$$

We also have, I think, that for $T > T_c$, no particles in the ground state. Why is this? I think this just comes out of the definition of T_c as the point where

$\mu = 0$: above T_c, $\mu < 0$. We had an expression for n at T_c:

$$n(0, T_c) = \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\epsilon^{1/2}\,d\epsilon}{e^{\beta(\epsilon)}-1} \tag{90}$$

$$= \frac{1}{4\pi^2}\left(\frac{2m}{\beta\hbar^2}\right)^{3/2}\zeta(\frac{3}{2})\Gamma(\frac{3}{2}) \tag{91}$$

I think that ultimately the right approach to deriving the values for C_V for $T > T_c$ will be to set these expressions equal, and solve for μ. Then, the integrals can be done numerically, which is where I believe the somewhat odd number 3.66 comes from.

5 1-D Ising Model Long-Range interactions

For this problem, we want to evaluate the Peierls argument for long-range interactions modelled by the Hamiltonian:

$$\mathcal{H} = -J\sum_{i\neq j}^{N}\frac{s_i s_j}{|i-j|^a} \tag{92}$$

In addition, we're given that $s \in \{-1, 1\}$, and $a > 0$. We want to show that the Peierls argument fails for $a < 2$, meaning that with a in that range, there is indeed a phase transition.

Like with the original argument, we can find the free energy A for $m = 0$ and $m = 1$. We note that the entropies are unchanged:

$$S_{m=0} < k_{\mathrm{B}}\log\frac{N}{2} \tag{93}$$

$$S_{m=1} = 0 \tag{94}$$

We need to find the energies. For $m = 1$:

$$U = \sum_{i\neq j}^{N}\frac{s_i s_j}{|i-j|^a} \tag{95}$$

$$= \sum_{i\neq j}^{N}\frac{1}{|i-j|^a} \tag{96}$$

$$\tag{97}$$

We can approximate this sum with an integral:

$$U \approx \frac{N^2}{L^2} \int_0^L dx \int_0^L dy \, \frac{1}{|x-y|^a} \tag{98}$$

We'll end up with nasty divergences if we don't properly attend to the condition in the sum that $i \neq j$. We can go one further, and notice that $i - j$ is never less than 1 for any allowed terms in the sum. We write

$$U \approx \frac{N^2}{L^2} \int_0^L dx \left(\int_0^{x-1} dy \, \frac{1}{(x-y)^a} + \int_{x+1}^L dy \, \frac{1}{(y-x)^a} \right) \tag{99}$$

We'll end up with some weird boundary terms that are possibly wrong, but let's forge a path forward hoping that the assumption that N is large will fix any problems.

$$U = \frac{N^2}{L^2} \int_0^L dx \left(-\frac{(x-y)^{-a+1}}{-a+1} \bigg|_0^{x-1} + \frac{(y-x)^{-a+1}}{-a+1} \bigg|_{x+1}^L \right) \tag{100}$$

$$U = \frac{N^2}{L^2} \int_0^L dx \left(-\frac{(1)^{-a+1} - (x)^{-a+1}}{-a+1} + \frac{(L-x)^{-a+1} - (1)^{-a+1}}{-a+1} \right) \tag{101}$$

$$U = \frac{N^2}{L^2} \int_0^L dx \, \frac{(L-x)^{-a+1} + x^{-a+1} - 2}{-a+1} \tag{102}$$

$$U = \frac{N^2}{L^2(-a+1)} \int_0^L dx \, (L-x)^{-a+1} + x^{-a+1} - 2 \tag{103}$$

$$U = \frac{N^2}{L^2(-a+1)} \left(\left(-\frac{(L-x)^{-a+2}}{-a+2} \right) + \frac{x^{-a+2}}{-a+2} - 2L \right) \bigg|_{x=0}^L \tag{104}$$

$$U = \frac{N^2}{L^2(-a+1)} \left(\frac{(L)^{-a+2}}{-a+2} + \frac{L^{-a+2}}{-a+2} - 2L \right) \bigg|_{x=0}^L \tag{105}$$

$$U = \frac{N^2}{L^2(-a+1)} \left(\frac{L^{-a+2}}{-a+2} + \frac{L^{-a+2}}{-a+2} - 2L \right) \tag{106}$$

$$U = \frac{2N^2}{L^2(1-a)} \left(\frac{L}{2-a} - \frac{2L - aL}{2-a} \right) \tag{107}$$

$$U = \frac{2N^2}{L^2(1-a)} \left(\frac{L}{2-a} - \frac{2L - aL}{2-a} \right) \tag{108}$$

