Assignment 7
Physics/ECE 176

Made available: Saturday, March 26, 2011
Due: by the beginning of class, Thursday, April 1, 2011.

Note: in this assignment, the non-Schroeder problems come after the Schroeder problems. Also, for this assignment, you can take the gloves off and use Mathematica in any way that helps you to get the answers more quickly.

Problem 1: Schroeder Problems

1. **Problems B.2 and B.3** on page 386 of Schroeder.

   Also show by an appropriate change of variables that one can evaluate arbitrary moments of the Gaussian function via the Gamma function:

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

   and verify that Eq. (1) is correct by using your results for Problems B.2 and B.3 for $\alpha = 1$, 2, 3, and 4. Also verify that Eq. (1) is correct for $\alpha = 1/2$ by using the Mathematica command `NIntegrate` to evaluate both sides of Eq. (1). By appropriate experiments, determine how many significant digits `NIntegrate` provides for this case.

   Note: you can learn about the `NIntegrate` command by clicking on the `Help/Documentation Center` menu option in a Mathematica notebook, then type "NIntegrate" in the SEARCH box.

2. **Problem 6.22** on page 234 of Schroeder but skip part (a).

   For part (c), you can calculate the average magnetization $\langle M\rangle$ via the relation

   $$\langle M\rangle = N\langle\mu_z\rangle = N\left\langle\frac{-E}{B}\right\rangle = -\frac{N}{B}\langle E\rangle, \tag{2}$$

   and you know how to calculate $\langle E\rangle$ in terms of the partition function. The algebra can be reduced somewhat by using the chain rule:

   $$\frac{\partial Z}{\partial\beta} = \frac{db}{d\beta}\frac{\partial Z}{\partial b}, \tag{3}$$

   where Schroeder defines $b = \beta\delta_\mu B$. To make the requested plot, you can use this Mathematica code:

```
f[ j_, b_ ] := (j + .5) Coth[ b (j + 0.5) ]  -  0.5 Coth[ b / 2 ] ;

Plot[
  { f[.5,b], f[1.,b], f[1.5,b], f[2.,b] } ,
  { b, 0, 5 }  ,
  PlotPoints -> 100 ,
  Frame -> True ,
  PlotRange -> { { 0., 5. }, { 0., 2.1 } }
]
```

3. **Problem 6.23** on page 236. You will need to experiment to make sure that you include enough terms in the exact formula Eq. (6.30) on page 235 of Schroeder to get a value that no longer depends on the number of terms included.

4. **Problem 6.32** on pages 240-241. This problem is rather satisfying in that you are able to relate an abstract microscopic property of a crystalline solid, the potential energy of how two particles interact, to an easily measurable macroscopic property, the linear thermal expansion coefficient. Some comments:

   - For part (b), make the substitution $y = x - x_0$ in the integral for $\overline{x}$ (bottom of page 240). Also recall that integrating an odd function over the real line $-\infty < x < \infty$ must give zero (why?).

   - For part (c), Schroeder's suggestion "assume that the cubic term is small, so its exponential can be expanded in a Taylor series" means to write

     $$e^{-\beta x} \approx e^{-\beta\left[u_0+ay^2+by^3\right]} \approx e^{-\beta u_0} e^{-\beta a y^2}\left(1-\beta b y^3\right), \tag{4}$$

     where $u_0 = u(x_0)$ and $y = x - x_0$. After looking for odd functions in the integrand that can be dropped since they contribute zero, you will end up with some moments of Gaussian integrals that you can evaluate via Eq. (1) above.

   - For part (d), make your life easy by using the Mathematica command `Series` to evaluate the Taylor series of the Lennard-Jones potential symbolically about $x = x_0$ like this:

     ```
     LJpotential = u0 ( (x0/x)^12 - 2 (x0/x)^6 )

     Plot[ LJpotential /. {u0 -> 1, x0 -> 1} , { x, 0.8, 2 } ]

     LJseries = Series[ LJpotential , { x, x0, 2.5 } ]
     ```

     You can then read off the coefficients a and b needed for Eq. (4) above from `LJseries`.

5. **Problem 6.34** on page 246.

6. **Problem 6.36** on page 246. Hint: Eq. (1) above.

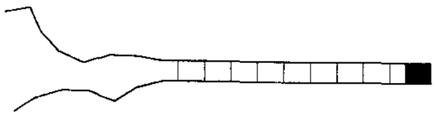
7. **Problem 6.38** on page 246. The Mathematica command `NIntegrate` is useful here.

8. **Problem 6.41** on page 247.

   For the 3D speed distribution, the rms speed $v_{\rm rms}$, the average speed $\overline{v}$, and the most likely speed $v_{\rm max}$ are in the ratio $\sqrt{3} : \sqrt{8/\pi} : \sqrt{2} \approx 1.22 : 1.13 : 1$. **What is the corresponding ratio $v_{\rm rms} : \overline{v} : v_{\rm max}$ for the 2D gas?**

Problem 2: Some quantitative details of the DNA-like zipper model

In this problem, you continue the Quiz 4 problem related to formation or unwinding of a two-strand DNA-like molecule by working out some quantitative details. Recall that the quiz problem introduced a simple zipper-like model of a biomolecule



that has N links such that each link is closed with energy 0 or open with energy $\epsilon > 0$. The zipper can unzip only from one side (say from the left as shown above) and the nth link from the left can open only if all the links to the left of it $(1, 2, \ldots, n-1)$ are already open. The Nth link on the right is always closed. The zipper is assumed to be in equilibrium with a surrounding reservoir with constant temperature T.

