Materials 218 Coding Assignment

Teams of 2 students are OK. Please attach a copy of your code with your submission, and submit to Sam Teicher.

1 Radial Distribution Function

The Radial Distribution Function $g(r)$ (**wiki**) can sometimes be obtained through appropriate Fourier transformation of experimental (X-ray, neutron *etc.*) scattering, and is a powerful technique to compare the local structure of liquids or glasses with those of crystals. Write functioning code (and create the plots) in any language (Matlab, Mathematica, python) to plot $g(r)$ for:

(a) A finite system of 101×101 points on a square lattice with unit separation between points.

(b) A random arrangement of 10,000 points generated within a square that is 100 unit lengths on edge.

(c) A Penrose tiling (wiki).

Data sets have been provided in the files: `lattice.dat`, `random.dat`, and `Penrose.dat`, for your convenience. You may choose to take the radial distribution function from the center of the lattice (with $r = 0$ at the center) even if, as in the random lattice, there is no point exactly at the center.

Answer the following questions:

1. $g(r)$ has asymptotic behavior for large r. Why?
2. Qualitatively, how does the radial distribution function of the ordered lattice differ from that of the random arrangement? Is the Penrose tiling $g(r)$ more like that of the random or the ordered lattice?

2 Structure Factor

The radial distribution function is directly related to the Structure Factor, a quantity that can be measured directly through probes such as X-ray diffraction:

$$S(\mathbf{q}) = 1 + \rho \int_V g(\mathbf{r}) e^{-iq\mathbf{r}} d\mathbf{r}$$

Perform a Fourier transform of your solutions for each lattice from the previous part as a rough estimate of the structure factor; plot your Fourier-transformed results: $\mathcal{F}[g(r)]$ (Be careful with the numerical Fourier transform here; your choice of integration region size (Δr) in the previous part can influence results).

Answer the following qualitative questions:

1. How do you expect the structure factor, $S(\mathbf{q})$ of the ordered lattice to look compared with that of the random lattice.

2. How does this relate to the difference between X-ray diffraction patterns for a crystalline material versus an amorphous material?

3. What would the 2D X-ray diffraction pattern of the provided Penrose tiling look like? Describe the unusual feature of the nature of order (long-range symmetry).

Additional Help

Sam Teicher will hold an two office hours in his office (MRL 2240) on Tuesday 1/22 and Thursday 1/24 (both 1 pm to 2 pm) to provide help with this assignment, especially for students with limited prior coding experience. Starter code for python can be provided (contact Sam).