Assignment 5
Physics/ECE 176

Made available: Saturday, February 12, 2011
Due: Friday, February 18, 2011, at my office by 3pm.

Problem 1: Surface areas of hyperspheres

Please read Appendix B.2 of Schroeder and do Schroeder problem B.8 below before doing Problem 1 so that you know the definition of the Gamma function $\Gamma(x)$ and its values for some representative arguments.

The surface area $A_d(r)$ of a hypersphere of radius r in d spatial dimensions is given by

$$A_d(r) = \frac{2\,\pi^{d/2}}{\Gamma\left(\frac{d}{2}\right)} r^{d-1}. \tag{1}$$

1. Use Eq. (1) to calculate a symbolic expression (in terms of π times a rational prefactor) and its numerical value of the surface area $A_d(1)$ of a unit hypersphere for $d = 4$ and $d = 5$. For example, for $d = 2$, the symbolic value is 2π and its numerical value is ≈ 6.3 to two digits. In Mathematica, numerical values of symbolic expressions can be obtained using the `N` function, for example `N[2 Pi] = 6.283` where `Pi` is Mathematica's symbol for π (and `E` is Mathematica's symbol for e).

2. The values for $A_d(1)$ for $d = 2, 3, 4, 5$ suggest incorrectly that $A_d(1)$ is an increasing function of d. Use Stirling's formula in the form $\Gamma(x+1) \approx \sqrt{2\pi x}\,(x/e)^x$ to show that, for large d, $A_d(1) \propto d^{-d/2} = e^{-[\ln(d)/2]d}$ actually decreases rapidly (a bit faster than exponentially rapidly) with increasing d.

3. In what spatial dimension does the numerical value of the surface area of a unit hypersphere reach a maximum value? Hint: use `Plot` to get a visual answer, there is no need to do any calculus here. Mathematica knows how to evaluate the Gamma function for all possible arguments (positive, negative, complex), just invoke `Gamma[x]`.

Problem 2: Heat Capacity $C_V(T)$ of an Einstein Solid

This problem is one of the most important in the course so please take the time to not just do it but think carefully about what steps you are taking and why. This problem shows you how to go from a mathematical expression for the multiplicity $\Omega(N, U)$ of an Einstein solid with N oscillators and energy $U = (hf)q$ all the way to the heat capacity $C_V(T)$ as a function of temperature, and how to use low-order Taylor series approximations to get some intuition about the low-temperature and high-temperature parts of the mathematical curve.

1. Use Stirling's formula to show that the multiplicity $\Omega(N, q)$ of an Einstein solid for any large values of N and q is approximately given by

$$\Omega(N, q) = \left(\frac{q+N}{q}\right)^q \left(\frac{q+N}{N}\right)^N. \tag{2}$$

   In your derivation, indicate clearly where you dropped certain multiplicative factors since they were just "large numbers" multiplying a "very large" number.

2. Use Eq. (2) to calculate the temperature $T = T(U)$ as a function of its thermal energy U.

Hints: $U = \epsilon q$, where $\epsilon = hf$ is the energy spacing between quantum harmonic oscillator levels, so in Eq. (2) you can express q in terms of U and ϵ. The entropy is give by $S = k \ln \Omega$ and you can use the chain rule to simplify your calculation of temperature:

$$\frac{1}{T} = \frac{\partial S}{\partial U} = \frac{\partial S}{\partial q}\frac{\partial q}{\partial U} = \frac{1}{\epsilon}\frac{\partial S}{\partial q}. \tag{3}$$

3. Invert your expression for $T = T(U)$ to find $U = U(T)$, the thermal energy as a function of T. Then differentiate to get the heat capacity $C_V(T) = \partial U/\partial T$. Your answer should be:

$$C_V = Nk\left(\frac{\epsilon}{kT}\right)^2 \frac{e^{\epsilon/(kT)}}{\left(e^{\epsilon/(kT)} - 1\right)^2}. \tag{4}$$