$$U = \frac{2N^2}{L^2(1-a)} \left(\frac{aL - L}{2-a} \right) \tag{109}$$

$$U = \frac{2N^2}{L} \frac{1}{a-2} \tag{110}$$

Now we need to find U for $m = 0$. Let's assume a domain wall erected halfway, so that $s(x) = 1$ for $x > \frac{L}{2}$ and $s(x) = -1$ for $x < \frac{L}{2}$. We note that there will be terms for $x, y < \frac{L}{2}$ and terms for $x, y > \frac{L}{2}$ These terms don't matter, because they'll be present in both the $m = 0$ and $m = 1$ integrals. We need only integrate for $x > \frac{L}{2}$ and $y < \frac{L}{2}$, and vice versa (and we'll add in a buffer of $\frac{1}{2}$ on each side, to maintain our inequality back from the sum).

$$\Delta U \approx \frac{N^2}{L^2} \int_{\frac{L}{2}+\frac{1}{2}}^{L} dx \int_{0}^{\frac{L}{2}-\frac{1}{2}} dy \, \frac{-1}{(x-y)^a} \tag{111}$$

$$= \frac{N^2}{L^2} \int_{\frac{L}{2}+\frac{1}{2}}^{L} dx \left(\frac{(x-y)^{-a+1}}{-a+1} \right) \Bigg|_{0}^{\frac{L}{2}-\frac{1}{2}} \tag{112}$$

$$= \frac{N^2}{L^2} \int_{\frac{L}{2}+\frac{1}{2}}^{L} dx \left(\frac{(x - \frac{L+1}{2})^{-a+1} - x^{-a+1}}{-a+1} \right) \tag{113}$$

We note at this point that in the end we're going to end up with something all over $-a+2$, with a form similar to the $U(m = 1)$. which means that the sign of ΔU (and ΔA) will change for $a < 2$. (And again, the $U(m = 1$ value itself didn't matter so much, because only the difference terms like this one are relevant). This means that the domain wall will go from being energetically disallowed to being energetically favourable. The other term, for $y > x$, will be the same. The dependence on N means that for large enough N, this will dominate the effect of the change in entropy, which was important for the Peierls argument.

6 Spin-1 Partition functions

We're told for this problem that we have a 1-D array of N spins $s_1, \ldots, s_N$, where $s_i \in \{-1, 0, 1\}$. We're also, importantly, given periodic boundary conditions $s_{N+1} = s_1$. Our Hamiltonian has no external field:

$$\mathcal{H} = -J \sum_{i=1}^{N} s_i s_{i+1} \tag{114}$$

We're asked to effectively find the transfer matrix, and show that the Helmholtz free energy A satisfies

$$A = -N k_{\mathrm{B}} T \log \lambda_+, \tag{115}$$

where λ_+ is the largest eigenvalue of the transfer matrix $\mathcal{T}$.

(a) Helmholtz free energy

We want to start by finding the partition function Q, as we know that $A = -k_\mathrm{B}T \log Q$. For Q, summing over all values of each spin:

$$
\begin{aligned}
Q &= \sum_{s_1} \cdots \sum_{s_N} e^{-\beta\mathcal{H}} && (116)\\
&= \sum_{s_1} \cdots \sum_{s_N} e^{-\beta\left(-J\sum_{i=1}^{N} s_i s_{i+1}\right)} && (117)\\
&= \sum_{s_1} \cdots \sum_{s_N} e^{\sum_{i=1}^{N} \beta J s_i s_{i+1}} && (118)\\
&= \sum_{s_1} \cdots \sum_{s_N} \prod_{i=1}^{N} e^{\beta J s_i s_{i+1}} && (119)
\end{aligned}
$$

This is the point where we can define a matrix $\mathcal{T}$ such that

$$\mathcal{T}_{ab} = e^{\beta J ab}, \tag{120}$$

where the indices run over possible spin values. Substituting this in for Q leads to:

$$
\begin{aligned}
Q &= \sum_{s_1} \cdots \sum_{s_N} \prod_{i=1}^{N} \mathcal{T}_{s_i s_{i+1}} && (121)\\
&= \sum_{s_1} \cdots \sum_{s_N} \mathcal{T}_{s_1 s_2} \mathcal{T}_{s_2 s_3} \cdots \mathcal{T}_{s_{N-1} s_N} \mathcal{T}_{s_N s_1} && (122)
\end{aligned}
$$