1. Use the partition function for this zipper model to show that the average number of open links $\langle n \rangle$ as a function of temperature is given by the expression:

$$\langle n \rangle = \frac{1}{e^{\beta\epsilon} - 1} - \frac{N}{e^{N\beta\epsilon} - 1}. \tag{5}$$

   Hint: $1 + x + \ldots + x^{K-1} = (1 - x^K)/(1 - x)$.

2. Calculate the leading-order functional behavior of Eq. (5) in the limit of small temperatures $kT \ll \epsilon$ and of high-temperatures $kT \gg \epsilon$. Use Mathematica to plot (as a function of the variable kT/ϵ) and so compare your two limiting behaviors with the exact answer Eq. (5) for $N = 10$ and discuss whether your plot for $\langle n \rangle$ makes scientific sense.

   Hint: "leading-order functional behavior" means to do some kind of expansion in powers of a small quantity until you find (and include) the first non-constant term.

Problem 3: A Box With A Tiny Cold Plate, Revisited

Redo Problem 2 of Assignment 2 for the most realistic case of isotropic molecular velocities and a Maxwell speed distribution by obtaining an analytical expression for the power dE/dt delivered by colliding molecules to a small cold plate of area A on the side of a vessel that contains an ideal equilibrium gas at temperature T. Discuss briefly how your answer differs from Eq. (4) of Assignment 2: does one gain much quantitative accuracy by using a speed distribution, compared to assuming all speeds are the same speed $v = v_{\rm rms}$?

Hint: The kinetic energy dE delivered to the area A over a short time Δt by all molecules with speeds in a range $[v, v + dv]$ along the θ, ϕ coordinate line of a spherical coordinate system centered on the area A is given by

$$dE = A[(v\cos(\theta))\Delta t] \times \frac{N}{V} \times \frac{\sin(\theta)\, d\theta\, d\phi}{4\pi} \times \frac{1}{2}mv^2 \times \mathcal{D}(v)\, dv, \tag{6}$$

where the last factor, $\mathcal{D}(v)\, dv$, is the new part of this problem and gives the fraction of molecules with a speed v in the range $[v, v + dv]$.

Alternatively, Eq. (6) could be derived more directly by observing that $dN \approx Av\cos(\theta)\Delta t \times (N/V) \times \mathcal{D}(\mathbf{v})\, d^3\mathbf{v}$ gives the number of molecules that will strike the area A in time Δt with a particular *velocity* vector $\mathbf{v}$, where $\mathcal{D}(\mathbf{v}) = (m/(2\pi kT))^{3/2} \exp(-\beta m v^2/2)$ is the Maxwell velocity distribution (not speed distribution). Changing this expression to spherical coordinates, $d^3\mathbf{v} \to v^2 \sin(\theta)\, dv\, d\theta\, d\phi$, leads to the same result.

Problem 4: Speed versus energy distribution of an equilibrium gas

In the context of discussing velocities and speeds of molecules in a gas that is thermodynamic equilibrium with constant temperature T, we have discussed probability densities (also called distribution functions) like the Maxwell speed distribution $\mathcal{D}(v)$ (Eq. (6.50) in Schroeder on page 244 of Schroeder) that give the relative probability of some quantity like the molecular speed v to take on some value.

One has to be a bit careful in using a distribution that describes one variable, say the speed v of a molecule, to gain intuition about the properties of some other variable that might depend on v. For example, because there is a range of molecular speeds in an equilibrium gas, there is a corresponding range of kinetic energies $E = (1/2)mv^2$. Is it the case that the most likely kinetic energy $E_{\rm max}$ is given by the most like speed $v_{\rm max}$ (using Schroeder's notation, see the bottom of page 244) so $E_{\rm max} = (1/2)mv_{\rm max}^2$?

Explore this situation by calculating directly the most likely kinetic energy $E_{\rm max}$ for molecules in an equilibrium ideal gas. Do this in two steps:

1. From $E = (1/2)mv^2$ we have $v = \sqrt{(2/m)E}$. Now change variables $v \to E$ in the normalization condition for the Maxwell speed distribution

$$1 = \int_0^\infty \mathcal{D}(v)\, dv, \tag{7}$$

   and deduce from the new integral what is the distribution function[1] $\mathcal{D}(E)$ for the kinetic energy.

2. From your expression for the probability density $\mathcal{D}(E)$ for the kinetic energy of molecules in an equilibrium gas, calculate the most likely kinetic energy E_{max} as determined by where $\mathcal{D}(E)$ has a local maximum. Is the most likely kinetic energy the one that corresponds to the most like speed v_{max}? If not, discuss how big is the error and why E_{max} is bigger or smaller than $(1/2)mv_{\mathrm{max}}^2$.

Problem 5: Time to Finish This Homework Assignment

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

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[1] It is a common but sometimes confusing practice in physics to use the same symbol to represent functions of a similar physical meaning, with the variable indicating what specific function is being considered. Thus $\mathcal{D}(v)$ is the Maxwell speed distribution but $\mathcal{D}(E)$ represents a different function, the distribution appropriate for the kinetic energy. A better notation would be something like $\mathcal{D}_{\mathrm{speed}}(v)$ and $\mathcal{D}_E(E)$.