4. Use Mathematica to plot Eq. (4) and include your plot with your homework assignment.

   Since Nk is a natural unit for heat capacity and the temperature T enters Eq. (4) only through the combination of symbols $x = kT/\epsilon \propto T$, plot Eq. (4) by plotting $C_V/(Nk)$ versus x; this avoids having to know values for N or ϵ. (A range $0 \le x \le 2$ should be fine.) Since $x \propto T$, you can think of the horizontal axis as still being the temperature axis. Note that $x = 1$ on the horizontal axis when $kT = \epsilon$, i.e., the thermal energy kT is comparable to the harmonic oscillator energy spacing.

5. Using the fact that

$$e^y \approx 1 + y + \frac{1}{2}y^2 + \frac{1}{6}y^3, \tag{5}$$

   for y sufficiently small (close to zero), **show that the high-temperature part of the heat capacity curve Eq. (4) behaves approximately like**

$$\frac{C_V(T)}{Nk} \approx 1 - \frac{1}{12}\left(\frac{\epsilon}{kT}\right)^2 + \ldots, \tag{6}$$

   for $kT \gg \epsilon$. The dots $\ldots$ in Eq. (6) represent higher powers of $\epsilon/(kT)$ that can be neglected as tiny for T sufficiently large.

   To get some intuition about when the high-temperature approximation Eq. (6) is qualitatively useful, **use Mathematica to plot Eq. (6) and Eq. (4) on the same plot and include that plot with your homework. Indicate with arrows and labels on your plot the range of x over which Eq. (6) is a useful approximation.**

   Note how Eq. (6) implies that the high-temperature limit $T \to \infty$ of C_V is none other than Nk, the equipartition value predicted for N oscillators, each with $f = 2$ degrees of freedom, i.e., Eq. (4) is consistent with the equipartition theorem for high temperatures.

   Some hints: the expression $y = 1/x = \epsilon/(kT)$ is small when T is large so first rewrite Eq. (4) in terms of the small quantity y:

$$\frac{C_V}{Nk} = \frac{y^2 e^y}{\left(e^y - 1\right)^2}. \tag{7}$$

   Now use Eq. (5) to second-order in the numerator and to third-order in the denominator and use your accumulated Taylor-series skills to obtain Eq. (6).

6. Now obtain a leading-order low-temperature approximation to the expression Eq. (4) by showing that

$$\frac{C_V}{Nk} \approx \left(\frac{\epsilon}{kT}\right)^2 e^{-\epsilon/(kT)}, \tag{8}$$

   when $kT \ll \epsilon$. Hint: As $T \to 0$, $y = \epsilon/(kT)$ becomes large and so $e^y \gg 1$.

Create a final Mathematical plot that combines your low-temperature approximation Eq. (8), your high-temperature approximation Eq. (6), and the full curve Eq. (4) on one plot and include that plot with your homework.

Describe over what range of x the low-temperature expression Eq. (8) qualitatively agree with Eq. (4). If you knew just the low- and high-temperature behaviors, would you be able to deduce the entire form of $C_V(T)$?

A comment: in case you are wondering, you can't simplify Eq. (8) further by trying to approximate $\exp(-\epsilon/(kT))$ by a truncated Taylor series around $T = 0$ because a function of the form $e^{-c/T}$ for c a positive constant is one of the rare functions that has infinitely many derivatives at $T = 0$ (as you should verify) but all the derivatives are zero (as you should also verify) and so the function does not have a Taylor series about $T = 0$. This situation arises frequently in thermal physics.

7. The expression Eq. (4) can be used to understand the vibrational motions of diatomic molecules. Looking only at the vibrational contribution to the heat capacity graph for H_2 in Fig. 1.13 on page 30, estimate the value of ϵ (this is the uniform spacing between energy levels of the quantum harmonic oscillator) for the vibrational motion of a H_2 molecule and compare your value with the experimental value of ΔE, which is 0.5 eV to one digit.

