# Physics 5403: Computational Physics – Project 6

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due date: Nov 1, 2022

## Scattering by periodic, quasiperiodic, and random chains

In this project you will explore the structure and scattering properties of a one-dimensional crystal, a quasicrystal and an amorphous (random) system.

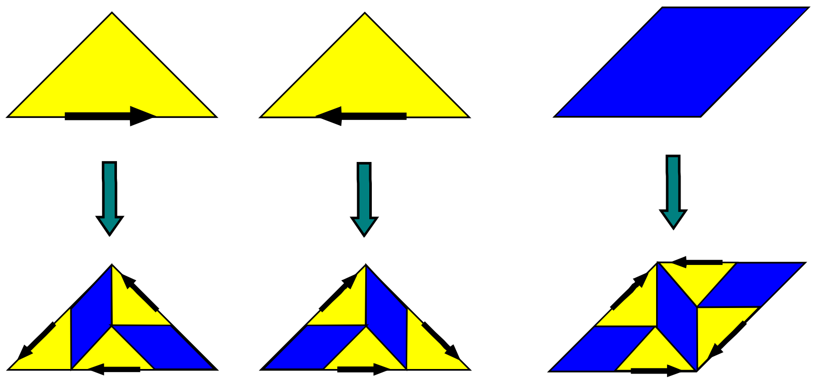
Consider a one-dimensional lattice of $N$ sites and lattice constant $a$. The sites can be occupied by two types of atoms, A or B. A crystal corresponds to a periodic arrangement of the atoms, for example ABABAB... or AABAABAAB... . A random sequence of A and B atoms is a model of an amorphous material. The Fibonacci sequence is one of the simplest examples of a quasicrystal. It is a sequence of A and B atoms that is generated by the repeated application of the inflation rule $A \to AB, \quad B \to A$, starting from A. The first few generations of the Fibonacci sequence are $A$, $AB$, $ABA$, $ABAAB$, and $ABAABABA$

For simplicity, the atomic potentials are approximated by $\delta$-functions, $u_{A,B}(x) = U_{A,B}\delta(x)$ with two different amplitudes. The goal of the project is to find the scattering intensity $I(q) \sim |V(q)|^2$ for each system where $V(q)$ is the Fourier transform of the total potential.

1. Write a program (or programs) which generates a Fibonacci chain of the desired length (using the inflation rule), the periodic sequences $ABABAB$... and $AABAABAAB$... as well as random sequences of $A$s and $B$s with probabilities $p$ and $1-p$).
2. For the Fibonacci chain, determine the ratio between the numbers of A and B atoms for each generation. Find an analytical results for the limit of an infinite chain and compare it to your numerical data.?
3. Write a program that calculates the scattering intensity $I(q) = |V(q)|^2$ for a given chain of atoms.
4. Compute $I(q)$ for the Fibonacci chain, for the two periodic chains, and for random chains with several $p$. Think about which $p$ would be interesting. (Make sure your data sets have length $2^M$ before applying the FFT.)
5. Plot the scattering intensities and describe their qualitative features. Vary the system size (say from $N = 1024$ to $N = 32768$) How do the $I(q)$ of the different chains change with size? What does this tell you? Which of the features you observe are sharp Bragg peaks?

## BONUS: Ammann-Beenker tiling (10 bonus points)

The Ammann-Beenker tiling is a 2d model of a quasicrystal with 8-fold symmetry. In addition to being of importance for the physics of quasicrystals this tiling is also strikingly beautiful. The pattern consists of 2 building blocks, a 45° rhombus and a square which we actually dissect into two isosceles triangles. The Ammann-Beenker tiling can be generated using the following inflation rules (note that we have to distinguish two classes of triangles):



An easy way the produce a nice-looking graph of the tiling consists in directly generating a postscript file. You will be given an example postscript file which shows how to draw a filled polygon.

1. Write a program which implements the above inflation rules to generate the Ammann-Beenker tiling starting from an arbitrary set of tiles. The output of the program should consist of a postscript file which plots the tiling.
2. Run the program starting from a configuration consisting of 8 rhombi forming a star.