We recognise this sum over repeated indices as basic matrix multiplication:

$$Q = \sum_{s_1} \mathcal{T}^{N}_{s_1 s_1} \tag{123}$$

It's important here that we had a periodic boundary condition, or we'd have some extra work to do for the first and last spin and the next step wouldn't be possible. We have only the s_1 index left to sum over, and we recognise here the trace of $\mathcal{T}^N$:

$$Q = \operatorname{Tr} \mathcal{T}^N \tag{124}$$

Why's this good? We know that $\operatorname{Tr} \mathcal{T} = \sum \lambda_i$, where the λ are the eigenvalues of $\mathcal{T}$, and we also know that $\operatorname{Tr} \mathcal{T}^N = \sum \lambda_i^N$. As with the examples of the transfer matrix method, we can make the assumption that the three eigenvalues for this Hamiltonian's transfer matrix have a T- and J- independent order, and name them λ_+, λ_0 and λ_- (where $\lambda_+ > \lambda_0 > \lambda_-$). Thus we write

$$Q = \operatorname{Tr} \mathcal{T}^N \tag{125}$$

$$= \lambda_+^N + \lambda_0^N + \lambda_-^N \tag{126}$$

$$= \lambda_+^N \left(1 + \left(\frac{\lambda_0}{\lambda_+}\right)^N + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right) \tag{127}$$

For sufficiently large N, the quantity in parentheses goes to 1 (because each parenthesised quantity therein contained goes to 0), so

$$Q = \lambda_+^N \tag{128}$$

The Helmholtz free energy is trivial:

$$A = -k_{\mathrm{B}} T \log Q \tag{129}$$

$$A = -k_{\mathrm{B}} T \log \left(\lambda_+^N\right) \tag{130}$$

$$A = -N k_{\mathrm{B}} T \log \lambda_+ \tag{131}$$

This is what we wanted to show for this part.

(b) The components of the transfer matrix

We can go back to (120):, $\mathcal{T}_{ab} = e^{\beta J ab}$, and recall that a and b ran over the values for the spins, $\{-1, 0, 1\}$. If either a or b is 0, $\mathcal{T}_{ab} = 1$, and the other components are only slightly more complicated:

$$\begin{array}{cc} & \begin{array}{ccc} s=1 & s=0 & s=-1 \end{array} \\ \mathcal{T} = & \begin{pmatrix} e^{\beta J} & 1 & e^{-\beta J} \\ 1 & 1 & 1 \\ e^{-\beta J} & 1 & e^{\beta J} \end{pmatrix} \begin{array}{c} s=1 \\ s=0 \\ s=-1 \end{array} \end{array} \tag{132}$$

(c) Equation for $\boldsymbol{\lambda_+}$

We want to find the eigenvalues of $\mathcal{T}$. Let's solve our standard eigenvalue equation:

$$0 = \det(\mathcal{T} - \lambda I) \tag{133}$$

$$= \det \begin{pmatrix} e^{\beta J} - \lambda & 1 & e^{-\beta J} \\ 1 & 1 - \lambda & 1 \\ e^{-\beta J} & 1 & e^{\beta J} - \lambda \end{pmatrix} \tag{134}$$

To spare my fingers the extra typing, we'll define $a = e^{\beta J}$ and $b = e^{-\beta J}$.

$$
\begin{aligned}
0 &= \det \begin{pmatrix} a-\lambda & 1 & b \\ 1 & 1-\lambda & 1 \\ b & 1 & a-\lambda \end{pmatrix} && (135) \\
&= (a-\lambda)\left((1-\lambda)(a-\lambda)-1\right) - \left((a-\lambda)-b\right) + b\left(1-(1-\lambda)\,b\right) && (136) \\
&= (a-\lambda)\left(a+\lambda^2-\lambda(1+a)-1\right) - a + \lambda + b + b\left(1-b+b\lambda\right) && (137) \\
&= (a-\lambda)\left(\lambda^2-\lambda(1+a)+a-1\right) - a + \lambda + b + b - b^2 + b^2\lambda && (138) \\
&= (a-\lambda)\left(\lambda^2-\lambda(1+a)+a-1\right) + \lambda(1+b^2) - a + 2b - b^2 && (139) \\
&= a\lambda^2 - \lambda(a+a^2) + a^2 - a - \lambda^3 + \lambda^2(1+a) - \lambda a + \lambda \\
&\qquad + \lambda(1+b^2) - a + 2b - b^2 && (140) \\
&= -\lambda^3 + \lambda^2\left(2a+1\right) + \lambda\left(-a-a^2-a+1+1+b^2\right) \\
&\qquad + a^2 - a - a + 2b - b^2 && (141) \\
&= -\lambda^3 + \lambda^2\left(2a+1\right) + \lambda\left(b^2-a^2-2a+2\right) + a^2 - b^2 - 2a + 2b && (142)
\end{aligned}
$$

This cubic equation seems rather ugly, but not unexpectedly so. I'm sure this can be simplified further by plugging in for a and b and writing some hyperbolic trig functions, but I don't think that helps, particularly given that we're not going to be solving this. It's exactly solvable though, and that's quite cool.