   Hint: One way to compare the theoretical curve Eq. (4) with the experimental data is to look for some representative feature that can be compared independently of physical units. For example, from your plot of Eq. (4), observe that the curve reaches half its maximum value when $x = \epsilon/(kT) \approx 1/3$.

Problem 3: Schroeder Problems

1. Problem B.7 on page 388. Hint: integration by parts.

2. Problem B.8 on page 388. Hint: In the expression for $\Gamma(1/2)$:

$$\Gamma\left(\frac{1}{2}\right) = \int_0^\infty x^{-1/2} e^{-x}\, dx, \tag{9}$$

   change the integration variable to $y = x^{1/2}$ and use Eq. (B.6) on page 386. (You need to memorize the value of the Gaussian integral Eq. (B.6) which is used often in physics, engineering, and mathematics.)

3. Problem 2.21 on page 66. In addition, please also answer the sentences in bold below as part of this problem.

   Note that this problem basically involves executing the Mathematica command

```
Manipulate[
  Plot[
    ( 4. z (1 - z) )^(10^a) ,
    { z, 0, 1 } ,
    PlotRange -> { 0, 1 }  (* make vertical axis range [0,1] *)
  ] ,
  { a, 0, 4 }               (* the Manipulate parameter *)
]
```

   Please explain briefly what this code is doing, e.g. what is being plotted as the parameter a varies from 0 to 4. Also discuss briefly what you learn from executing this code.

   Note that for larger powers of N, the plots show artifacts, e.g. the peak at $z = 1/2$ doesn't reach all the way up to 1 which mathematically it must since the maximum value of the function $4z(1-z)$ is 1, which is unchanged no matter what power N the function is raised to. When using any visualization software like Mathematica or Matlab, you should always be wary and you should think of ways to determine whether your plot makes sense or not.

These artifacts are consequences of Mathematica's heuristic plotting algorithm, which unfortunately is not discussed anywhere, presumably because the algorithm is proprietary. The `Plot` algorithm first samples the function to be plotted with a modest number of equally spaced points, then evaluates the function at some extra points based on the mathematical structure of the crude plot. The problem here is that the function $f(z)^N$ is becoming so narrow with increasing N that the default number of sampling points that `Plot` starts with is too few to determine a reasonable structure of the curve.

You can override Mathematica's heuristic algorithm by telling `Plot` explicitly how many initial sampling points to use via the `PlotPoints` option. Thus re-execute the above Mathematica code (you don't have to include the second plot in your homework nor discuss it) with this option

```
PlotPoints -> 200     (* use many more initial sampling points *)
```

added to the `Plot` command. You should verify that the plots now have a correct peak for all powers. Note that you don't want to go overboard with the option `PlotPoints` since, on a computer screen with perhaps 100 pixels per inch, you can't plot more than about 1,000 points on a screen and actually see the points.

Even though the peak is now correct, discuss briefly whether the width of the curve $f(z)^N$ for large N is also correct, by using your analytical knowledge of what the width should be according to the Gaussian that approximates this curve. (The discussion of Figure 2.7 in Schroeder on pages 65-66 may be helpful here.)

It is also insightful to use Mathematica to compare the function $[f(z)]^N$ for $f(z) = 4z(1-z)$ with the Gaussian that it presumably asymptotes to for large N. According to our discussion in class about how a high power of a function $f(z)$ look like a Gaussian near its global maximum $z_{\max}$ with value $f_{\max}$, the Gaussian approximating $[4z(1-z)]^N$ for large N should be:

$$f(z)^N \approx f_{\max}^N \exp\left[-N\frac{|f''(z_{\max})|}{2f_{\max}}(z-z_{\max})^2\right] \tag{10}$$

$$= \exp\left[-4N\left(z-\frac{1}{2}\right)^2\right], \tag{11}$$

since here $f_{\max} = 1$ and $|f''(z_{\max})| = 8$.

