Reciprocal space and Fourier transforms

The aim of this practical is to give you a chance to develop your intuition about the relationship between real space and reciprocal space. There are two halves to the practical. The first makes use of a great java tool developed by Nicolas Schoeni and Gervais Chapuis of EPH Lausanne: it allows us to draw all sorts of objects or repeating patterns and investigate their Fourier transforms. The second half focusses a little more on the maths involved, and the idea is that the maths should supplement the pictorial interpretation developed in the first half. The java applet is available on the web at

http://rock.esc.cam.ac.uk/~alg44/teaching_ib_bd1.html

and if you have some spare time it is worth having a go – reciprocal space can be very counterintuitive.

Begin the practical by downloading the java program from the above web address, and open the file. A new window similar to that shown above should appear (perhaps after 30 seconds or so).
Diffraction from rectangular slits

For this first part, we want to investigate the Fourier transform of different types of rectangular slits, and so we want to turn off the “periodicity” option: do this by unchecking the box. The red rectangle in the drawing field should disappear. We are also only going to worry about the intensity, rather than the phase, of the Fourier transform, so in the “Show” panel on the right-hand side, select the radio button. Also, slide the “Contrast” slider to the extreme left-hand side.

(i) Select the “line” drawing tool from the drop-down menu in the “Draw” panel. Change the width of the line to 1, either with the down arrow next to the field, or by entering the number directly; however, if you enter the number you must hit return afterwards so that the change actually occurs. Draw a line from one side of the large gridded field labelled “image” to the other side. Now click the button in the “Transform” panel. Describe what you observe in the Fourier transform (shown on the right hand side).

(ii) Clear the drawing field by clicking in the “Draw” panel. Now draw another line, using a new position or a new angle – remember, though, to keep it running from one edge of the screen to the other. Keep repeating the process, looking at the Fourier transform each time, and see if you can come to a general conclusion about the form of the Fourier transform for arbitrary lines.

(iii) Now investigate what effect is produced by changing the thickness of the line. Clear the image field, draw in the centre a horizontal line that spans the entire box, and calculate the Fourier transform. Now, increase the line width to 10. Draw a new horizontal line over the existing line. Recalculate the Fourier transform, noting how it changes. Increase the line width again to 50 and repeat the process. What is the general relationship between lines of varying thicknesses and their Fourier transforms?

(iv) Clear the drawing field, and draw a new horizontal line (keeping the line-width at 50) that doesn’t quite reach the edges of the box. Calculate the Fourier transform and describe how it changes. Clear the field again, and draw another slightly shorter line and calculate its Fourier transform. Repeat this process, drawing a shorter line each time until all you are left with is a 50 × 50 square in the centre of the drawing field. Describe your observations.

(v) Now increase the line-width to 100, and draw a new square on top of the existing one (which should be in the centre of the “image” field). Describe how the Fourier transform has changed. Keep increasing the line-widths and looking at the Fourier transforms until the entire box is filled. Describe the Fourier transform at this point – you might need to use the “Zoom” slider to see what is going on near the centre of the transform field.
Phases

For the second part we are going to use the “circle” drawing tool; select this (the solid circle, and not the “fuzzy” circle) from the drop-down menu in the “Draw” panel. We are now going to be looking at both phases and intensities. We can change between the two views by clicking the Complex or Magnitude² radio buttons in the “Show” panel.

(vi) Clear the image field and change the line-width to 1. Draw a single point somewhere near to the centre of the screen, and describe the Fourier transform in terms of both its phase and magnitude across reciprocal space. Repeat the procedure (clearing the image field each time), placing the point in different locations. What general comments can you make about the Fourier transform?

(vii) Finish up with your dot somewhere near the centre of the image field and have the Fourier transform panel in “Complex” view. Now increase the line-width to 5, and place a new single dot on top of your existing one. How have things changed in reciprocal space? Increase the line-width again to 10, and then to 50 and repeating the process each time.

(viii) Return the line-width to 1, clear the field, and experiment with placing two dots in different places and at different relative orientations. What general conclusions can you draw about the form of the intensities and the phases in reciprocal space?

Convolution

(ix) Clear the field and place two dots near the centre, one gridline apart in a horizontal direction. The Fourier transform should look something like:

![Fourier transform of two adjacent dots](image)

Now, increase the line-width to 10, and place two new dots on top of the existing ones. Explain exactly how the new Fourier transform can be interpreted in terms of the Fourier transform shown above, and that of a single dot of diameter 10 (calculated in part (iv) above). Make explicit reference to the convolution theorem in your answer.
Periodicity

We are now going to take a look at periodic patterns, so make sure the check-box is ticked and that the image field is cleared. Double check that the drawing tool is set to the filled circle tool with a line-width of 1 and that you are viewing the Fourier transform in magnitude mode.

(x) Place a single dot somewhere within the unit cell and calculate the Fourier transform. Hopefully you will now see a grid of points – these are the reciprocal lattice points. Sketch this lattice, assigning the reciprocal unit cell. Explain how this reciprocal cell is related to the real space cell.

(xi) You may notice that there is a trail of intensity between adjacent reciprocal lattice points. Using the convolution theorem, and in light of your answer to part (v) above, can you explain this spurious intensity?

(xii) Reset the image field, and place a new point of size 10 in the lower left-hand quadrant of the unit cell, so that it looks something like the left-hand image below. Calculate the Fourier transform and explains how and why it differs from that in part (xi). Now add a second point in the upper right-hand quadrant, so that it looks like the right-hand image below. Calculate the Fourier transform and explain the difference observed.

(xiii) Finally, experiment with changing the dimensions and angle of the unit cell. See if you can predict what the reciprocal lattice will look like before calculating the Fourier transform.

There are plenty of ways to continue exploring Fourier transforms using this java tool. If you have time during the practical, or want some more practice outside practical hours, some extension ideas involve using the mask feature, calculating back Fourier transforms (using the button), and you can even load in image files (from e.g. the web or another drawing program) using the button.
Calculating scattering from a pair of points

(xiv) Recall the general expression for the structure factor for a collection of particles:

$$F(Q) = \sum_j f_j \exp(iQ \cdot r_j).$$

Consider the case of a pair of atoms of scattering factor $f$ at $\pm(p, 0, 0)$. Write an expression the intensity distribution $|F(Q)|^2$ for $Q = 2\pi(q_x, 0, 0)$. How does $|F(Q)|^2$ vary for $Q$ along the other two directions in reciprocal space? Show how your answer relates to what you observed in part (viii) above.

Calculating scattering from a benzene “molecule”

(xv) Let us consider a benzene molecule as six point particles arranged at the vertices of a hexagon:

We are going to try to calculate the structure factor $F(Q)$ for this molecule using the result of part (xiv) above for each of the three pairs of atoms rotated by $\pm120^\circ$. Below we have the three structure factors superimposed in a two-dimensional section, where the lines of maxima and minima are shown as solid and dashed lines, respectively. The total scattering factor will be given by the sum of the three individual contributions, and the intensity the square of this sum.
Using circles of different colours or sizes, mark on the diagram the points where the intensity will have local maxima of values 36 and 4.

(xvi) Draw a benzene “molecule” in the java applet window, using a line-width of 5 for the points. Naturally, make sure that you have the periodicity function turned off. Things work reasonably well if the molecule is about two grid-lines in diameter:

(xvii) How well does your predicted diffraction pattern compare with that calculated by the applet? You may find the zoom feature useful!

(xviii) Use convolution theory and your thoughts in part (ix) above to predict the diffraction pattern for two benzene molecules placed side by side:

and then see how well you have done by calculating the Fourier transform using the applet.