

Statistical Mechanics Assignment 5

Due: March 6, 11:00 a.m.

Marks: 20

Generate (e.g. in a spreadsheet) ensembles of freely jointed polymers in three dimensions for several different values of n , the number of monomers. Calculate the average and standard deviation of the radius of gyration for your ensemble. How does the average radius of gyration compare to the theoretical value? Your report should include a clear description of the computing methods used, including any equations you used.

Hints: You might as well take $\ell = 1$, since this parameter just sets the length scale for your simulations. A freely jointed polymer has random bond angles. This corresponds to choosing a random orientation in three-dimensional space for the vector connecting monomers i and $i + 1$. The easiest way to do this is to think in terms of spherical polar coordinates (figure 1 and Appendix B of the textbook.) The angles θ and ϕ have the following ranges: $\theta \in [0, \pi]$, $\phi \in [0, 2\pi)$. The relationship between the (r, θ, ϕ) and (x, y, z) coordinates is

$$\begin{aligned}x &= r \sin \theta \cos \phi, \\y &= r \sin \theta \sin \phi, \\z &= r \cos \theta.\end{aligned}$$

Random values of θ and ϕ can therefore be used to produce a randomly oriented vector.

The following comments assume that you will use a spreadsheet. However, you are free to use some other computing environment if you think it will be more convenient.

You will probably need to spend a bit of time planning before you actually try to create the spreadsheet. There are two ways to set up this calculation: You can either put your ensemble on one large worksheet, or put one polymer on each worksheet and just have a large number of polymers. If you go the former route, be aware that Excel is limited to a maximum of 256 columns.

There are a few spreadsheet functions we haven't used before that you may find useful. The first is `SUMSQ()`. This function computes the sum of the squares of some numbers, usually given as a range in the argument of the function, so `SUMSQ(A1:A10)` calculates the sum of squares of the values stored in cells A1 to A10.

One of the ways to generate data for different values of n is to make polymers for the largest value of n you intend to include, and then look at statistics for the first n monomers in each polymer. To do this, you somehow have to adjust formulas for all the polymers in your ensemble at once. One way to do this is to use the `INDIRECT()` function. `INDIRECT()` interprets the contents of a cell as a cell address or range, and returns the contents of those cells. These can then be summed, averaged, etc. For example, suppose that cell A1 contains the character string `B2:B50`. Then the formula `COUNT(INDIRECT(A1))` will count the number

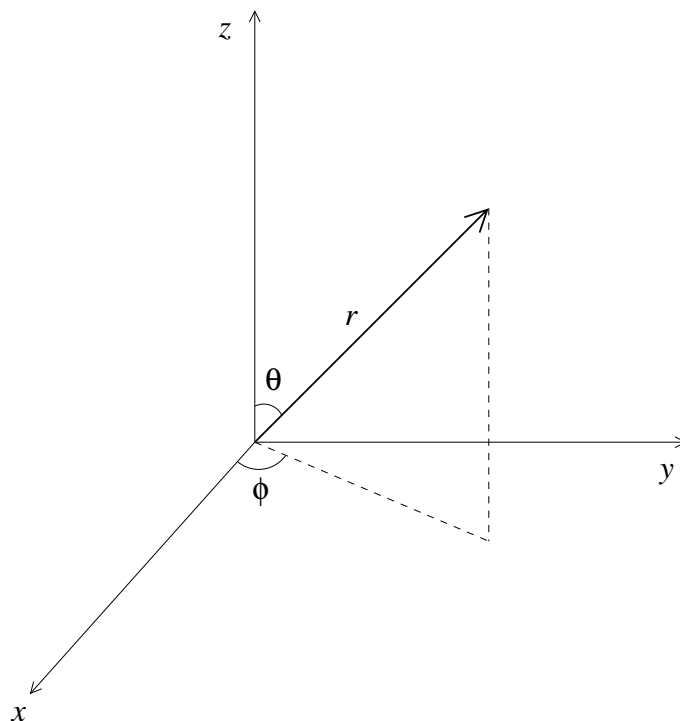


Figure 1: Spherical polar coordinates

of nonblank entries in the range B2:B50. The advantage of `INDIRECT()` is that, if you set up your worksheets with the data for your polymers in the same cells in each worksheet, then you can change the range of a sum in *each* worksheet by changing the range in one cell to which all the worksheets refer. Continuing the example above, if you wanted to carry out the same counting operation in one or more additional worksheets and the range was stored in cell A1 of worksheet **Sheet1**, you could use `COUNT(INDIRECT(Sheet1!A1))`.

If you go with the multiple-worksheet solution, you may also need to apply some operations across a range of worksheets. For instance, suppose you want to count up the number of values in cell B1500 in all your worksheets. Then you would type `COUNT(Sheet1:Sheet_last!B1500)`, where **Sheet1** and **Sheet_last** are the names of the first and last worksheets to which you want to apply this operation.

I would suggest that you figure out how to do the calculations with just a few polymers at first. Once you're reasonably sure that you have the calculations working correctly, you can make additional copies. If you are going with the multiple worksheet solution, note that you can copy several worksheets at once by clicking on the tab of the first one, then shift-click on the tab of the last one to copy. This selects a range of worksheets. Having done this, use the **Move or Copy Worksheet** item in the **Edit** menu. If you repeat this process several times, you can generate 2,4,8,... copies of a particular worksheet reasonably quickly.