Thus also execute the Mathematica code:

```
Manipulate[
  Plot[
    {
      ( 4. z (1 - z) )^(10^a),
      Exp[ - 4 10^a (z - 1/2)^2 ]  (* compare with Gaussian *)
    } ,
    { z, 0, 1 },
    PlotRange -> { 0, 1 } ,  (* make vertical axis range [0,1] *)
    PlotPoints -> 200
  ] ,
  { a, 0, 4 }  (* the Manipulate parameter *)
]
```

and summarize what you learn: how large does a power N have to become for a Gaussian to describe $f(z)^N$ well?

4. Problem 2.23 on page 67. Note: use Stirling's formula to answer part (a). Your answer should be

$$\Omega_{\rm max} = \left(\frac{2}{\pi N}\right)^{1/2} 2^N . \tag{12}$$

5. Problem 2.24 on page 67.

   Some comments:

   (a) You have solved part (a) already while answering Problem 2.23(a) so don't do this a second time.

   (b) Part (b) will perhaps be the most challenging part of this assignment algebraically so let me give you some suggestions to help you on your way. Using Stirling's approximation, show as a first step that the multiplicity $\Omega(N_\uparrow)$ of a two-state paramagnet consisting of N magnetic dipoles can, for large values of N, $N_\uparrow$, and $N_\downarrow$ can be approximated as:

$$\Omega = \frac{N!}{N_\uparrow! N_\downarrow!} \approx \left(\frac{N}{2\pi N_\uparrow N_\downarrow}\right)^{1/2} \frac{N^N}{N_\uparrow^{N_\uparrow} N_\downarrow^{N_\downarrow}}, \tag{13}$$

   where the number $N_\uparrow$ of up spins and the number $N_\downarrow$ of down spins satisfy

$$N_\uparrow + N_\downarrow = N. \tag{14}$$

   Because the denominator $N_\uparrow^{N_\uparrow} N_\downarrow^{N_\downarrow}$ has big numbers raised to different exponents, Eq. (13) can not be written in the form $f(N_\uparrow)^N$ so we cannot use Eq. (10), that high powers of a function with a single global maximum looks like a Gaussian near the global maximum. Instead, you can use the more direct argument of Schroeder on page 65. We know that the maximum multiplicity will occur for $N_\uparrow = N_\downarrow = N/2$ and we can anticipate (and verify later) that the multiplicity will be sharply peaked about the maximum value. So we can write

$$N_\uparrow = \frac{N}{2} + x, \qquad N_\downarrow = \frac{N}{2} - x, \tag{15}$$

   where the variable x expresses how far we are from the position $N/2$ of the maximum. If the peak near the maximum is extremely narrow, then we only have to consider Eq. (13) near its maximum, i.e. we can assume that the variable x in Eq. (15) is small:

$$x \ll \frac{N}{2}. \tag{16}$$

   Now follow the ideas of page 65 of Schroeder in three steps: eliminate $N_\uparrow$ and $N_\downarrow$ everywhere in terms of $N/2 \pm x$; take the log of the multiplicity; and simplify several expressions of the form $\ln(a+\epsilon) \approx \ln(a) + \epsilon/a$ where $\epsilon/a \ll 1$. When the dust clears, you should obtain the answer

$$\Omega \approx \left(\frac{2}{\pi N}\right)^{1/2} 2^N \, e^{-(2/N)x^2}. \tag{17}$$

   (The 2 in the argument $-(2/N)x^2$ of the exponent in Eq. (17) is *not* a mistake.) Note how this result reduces to your answer in (a) for $x = 0$.

6. Problem 2.26 on page 72. Then use $S = k \ln \Omega$ and Stirling's formula to derive the two-dimensional version of the Sackur-Tetrode equation for the entropy $S(U, A, N)$ of N atoms on a two-dimensional surface of area A:

$$S = Nk\left(2 + \ln\left[\frac{A}{N}\left(\frac{2\pi m}{h^2}\frac{U}{N}\right)\right]\right). \tag{18}$$

Problem 4: Time to Finish This Homework Assignment

Please tell me the approximate time in hours that it took you to complete this homework assignment.